



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 05:12 AM UTC

PDB ID : 6W2S / pdb_00006w2s
EMDB ID : EMD-21529
Title : Structure of the Cricket Paralysis Virus 5-UTR IRES (CrPV 5-UTR-IRES)
bound to the small ribosomal subunit in the open state (Class 1)
Authors : Neupane, R.; Pisareva, V.; Rodriguez, C.F.; Pisarev, A.; Fernandez, I.S.
Deposited on : 2020-03-08
Resolution : 3.47 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

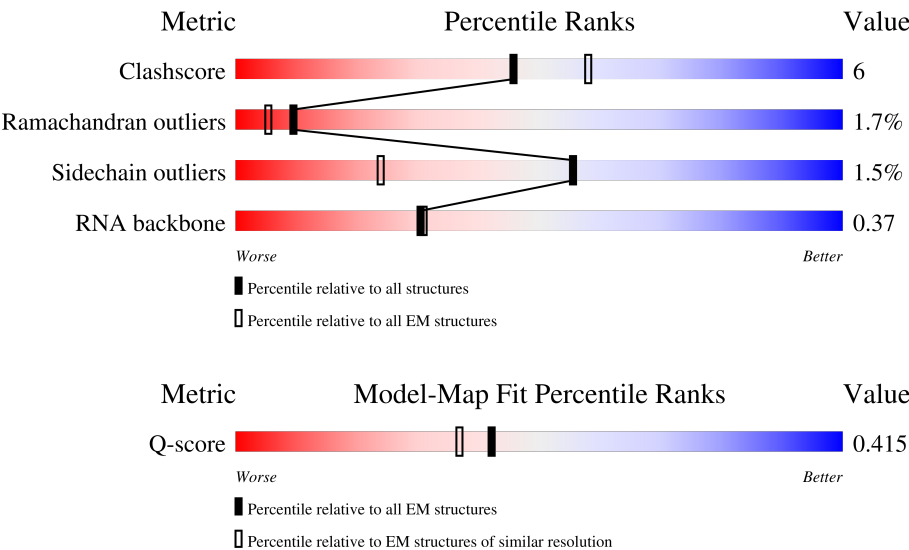
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.47 Å.

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



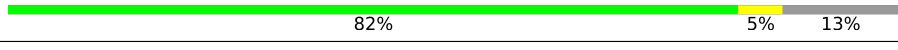
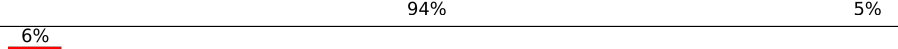
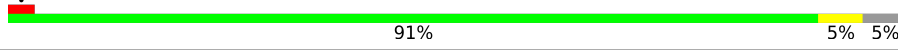
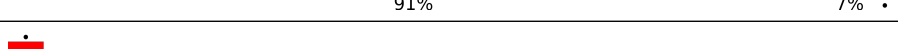
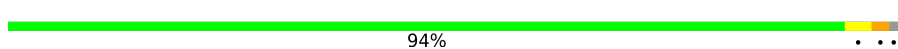
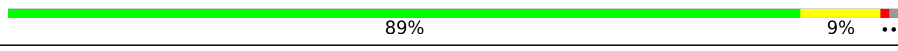
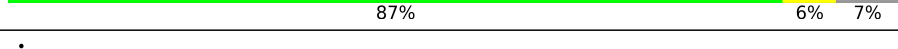
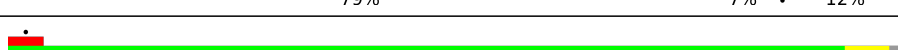
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13733 (2.97 - 3.97)

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	A	1697	
2	0	377	
3	B	295	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	C	264	
5	D	255	
6	F	263	
7	H	249	
8	I	194	
9	J	208	
10	K	194	
11	M	158	
12	O	151	
13	P	151	
14	W	83	
15	X	130	
16	Y	143	
17	Z	134	
18	b	115	
19	c	84	
20	f	133	
21	E	281	
22	G	204	
23	L	149	
24	N	132	
25	Q	145	
26	R	172	
27	S	135	
28	T	152	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	U	145	
30	V	119	
31	a	125	
32	d	69	
33	e	56	
34	g	156	
35	h	317	
36	1	1362	
37	2	913	
38	3	462	
39	4	364	
40	5	363	
41	6	218	
42	7	607	
43	8	374	

2 Entry composition

There are 45 unique types of molecules in this entry. The entry contains 106911 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1697	Total	C	N	O	P	0	0
			36229	16171	6507	11855	1696		

- Molecule 2 is a RNA chain called CrPV 5'-UTR IRES.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	0	339	Total	C	N	O	P	0	0
			7205	3222	1255	2389	339		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	569	U	C	conflict	GB 8895506
0	570	U	C	conflict	GB 8895506
0	571	U	A	conflict	GB 8895506
0	572	U	C	conflict	GB 8895506
0	574	U	C	conflict	GB 8895506
0	575	U	G	conflict	GB 8895506
0	729	G	-	expression tag	GB 8895506
0	730	G	-	expression tag	GB 8895506
0	731	A	-	expression tag	GB 8895506
0	732	U	-	expression tag	GB 8895506
0	733	C	-	expression tag	GB 8895506

- Molecule 3 is a protein called uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	217	Total	C	N	O	S	0	0
			1706	1084	296	318	8		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	114	THR	ALA	conflict	UNP G1TWL4
B	135	THR	MET	conflict	UNP G1TWL4
B	155	ARG	HIS	conflict	UNP G1TWL4
B	162	PRO	LEU	conflict	UNP G1TWL4

- Molecule 4 is a protein called eS1.

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

- Molecule 5 is a protein called uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	221	Total	C	N	O	S	0	0
			1717	1113	296	299	9		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	57	ASN	ASP	conflict	UNP G1SWM1
D	97	PHE	CYS	conflict	UNP G1SWM1
D	181	PRO	LEU	conflict	UNP G1SWM1
D	191	VAL	-	insertion	UNP G1SWM1

- Molecule 6 is a protein called eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	262	Total	C	N	O	S	0	0
			2072	1323	384	357	8		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	25	GLY	SER	conflict	UNP G1TK17
F	156	VAL	MET	conflict	UNP G1TK17

- Molecule 7 is a protein called eS6.

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

- Molecule 8 is a protein called eS7.

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

- Molecule 9 is a protein called eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 10 is a protein called uS4.

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

- Molecule 11 is a protein called uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	143	Total	C	N	O	S	0	0
			1175	749	222	198	6		

- Molecule 12 is a protein called uS15.

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

- Molecule 13 is a protein called uS11.

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

- Molecule 14 is a protein called eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	W	83	Total	C	N	O	S	0	0
			634	390	116	123	5		

- Molecule 15 is a protein called uS8.

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

- Molecule 16 is a protein called uS12.

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

- Molecule 17 is a protein called eS24.

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

- Molecule 18 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	b	101	Total	C	N	O	S	0	0
			816	509	170	132	5		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 19 is a protein called eS27.

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

- Molecule 20 is a protein called eS30.

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

- Molecule 21 is a protein called uS3.

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

- Molecule 22 is a protein called uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	G	191	Total	C	N	O	S	0	0
			1499	937	283	272	7		

- Molecule 23 is a protein called eS10.

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

- Molecule 24 is a protein called eS12.

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

- Molecule 25 is a protein called uS19.

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

- Molecule 26 is a protein called uS9.

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

- Molecule 27 is a protein called eS17.

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

- Molecule 28 is a protein called uS13.

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

- Molecule 29 is a protein called eS19.

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

- Molecule 30 is a protein called uS10.

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

- Molecule 31 is a protein called eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	a	75	Total	C	N	O	S	0	0
			598	382	111	104	1		

- Molecule 32 is a protein called eS28.

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

- Molecule 33 is a protein called eS29.

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

- Molecule 34 is a protein called eS31.

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

- Molecule 35 is a protein called RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	h	312	Total	C	N	O	S	0	0
			2429	1531	423	463	12		

- Molecule 36 is a protein called Eukaryotic translation initiation factor 3 subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	1	534	Total	C	N	O	S	0	0
			4377	2770	778	808	21		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	2	547	Total	C	N	O	S	0	0
			4446	2791	785	837	33		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	671	GLU	VAL	conflict	UNP G1U971

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	3	419	Total	C	N	O	S	0	0
			3465	2220	586	639	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	4	272	Total	C	N	O	S	0	0
			2111	1330	359	410	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	5	324	Total	C	N	O	S	0	0
			2624	1654	452	503	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	6	215	Total	C	N	O	S	0	0
			1737	1109	285	330	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	7	372	Total	C	N	O	S	0	0
			3109	2010	519	563	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	8	365	Total	C	N	O	S	0	0
			2918	1850	493	558	17		

- Molecule 44 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
44	A	1	Total	Mg	0
			1	1	

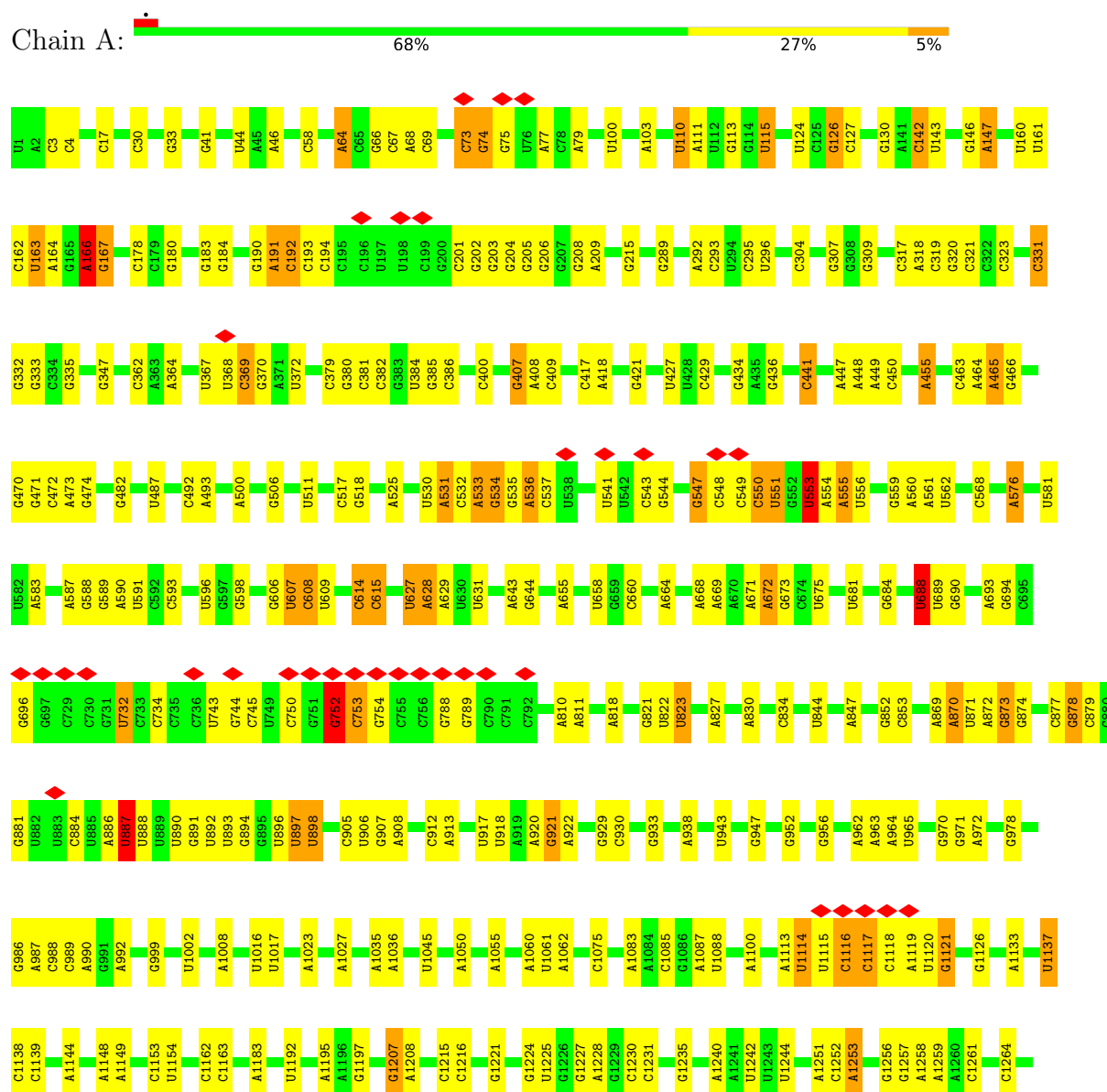
- Molecule 45 is ZINC ION (CCD ID: ZN) (formula: Zn).

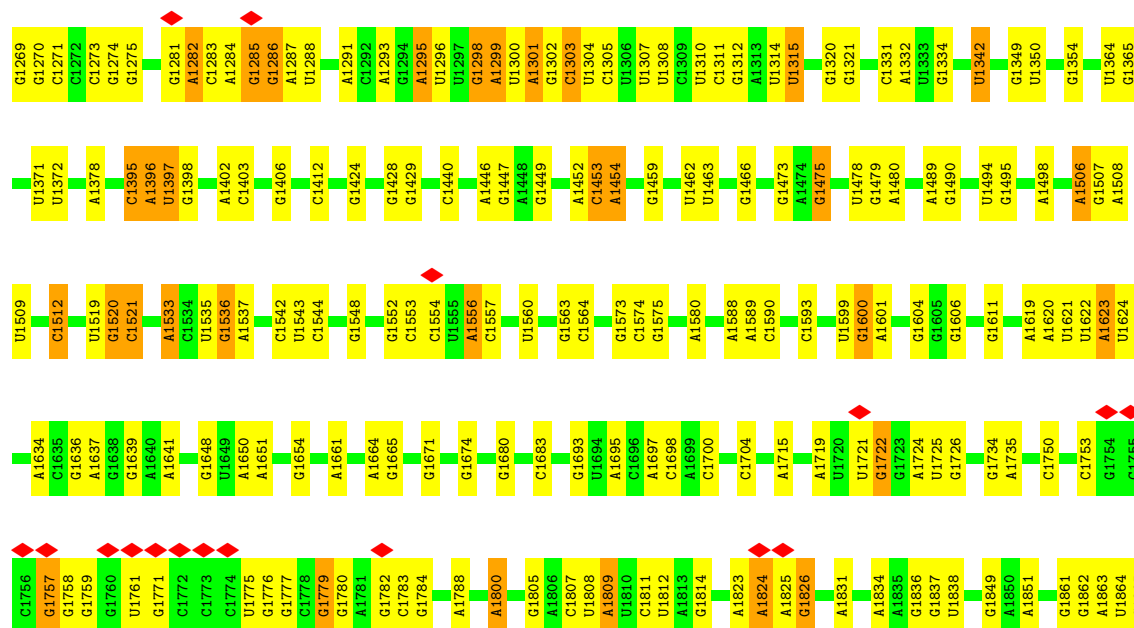
Mol	Chain	Residues	Atoms		AltConf
45	b	1	Total	Zn	0
			1	1	

3 Residue-property plots

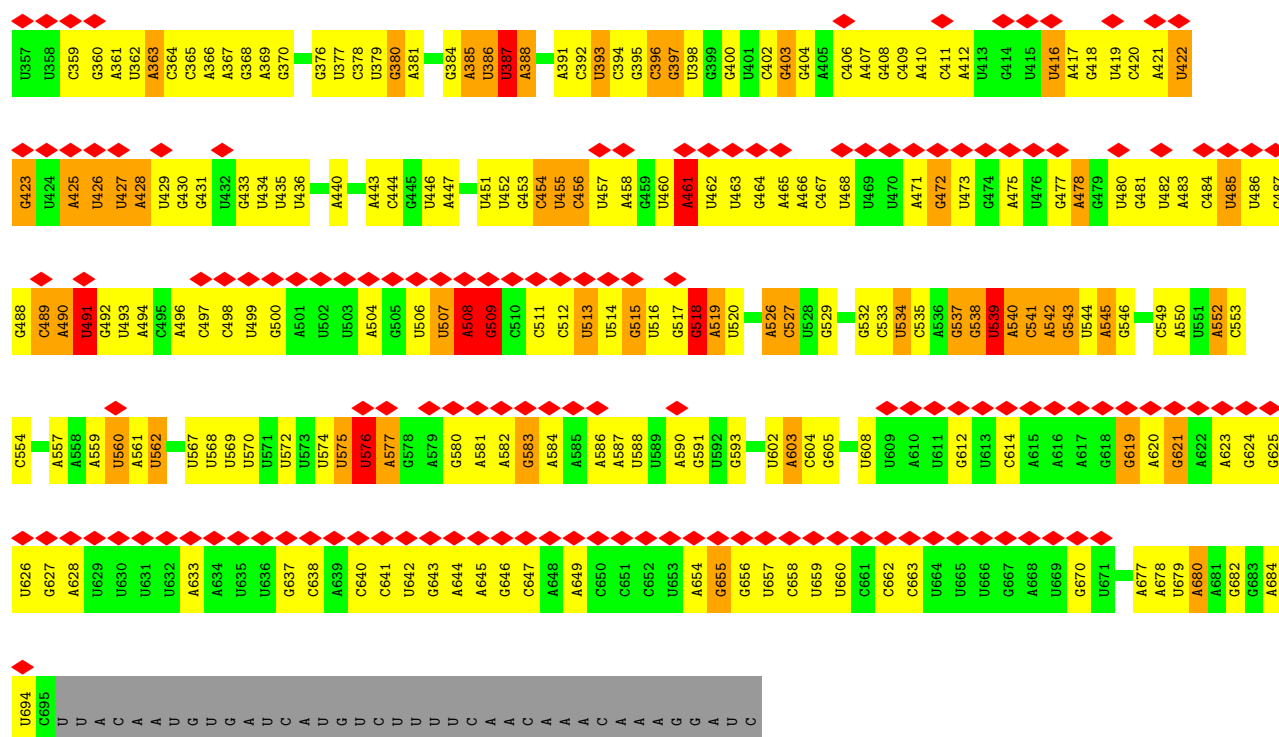
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 18S rRNA



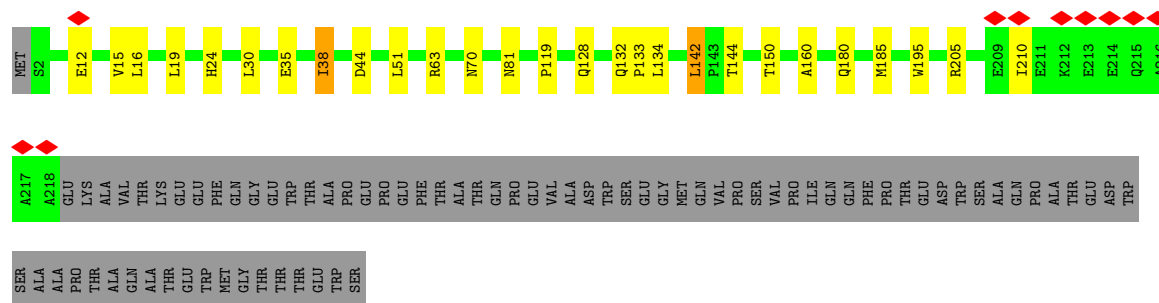


• Molecule 2: CrPV 5'-UTR IRES

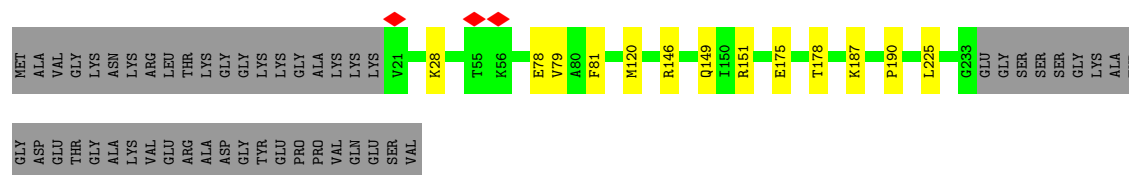
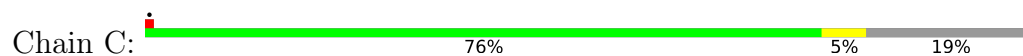


• Molecule 3: uS2

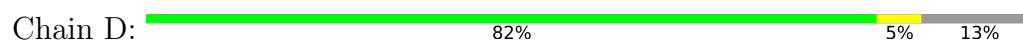




- Molecule 4: eS1



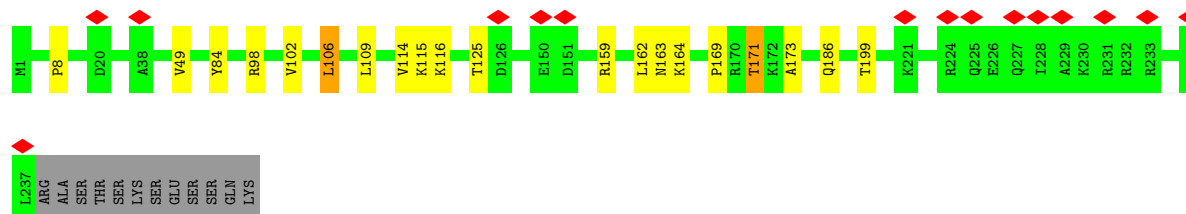
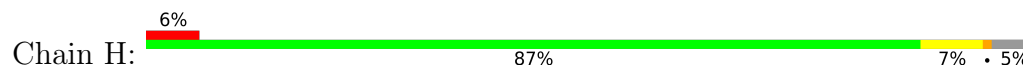
- Molecule 5: uS5



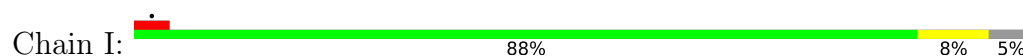
- Molecule 6: eS4

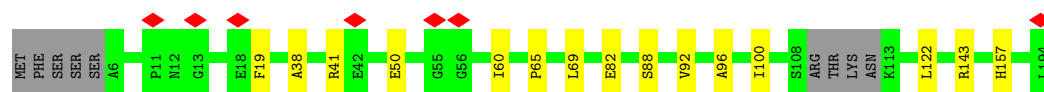


- Molecule 7: eS6

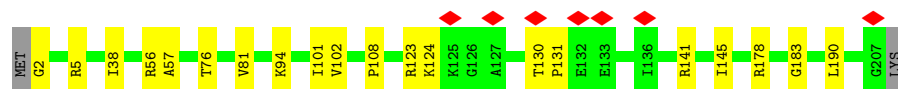
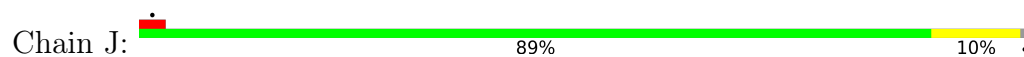


- Molecule 8: eS7

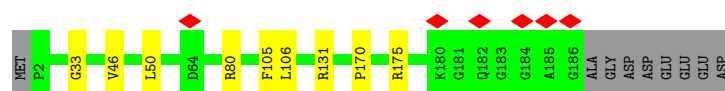




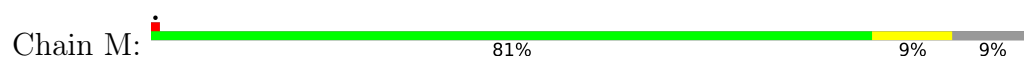
- Molecule 9: eS8



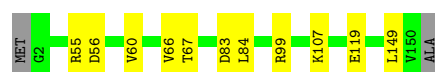
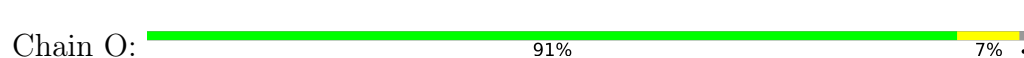
- Molecule 10: uS4



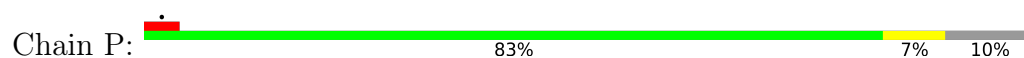
- Molecule 11: uS17



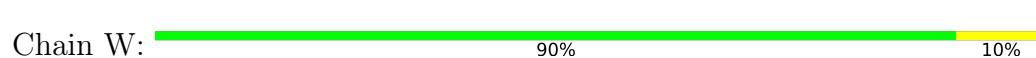
- Molecule 12: uS15



- Molecule 13: uS11



- Molecule 14: eS21



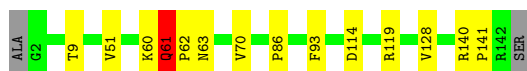
- Molecule 15: uS8





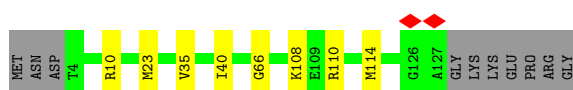
• Molecule 16: uS12

Chain Y: 89% 9% ..



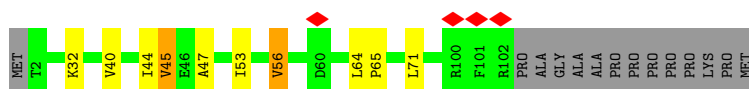
• Molecule 17: eS24

Chain Z: 87% 6% 7%



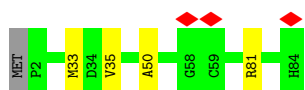
• Molecule 18: eS26

Chain b: 79% 7% 12%



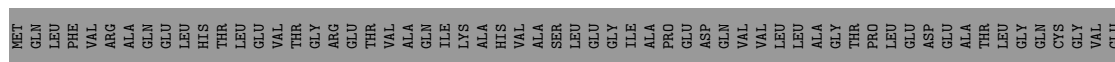
• Molecule 19: eS27

Chain c: 94% 5% .



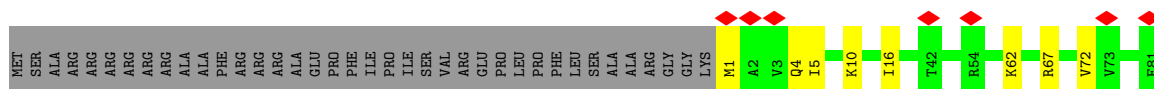
• Molecule 20: eS30

Chain f: 6% 41% 57%



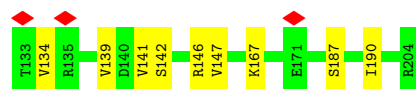
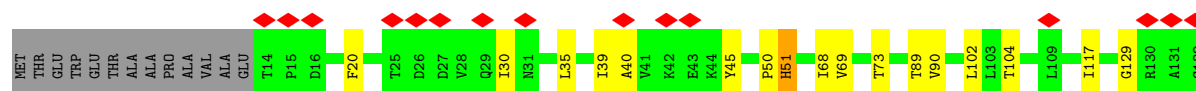
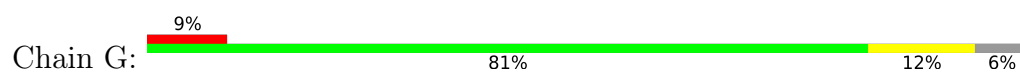
• Molecule 21: uS3

Chain E: 6% 74% 6% 19%

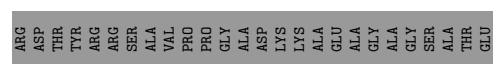
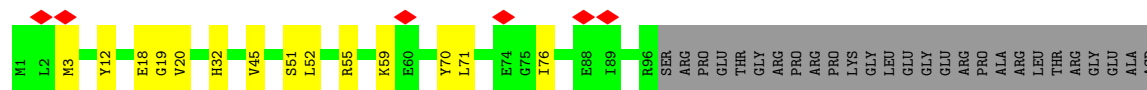




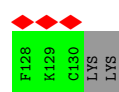
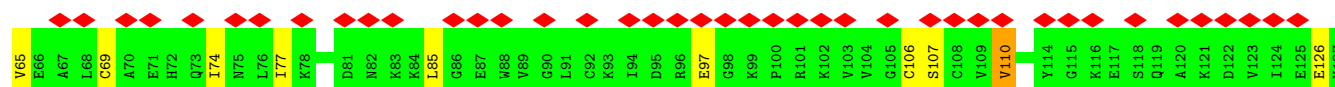
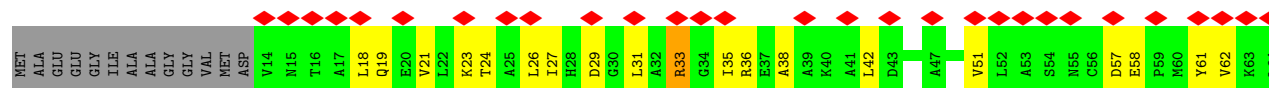
- Molecule 22: uS7



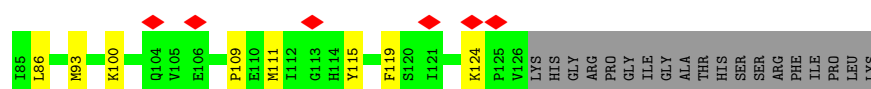
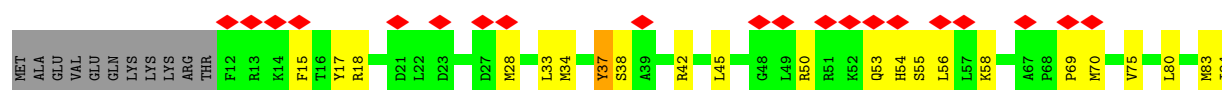
- Molecule 23: eS10



- Molecule 24: eS12

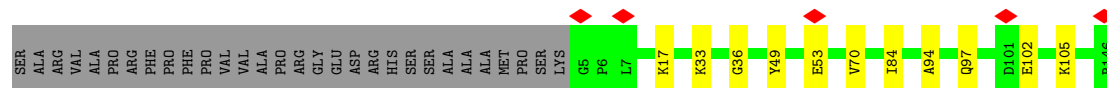


- Molecule 25: uS19



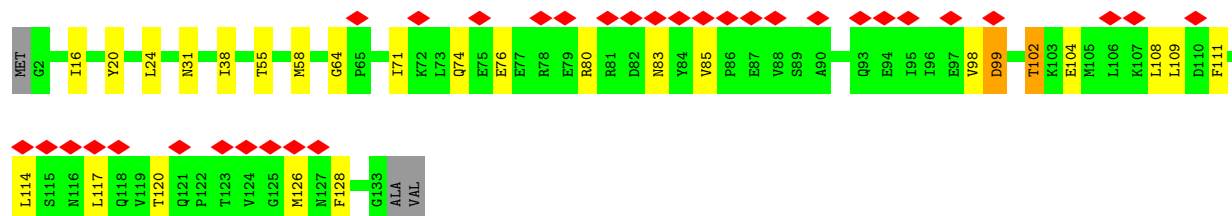
- Molecule 26: uS9

Chain R: 



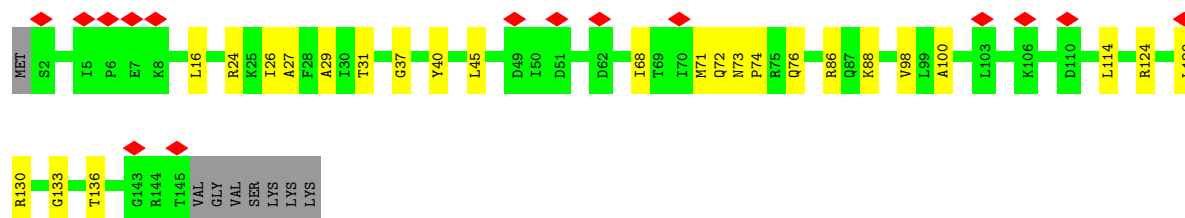
- Molecule 27: eS17

Chain S: 

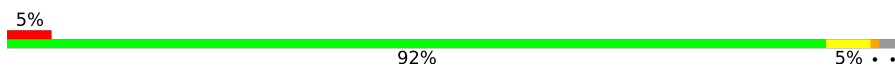


- Molecule 28: uS13

Chain T: 



- Molecule 29: eS19

Chain U: 



- Molecule 30: uS10

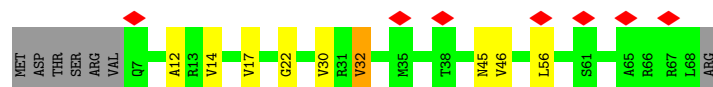
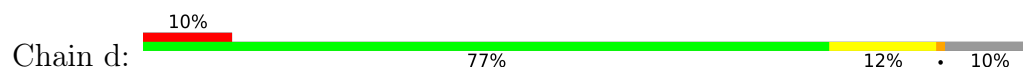
Chain V: 



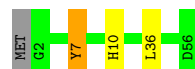
- Molecule 31: eS25

Chain a: 

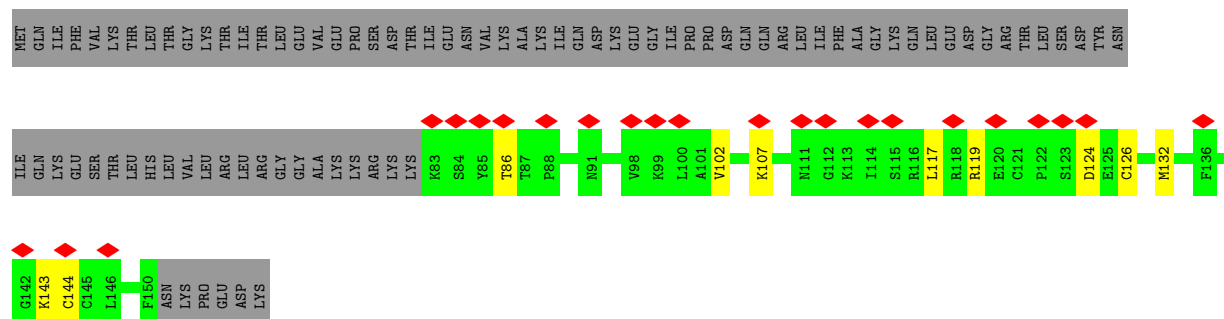
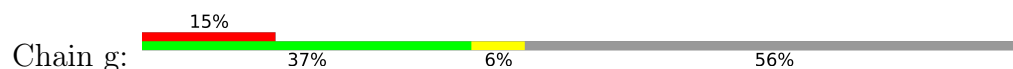
- Molecule 32: eS28



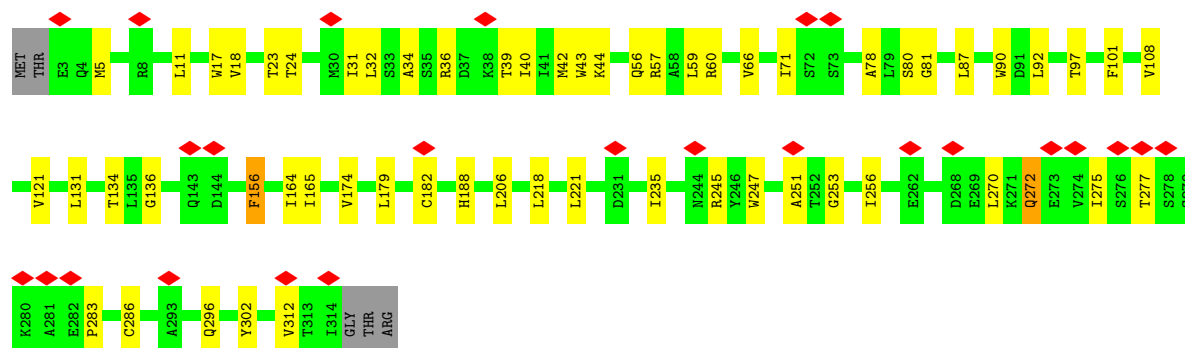
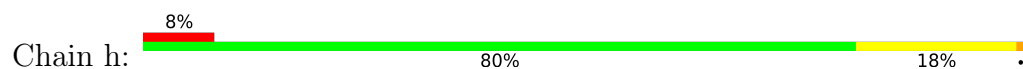
- Molecule 33: eS29



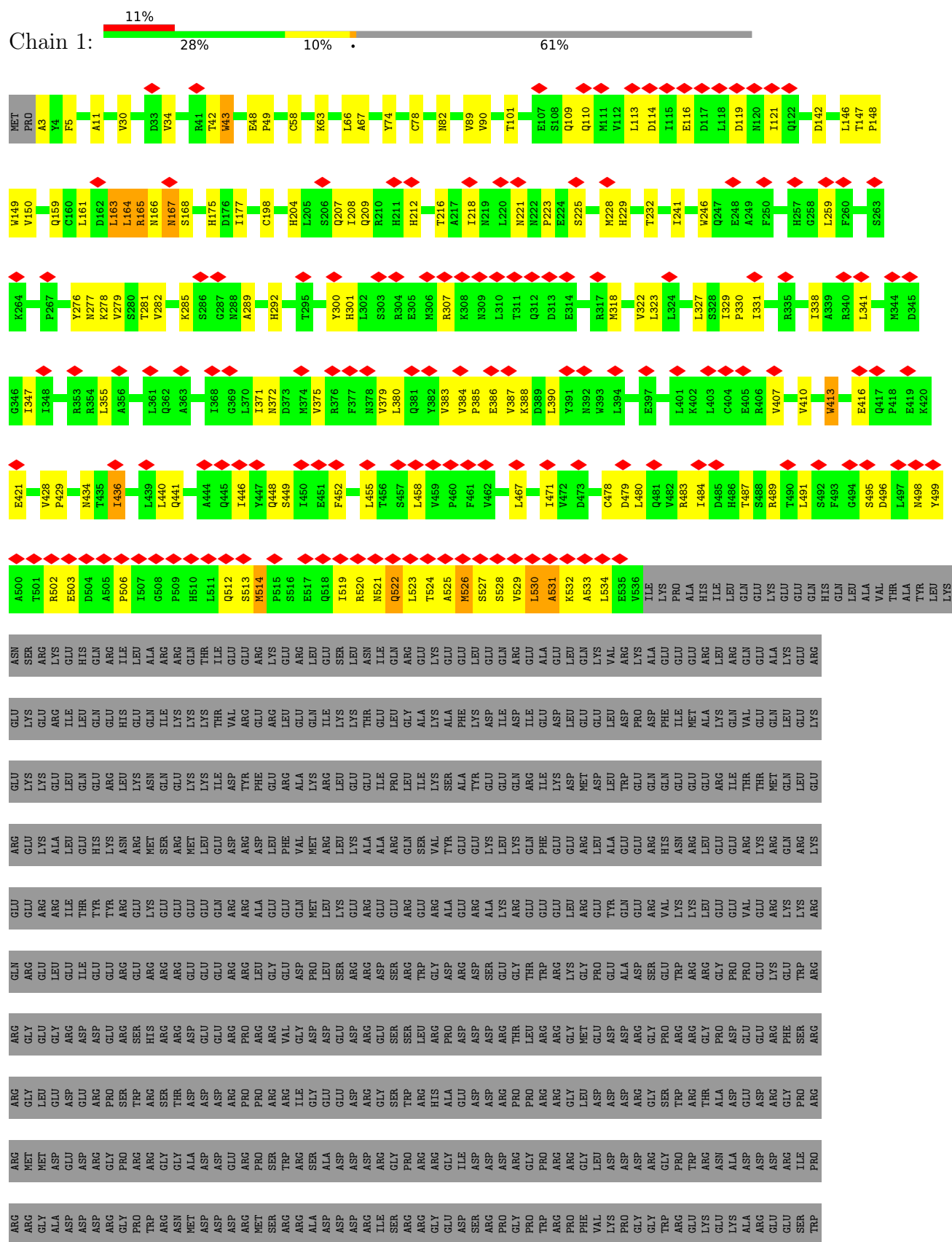
- Molecule 34: eS31



- Molecule 35: RACK1



● Molecule 36: Eukaryotic translation initiation factor 3 subunit A



LYS	ASP	ALA	ARG	PRO	GLY
ASP	ARG	ASP	ALA	ALA	PRO
GLU	GLU	ASP	ARG	GLU	ARG
SER	SER	ARG	LYS	SER	GLU
LEU	LEU	LYS	LYS	SER	SER
ARG	ARG	ASP	ASP	SER	ARG
ARG	ARG	ASP	ASP	TRP	PRO
THR	THR	ASP	ASP	ARG	PRO
LYS	LYS	ALA	ALA	ASP	GLU
ASN	ASN	GLU	GLU	SER	GLU
GLU	GLU	GLU	ARG	SER	ARG
THR	THR	ARG	ARG	ARG	GLU
ASP	ASP	ASP	ASP	ARG	TRP
GLU	GLU	PRO	PRO	ASP	GLU
ASP	ASP	PRO	ARG	ASP	ARG
GLY	GLY	ARG	ARG	ARG	GLU
TRP	TRP	VAL	VAL	ASP	ASP
THR	THR	VAL	SER	ARG	ASP
THR	THR	ARG	ARG	GLU	ARG
VAL	VAL	PRO	ARG	ARG	GLU
ARG	ARG	PRO	PRO	ASP	ASN
ARG	ARG	VAL	VAL	ARG	PRO
ARG	ARG	LEU	LEU	ARG	ASP
		SER	SER	ARG	ASP
		ARG	ARG	GLU	ARG
		ASP	ASP	ARG	GLU
		ARG	ARG	ASP	GLU
		ARG	ARG	ASP	ASN
		ARG	ARG	ASP	ASP
		ASP	ASP	ARG	LYS
		ARG	ARG	ASP	ASP
		ARG	ARG	ASP	ASP
		ARG	ARG	LEU	PRO
		ARG	ARG	ARG	GLU
		ASP	ASP	ARG	ARG
		GLU	GLU	ASP	GLU
		ARG	ARG	ASP	ASP
		GLY	GLY	ASP	GLY
		GLU	GLU	ARG	ASP
		GLU	GLU	PRO	PHE
		GLU	GLU	LEU	ARG
		GLY	GLY	ARG	ARG
		LYS	LYS	SER	PRO
		LYS	LYS	GLU	ASP
		LYS	LYS	ARG	ASP
		THR	THR	ASP	GLU
		THR	THR	GLU	GLY
		SER	SER	VAL	GLY
		TRP	TRP	SER	TRP
		ALA	ALA	SER	ARG
		GLU	GLU	TRP	GLY

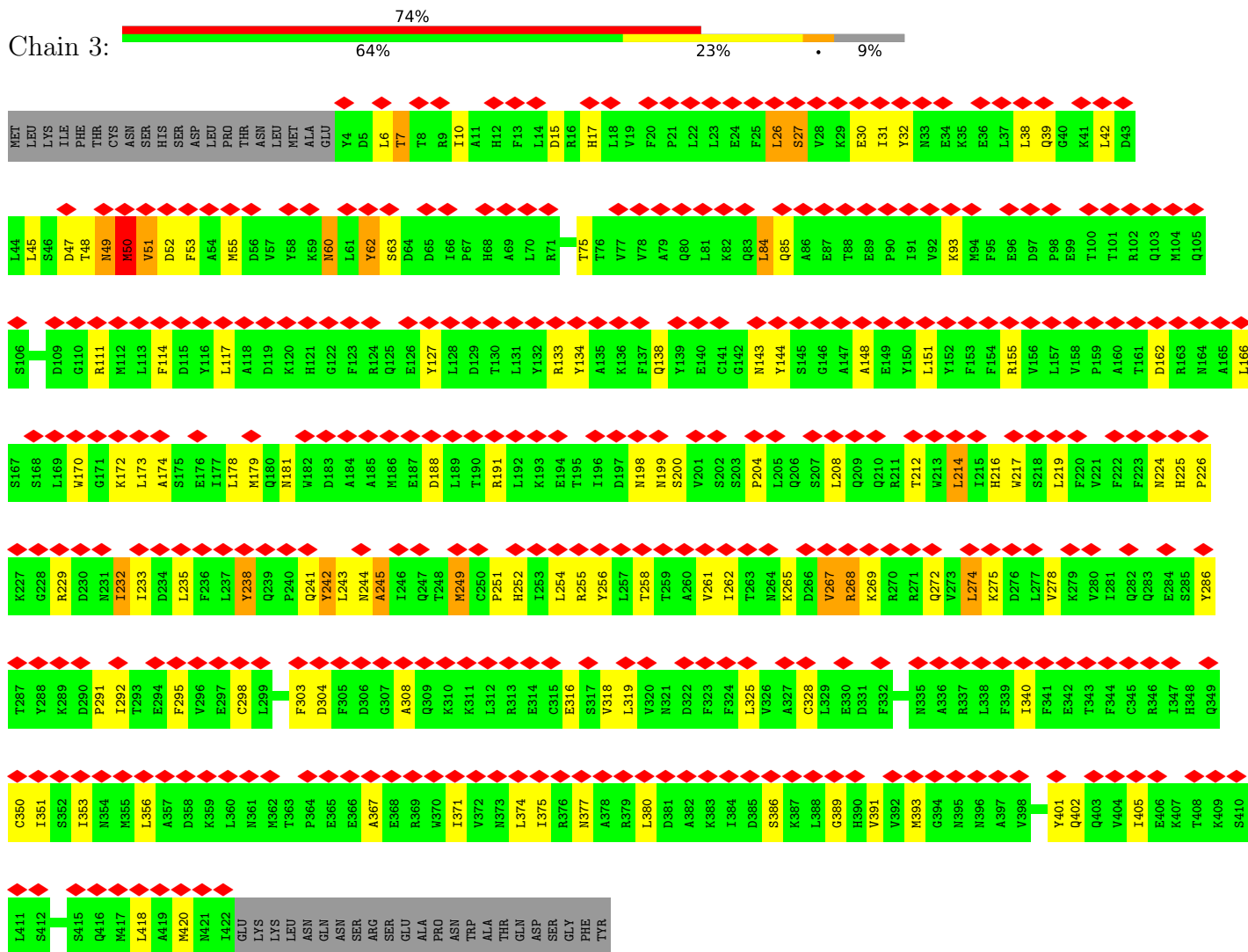
- Molecule 37: Eukaryotic translation initiation factor 3 subunit C

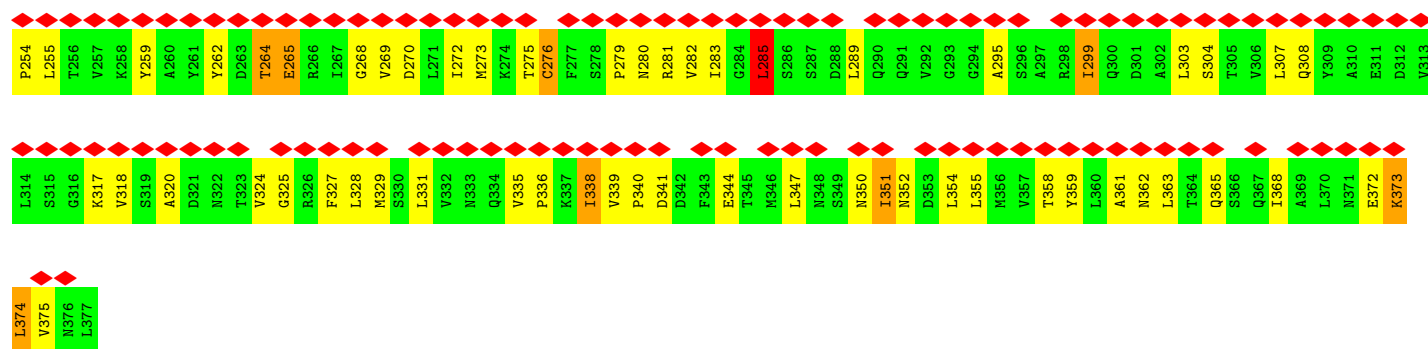
[illegible]

ARG	ARG	A833	G747	H674	S529	Q436	◆	TRP
LYS	LYS	S834	D748	◆	S530	P437	◆	GLU
ASN	ASN	L835	◆	I677	K531	R438	◆	ARG
GLU	GLU	D836	F755	◆	S532	L439	◆	VAL
GLY	GLY	Q837	W756	E683	E533	V440	◆	GLY
TYR	TYR	◆	I757	◆	◆	R441	◆	ARG
MET	MET	P838	◆	Y686	Q634	G442	◆	GLY
ARG	ARG	T839	W766	L687	D535	C443	◆	VAL
ARG	ARG	Q840	D767	P688	Q536	T444	◆	PRO
GLY	GLY	T841	W768	S689	Q536	T444	◆	LEU
GLY	GLY	◆	◆	A690	A537	L445	◆	VAL
TYR	TYR	W842	◆	M691	E538	T446	◆	LYS
ARG	ARG	W843	W778	◆	L692	V447	◆	GLU
GLN	GLN	H844	◆	L693	M539	V448	◆	LYS
GLN	GLN	H845	K782	Y697	E540	E449	◆	PRO
GLN	GLN	R846	W783	◆	◆	◆	◆	LYS
SER	SER	T847	W784	M698	E549	E454	◆	MET
GLN	GLN	E848	E785	◆	◆	◆	◆	PHE
THR	THR	P849	◆	◆	◆	◆	◆	ALA
ALA	ALA	T850	L788	A699	Y556	T462	◆	ALA
TYR	TYR	◆	W789	A700	A557	D463	◆	LYS
◆	◆	A851	R790	H701	K558	P464	◆	GLY
◆	◆	Q852	◆	E702	D559	◆	◆	THR
◆	◆	Q853	◆	S703	R560	C480	◆	GLY
◆	◆	H854	L792	◆	◆	I483	◆	I324
◆	◆	L855	F793	◆	◆	◆	◆	T326
◆	◆	A856	T794	R706	I564	R488	◆	D346
◆	◆	L857	W795	R707	H572	E491	◆	L356
◆	◆	Q858	S796	M709	◆	E492	◆	◆
◆	◆	◆	S797	I710	L578	K493	◆	I360
◆	◆	L859	W798	◆	H579	◆	◆	◆
◆	◆	A860	◆	F714	L590	GLY	◆	◆
◆	◆	E861	W799	H715	◆	THR	◆	E363
◆	◆	K862	D800	H716	H593	T496	◆	N364
◆	◆	L863	S801	◆	Q594	E497	◆	N365
◆	◆	Q864	◆	L718	L594	E498	◆	L366
◆	◆	S865	H804	R719	Q595	I499	◆	◆
◆	◆	L866	E866	◆	D596	C500	◆	G367
◆	◆	◆	T806	W720	H597	R501	◆	E368
◆	◆	W867	L807	G721	I598	V502	◆	◆
◆	◆	◆	◆	E722	◆	◆	◆	◆
◆	◆	E868	S808	R723	P603	R505	◆	V372
◆	◆	N869	D809	Q724	◆	R506	◆	◆
◆	◆	◆	◆	P725	L608	I507	◆	K375
◆	◆	◆	◆	◆	◆	◆	◆	◆
◆	◆	N870	E812	L726	◆	◆	◆	I378
◆	◆	◆	L813	L727	M613	T510	◆	I379
◆	◆	ARG	L815	◆	◆	◆	◆	◆
◆	◆	VAL	P816	P730	K513	C404	◆	C404
◆	◆	ASP	◆	E731	F514	◆	◆	◆
◆	◆	ASP	◆	◆	◆	◆	◆	◆
◆	◆	HIS	R734	I618	L616	A414	◆	◆
◆	◆	LYS	H819	◆	Q617	◆	◆	◆
◆	◆	GLN	S820	F735	◆	A518	◆	I418
◆	◆	GLY	I821	W736	K627	H519	◆	F419
◆	◆	THR	◆	◆	◆	Q520	◆	◆
◆	◆	◆	1822	V737	◆	R521	◆	E422
◆	◆	TYR	S823	W738	D635	Q522	◆	M423
◆	◆	GLY	K824	A739	◆	L523	◆	◆
◆	◆	GLY	H825	A740	R641	T524	◆	E427
◆	◆	PHE	1826	◆	◆	P525	◆	◆
◆	◆	ARG	1827	K742	L651	T524	◆	◆
◆	◆	ASP	M828	A743	L652	P526	◆	V434
◆	◆	GLN	W829	M744	R653	P527	◆	D435
◆	◆	LYS	◆	K745	◆	◆	◆	◆
◆	◆	ASP	E830	W746	R667	Q528	◆	◆
◆	◆	GLY	L831	◆	R668	◆	◆	◆
◆	◆	TYR	◆	◆	◆	◆	◆	◆

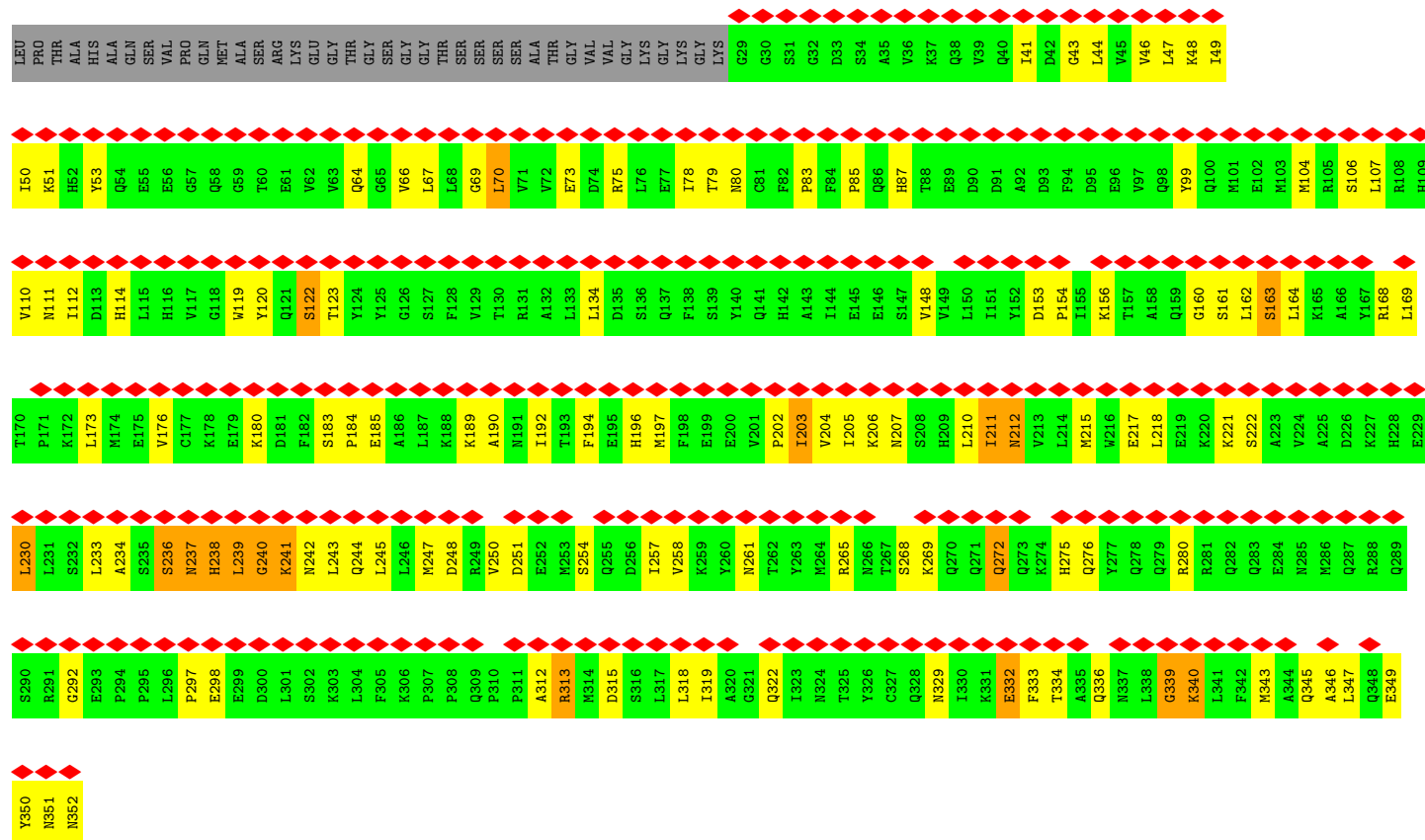
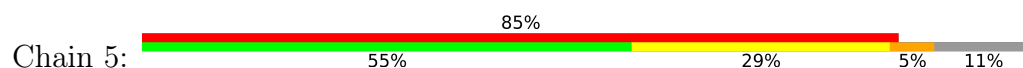
• Molecule 38: Eukaryotic translation initiation factor 3 subunit E

Chain 3:

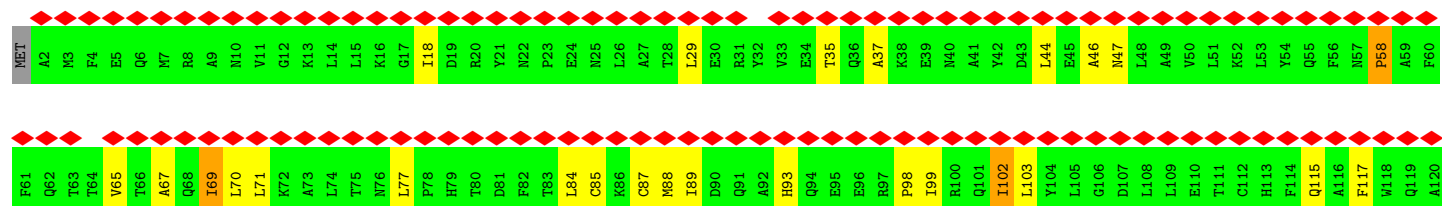
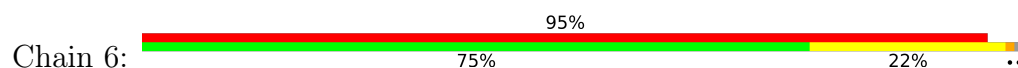


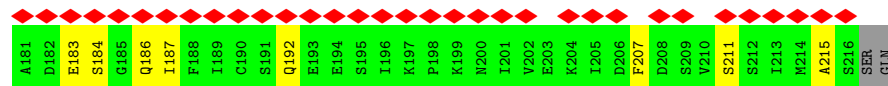


• Molecule 40: Eukaryotic translation initiation factor 3 subunit H

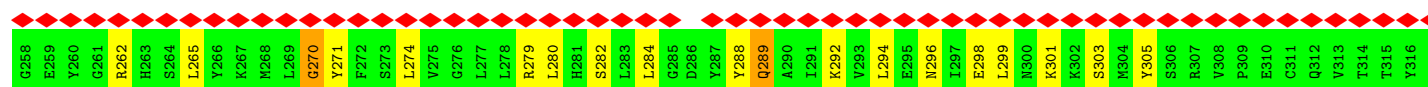
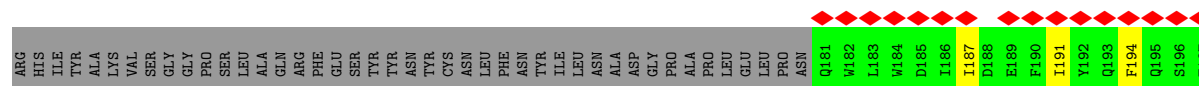
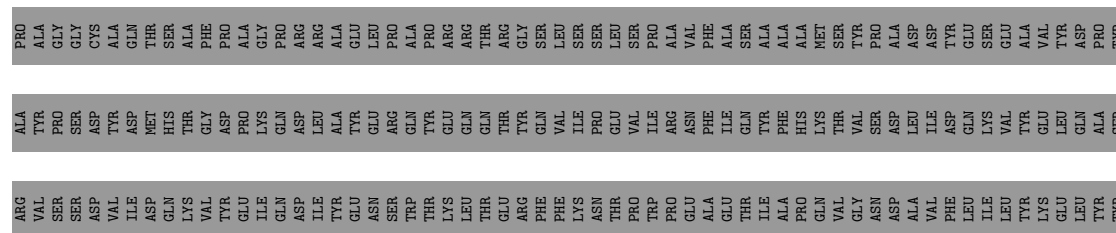


• Molecule 41: Eukaryotic translation initiation factor 3 subunit K





• Molecule 42: Eukaryotic translation initiation factor 3 subunit L





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	36100	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	56.90	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.154	Depositor
Minimum map value	-0.093	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	424.2, 424.2, 424.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0605, 1.0605, 1.0605	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.37	0/40505	0.70	15/63112 (0.0%)
2	O	0.41	2/8053 (0.0%)	0.78	14/12543 (0.1%)
3	B	1.03	0/1743	1.48	2/2370 (0.1%)
4	C	1.06	0/1756	1.48	0/2350
5	D	1.05	0/1754	1.46	0/2370
6	F	1.05	0/2114	1.39	0/2843
7	H	1.05	0/1946	1.51	0/2590
8	I	1.06	0/1510	1.47	2/2022 (0.1%)
9	J	1.05	0/1715	1.45	0/2287
10	K	1.03	0/1550	1.55	0/2069
11	M	1.03	0/1195	1.31	0/1597
12	O	1.03	0/1226	1.57	0/1649
13	P	1.06	0/1029	1.46	1/1380 (0.1%)
14	W	1.08	0/641	1.55	0/858
15	X	1.04	0/1051	1.47	0/1406
16	Y	1.06	0/1116	1.45	0/1490
17	Z	1.04	0/1028	1.44	0/1366
18	b	1.05	0/830	1.43	0/1112
19	c	1.05	0/665	1.39	0/891
20	f	1.04	0/462	1.53	0/607
21	E	1.06	0/1796	1.50	0/2417
22	G	1.07	0/1521	1.61	0/2046
23	L	1.01	0/834	1.46	0/1125
24	N	1.07	0/918	1.52	2/1233 (0.2%)
25	Q	1.04	0/974	1.43	4/1301 (0.3%)
26	R	1.07	0/1146	1.49	0/1534
27	S	1.06	0/1082	1.55	0/1452
28	T	1.05	0/1208	1.52	0/1618
29	U	1.05	0/1115	1.56	0/1493
30	V	1.07	0/805	1.41	0/1081
31	a	1.08	0/604	1.53	0/810
32	d	1.09	0/490	1.35	1/656 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	e	1.02	0/470	1.34	0/623
34	g	1.06	0/567	1.38	0/753
35	h	1.08	0/2486	1.36	2/3384 (0.1%)
36	1	1.05	0/4460	1.54	0/6034
37	2	1.07	0/4522	1.52	4/6102 (0.1%)
38	3	1.06	0/3538	1.55	10/4786 (0.2%)
39	4	1.09	2/2149 (0.1%)	1.59	3/2920 (0.1%)
40	5	1.03	0/2674	1.53	5/3606 (0.1%)
41	6	1.13	3/1772 (0.2%)	1.53	1/2396 (0.0%)
42	7	1.10	6/3185 (0.2%)	1.55	7/4296 (0.2%)
43	8	1.10	1/2963 (0.0%)	1.60	2/3998 (0.1%)
All	All	0.84	14/113168 (0.0%)	1.20	75/162576 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
16	Y	0	1
18	b	0	1
22	G	0	1
25	Q	0	1
27	S	0	1
36	1	0	4
37	2	0	4
38	3	0	6
39	4	0	3
40	5	0	6
42	7	0	3
43	8	0	4
All	All	0	35

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	6	69	ILE	CG1-CD1	-13.66	0.98	1.51
42	7	187	ILE	CG1-CD1	-11.74	1.05	1.51
39	4	351	ILE	CG1-CD1	10.68	1.93	1.51
42	7	382	ILE	CG1-CD1	-9.25	1.15	1.51
42	7	240	ILE	CG1-CD1	-6.64	1.25	1.51
42	7	530	ILE	CG1-CD1	-6.38	1.26	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	0	509	G	C1'-N9	-6.32	1.38	1.48
41	6	148	ILE	CG1-CD1	-5.88	1.28	1.51
2	0	576	U	C1'-N1	5.82	1.57	1.48
42	7	547	ILE	CG1-CD1	-5.78	1.29	1.51
39	4	299	ILE	CG1-CD1	-5.73	1.29	1.51
43	8	313	ILE	CG1-CD1	5.36	1.72	1.51
41	6	102	ILE	CG1-CD1	-5.12	1.31	1.51
42	7	191	ILE	CG1-CD1	-5.09	1.31	1.51

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	7	382	ILE	CB-CG1-CD1	12.87	140.82	113.80
42	7	240	ILE	CB-CG1-CD1	10.79	136.47	113.80
1	A	688	U	C2'-C3'-O3'	10.01	124.51	109.50
42	7	187	ILE	CB-CG1-CD1	9.74	134.25	113.80
2	0	387	U	C4'-C3'-O3'	7.99	121.39	109.40
1	A	870	A	C4'-C3'-O3'	7.89	121.24	109.40
40	5	236	SER	CA-C-O	-7.76	111.63	120.24
41	6	69	ILE	CB-CG1-CD1	7.63	129.82	113.80
1	A	627	U	C4'-C3'-O3'	7.35	120.43	109.40
2	0	655	G	C4'-C3'-O3'	7.11	120.06	109.40
2	0	518	G	C4'-C3'-O3'	7.08	120.03	109.40
1	A	166	A	C2'-C3'-O3'	7.07	124.30	113.70
1	A	752	G	C4'-C3'-O3'	7.00	119.90	109.40
2	0	485	U	C2'-C3'-O3'	6.89	124.04	113.70
2	0	425	A	C2'-C3'-O3'	6.59	119.39	109.50
42	7	424	VAL	N-CA-C	-6.54	106.60	111.90
2	0	416	U	C4'-C3'-O3'	6.41	119.01	109.40
42	7	486	PHE	CA-C-N	6.37	133.17	121.70
42	7	486	PHE	C-N-CA	6.37	133.17	121.70
1	A	1137	U	C2'-C3'-O3'	6.27	123.10	113.70
43	8	325	ILE	CB-CG1-CD1	6.18	126.78	113.80
43	8	115	LYS	CB-CA-C	5.92	122.19	110.42
1	A	553	U	C2'-C3'-O3'	5.88	118.32	109.50
40	5	237	ASN	N-CA-CB	5.87	119.42	110.44
2	0	461	A	C2'-C3'-O3'	5.80	118.20	109.50
1	A	465	A	C2'-C3'-O3'	5.61	117.91	109.50
24	N	85	LEU	CA-C-N	5.58	126.14	119.94
24	N	85	LEU	C-N-CA	5.58	126.14	119.94
37	2	491	GLU	CA-C-N	5.57	127.68	120.44
37	2	491	GLU	C-N-CA	5.57	127.68	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	887	U	C4'-C3'-O3'	5.56	117.74	109.40
1	A	1295	A	C2'-C3'-O3'	5.55	122.03	113.70
32	d	22	GLY	CA-C-O	-5.55	118.14	122.52
2	0	560	U	C3'-C2'-O2'	5.53	119.00	110.70
2	0	619	G	C2'-C3'-O3'	5.52	117.79	109.50
42	7	333	ILE	CB-CG1-CD1	5.51	125.38	113.80
40	5	332	GLU	CB-CA-C	5.50	119.60	110.90
1	A	555	A	C4'-C3'-O3'	5.49	117.64	109.40
38	3	268	ARG	CA-C-N	5.46	131.53	121.70
38	3	268	ARG	C-N-CA	5.46	131.53	121.70
37	2	603	PRO	N-CA-C	5.39	117.28	110.70
38	3	340	ILE	CB-CG1-CD1	5.38	125.10	113.80
8	I	65	PRO	CA-C-N	5.37	125.58	120.43
8	I	65	PRO	C-N-CA	5.37	125.58	120.43
35	h	80	SER	CA-C-N	5.36	125.29	121.65
35	h	80	SER	C-N-CA	5.36	125.29	121.65
2	0	456	C	C3'-C2'-O2'	5.36	118.73	110.70
1	A	110	U	C2'-C3'-O3'	5.35	121.72	113.70
25	Q	55	SER	CA-C-N	5.35	127.76	120.54
25	Q	55	SER	C-N-CA	5.35	127.76	120.54
40	5	238	HIS	CB-CA-C	5.29	121.89	110.41
2	0	539	U	N1-C1'-C2'	5.23	119.85	112.00
1	A	1395	C	C3'-C2'-O2'	5.22	118.53	110.70
38	3	39	GLN	CA-C-N	5.17	125.68	119.94
38	3	39	GLN	C-N-CA	5.17	125.68	119.94
2	0	508	A	C2'-C3'-O3'	5.15	117.22	109.50
39	4	265	GLU	N-CA-CB	5.15	117.42	109.91
38	3	249	MET	CA-C-N	5.14	127.52	122.28
38	3	249	MET	C-N-CA	5.14	127.52	122.28
2	0	491	U	C3'-C2'-O2'	5.11	118.37	110.70
25	Q	38	SER	CA-C-N	5.11	127.64	120.28
25	Q	38	SER	C-N-CA	5.11	127.64	120.28
40	5	292	GLY	CA-C-O	-5.10	118.78	122.45
2	0	560	U	C2'-C3'-O3'	5.09	121.33	113.70
3	B	81	ASN	CA-C-N	5.07	127.03	120.44
3	B	81	ASN	C-N-CA	5.07	127.03	120.44
1	A	1824	A	C3'-C2'-O2'	5.07	118.30	110.70
38	3	50	MET	CA-C-N	5.04	131.05	121.97
38	3	50	MET	C-N-CA	5.04	131.05	121.97
13	P	144	GLY	CA-C-O	-5.03	118.21	122.29
39	4	285	LEU	CA-C-N	5.03	127.28	120.65
39	4	285	LEU	C-N-CA	5.03	127.28	120.65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	553	U	C4'-C3'-O3'	5.01	116.92	109.40
37	2	843	VAL	N-CA-C	-5.01	107.82	112.43
38	3	251	PRO	N-CA-CB	-5.00	98.00	103.25

There are no chirality outliers.

All (35) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
36	1	165	ARG	Peptide
36	1	483	ARG	Peptide
36	1	498	ASN	Peptide
36	1	514	MET	Peptide
37	2	564	ILE	Peptide
37	2	651	LEU	Peptide
37	2	716	HIS	Peptide
37	2	782	LYS	Peptide
38	3	27	SER	Peptide
38	3	278	VAL	Peptide
38	3	47	ASP	Peptide
38	3	49	ASN	Peptide
38	3	50	MET	Peptide
38	3	60	ASN	Peptide
39	4	243	VAL	Peptide
39	4	373	LYS	Peptide
39	4	374	LEU	Peptide
40	5	122	SER	Peptide
40	5	180	LYS	Peptide
40	5	210	LEU	Peptide
40	5	221	LYS	Peptide
40	5	272	GLN	Peptide
40	5	312	ALA	Peptide
42	7	225	HIS	Peptide
42	7	376	THR	Peptide
42	7	423	PRO	Peptide
43	8	115	LYS	Peptide
43	8	117	THR	Peptide
43	8	13	ASP	Peptide
43	8	332	VAL	Peptide
22	G	129	GLY	Peptide
25	Q	54	HIS	Peptide
27	S	64	GLY	Peptide
16	Y	61	GLN	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
18	b	45	VAL	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	36229	0	18304	160	0
2	O	7205	0	3626	56	0
3	B	1706	0	1698	21	0
4	C	1729	0	1803	6	0
5	D	1717	0	1812	17	0
6	F	2072	0	2175	10	0
7	H	1923	0	2089	13	0
8	I	1488	0	1582	7	0
9	J	1686	0	1772	12	0
10	K	1525	0	1640	5	0
11	M	1175	0	1249	8	0
12	O	1202	0	1289	5	0
13	P	1016	0	1039	8	0
14	W	634	0	629	5	0
15	X	1034	0	1080	4	0
16	Y	1098	0	1167	7	0
17	Z	1011	0	1083	5	0
18	b	816	0	867	10	0
19	c	651	0	672	1	0
20	f	457	0	502	2	0
21	E	1768	0	1866	13	0
22	G	1499	0	1540	12	0
23	L	810	0	836	7	0
24	N	908	0	939	14	0
25	Q	956	0	1002	15	0
26	R	1128	0	1195	6	0
27	S	1068	0	1121	17	0
28	T	1190	0	1249	17	0
29	U	1097	0	1130	5	0
30	V	795	0	862	3	0
31	a	598	0	656	3	0
32	d	488	0	514	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	e	459	0	452	3	0
34	g	555	0	567	4	0
35	h	2429	0	2386	32	0
36	1	4377	0	4433	153	0
37	2	4446	0	4444	126	0
38	3	3465	0	3446	73	0
39	4	2111	0	2105	178	0
40	5	2624	0	2591	261	0
41	6	1737	0	1706	34	0
42	7	3109	0	3084	70	0
43	8	2918	0	2950	68	0
44	A	1	0	0	0	0
45	b	1	0	0	0	0
All	All	106911	0	87152	1184	0

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

All (1184) 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)
5:D:127:PHE:CD1	5:D:141:LEU:HD21	1.26	1.61
5:D:127:PHE:CD1	5:D:141:LEU:CD2	1.95	1.50
36:1:523:LEU:HA	36:1:526:MET:SD	1.71	1.30
37:2:710:ILE:O	37:2:714:PHE:HD2	1.09	1.29
36:1:526:MET:HG2	40:5:236:SER:O	1.26	1.28
36:1:526:MET:CB	40:5:237:ASN:HA	1.64	1.28
37:2:710:ILE:O	37:2:714:PHE:CD2	1.88	1.27
39:4:351:ILE:HA	40:5:343:MET:SD	1.82	1.19
37:2:710:ILE:HB	37:2:714:PHE:CE2	1.81	1.15
39:4:354:LEU:HD12	40:5:343:MET:SD	1.86	1.15
36:1:526:MET:HB3	40:5:237:ASN:HA	1.18	1.14
36:1:526:MET:CG	40:5:237:ASN:HA	1.77	1.13
36:1:526:MET:HB3	40:5:237:ASN:CA	1.81	1.11
39:4:124:ASP:C	40:5:111:ASN:HD21	1.65	1.04
37:2:493:LYS:HG2	37:2:498:GLU:OE2	1.60	1.02
36:1:534:LEU:HB2	40:5:230:LEU:HD13	1.40	1.01
39:4:365:GLN:HG3	40:5:329:ASN:HB3	1.44	1.00
36:1:530:LEU:HD21	40:5:234:ALA:HB2	1.45	0.98
36:1:526:MET:HG2	40:5:236:SER:C	1.92	0.95
39:4:358:THR:HG22	40:5:336:GLN:HA	1.49	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:127:PHE:CE1	5:D:141:LEU:HD21	2.03	0.93
39:4:279:PRO:HA	39:4:280:ASN:HB3	1.51	0.93
5:D:127:PHE:CE1	5:D:141:LEU:CD2	2.53	0.92
37:2:493:LYS:CG	37:2:498:GLU:OE2	2.17	0.92
5:D:127:PHE:CD1	5:D:141:LEU:HD22	2.04	0.91
3:B:70:ASN:ND2	5:D:274:MET:SD	2.43	0.91
36:1:526:MET:HB3	40:5:237:ASN:CB	2.00	0.90
37:2:710:ILE:CB	37:2:714:PHE:CE2	2.57	0.88
2:0:534:U:O2	2:0:543:G:N2	2.08	0.85
36:1:523:LEU:HD12	36:1:526:MET:SD	2.17	0.85
37:2:855:LEU:HB3	40:5:258:VAL:HB	1.58	0.85
39:4:124:ASP:C	40:5:111:ASN:ND2	2.35	0.84
18:b:56:VAL:HG12	18:b:56:VAL:O	1.76	0.84
39:4:358:THR:HA	40:5:336:GLN:HG2	1.59	0.84
36:1:534:LEU:CB	40:5:230:LEU:HD13	2.07	0.83
37:2:855:LEU:HB3	40:5:258:VAL:CB	2.07	0.83
36:1:523:LEU:HD13	40:5:241:LYS:HB2	1.60	0.83
39:4:116:PRO:HB2	40:5:47:LEU:HD13	1.60	0.82
39:4:351:ILE:CA	40:5:343:MET:SD	2.68	0.82
38:3:371:ILE:HG21	38:3:391:VAL:HG21	1.61	0.81
37:2:710:ILE:CG1	37:2:714:PHE:HE2	1.94	0.81
39:4:125:SER:N	40:5:111:ASN:HD21	1.79	0.81
28:T:124:ARG:NH1	28:T:130:ARG:O	2.14	0.80
40:5:261:ASN:HB3	40:5:265:ARG:HH12	1.45	0.80
39:4:354:LEU:HD13	40:5:339:GLY:C	2.06	0.79
36:1:526:MET:CB	40:5:237:ASN:CA	2.48	0.78
40:5:67:LEU:HD22	40:5:78:ILE:HD13	1.65	0.78
37:2:710:ILE:HD12	37:2:714:PHE:CZ	2.18	0.78
1:A:1192:U:OP2	16:Y:119:ARG:NH2	2.17	0.77
36:1:277:ASN:O	36:1:281:THR:HG23	1.85	0.77
36:1:520:ARG:NH2	36:1:521:ASN:OD1	2.17	0.76
37:2:794:THR:O	37:2:839:THR:OG1	2.03	0.76
2:0:537:G:O2'	2:0:540:A:N1	2.18	0.76
37:2:855:LEU:HB3	40:5:258:VAL:CA	2.16	0.76
39:4:373:LYS:HA	39:4:375:VAL:HG12	1.68	0.75
37:2:710:ILE:C	37:2:714:PHE:CD2	2.63	0.75
36:1:446:ILE:HG23	43:8:313:ILE:HG13	1.67	0.75
36:1:526:MET:CG	40:5:236:SER:O	2.22	0.75
37:2:869:ASN:CG	40:5:272:GLN:HB2	2.12	0.75
36:1:526:MET:HE3	40:5:240:GLY:N	2.03	0.74
40:5:329:ASN:HA	40:5:332:GLU:HB2	1.68	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:7:486:PHE:H	42:7:487:ARG:C	1.95	0.74
37:2:483:ILE:HD11	37:2:505:ARG:HB3	1.70	0.74
36:1:520:ARG:NH2	40:5:243:LEU:O	2.21	0.73
38:3:49:ASN:HA	38:3:50:MET:HB2	1.68	0.73
42:7:241:ASN:HD22	42:7:423:PRO:HA	1.52	0.73
36:1:526:MET:SD	40:5:237:ASN:HA	2.28	0.73
36:1:530:LEU:O	36:1:532:LYS:N	2.22	0.73
1:A:1473:G:O2'	1:A:1475:G:N2	2.22	0.73
5:D:127:PHE:CE1	5:D:141:LEU:HD22	2.22	0.73
39:4:375:VAL:O	40:5:313:ARG:HD2	1.88	0.73
20:f:112:ASN:HA	20:f:116:VAL:HG12	1.71	0.72
39:4:354:LEU:O	39:4:358:THR:HG23	1.89	0.72
36:1:441:GLN:HE21	36:1:479:ASP:HB3	1.54	0.72
3:B:70:ASN:CG	5:D:274:MET:SD	2.73	0.71
36:1:523:LEU:HA	36:1:526:MET:CG	2.21	0.71
39:4:123:VAL:HG21	40:5:44:LEU:HD22	1.72	0.71
40:5:41:ILE:HG12	40:5:78:ILE:HD12	1.72	0.70
38:3:111:ARG:HA	38:3:114:PHE:HB2	1.73	0.70
36:1:101:THR:HG22	36:1:149:TRP:HB3	1.74	0.70
39:4:373:LYS:HD2	40:5:322:GLN:CD	2.17	0.70
28:T:16:LEU:HD11	28:T:72:GLN:HE21	1.56	0.69
37:2:870:ASN:HD22	40:5:272:GLN:NE2	1.91	0.69
39:4:354:LEU:CD1	40:5:343:MET:SD	2.76	0.69
36:1:229:HIS:HB3	36:1:259:LEU:HD11	1.74	0.69
39:4:362:ASN:CG	40:5:336:GLN:HE22	2.00	0.69
36:1:523:LEU:CD1	36:1:526:MET:SD	2.81	0.69
1:A:1693:G:H21	1:A:1834:A:H8	1.40	0.69
41:6:115:GLN:HE22	42:7:491:LEU:HB3	1.57	0.69
39:4:361:ALA:HB1	40:5:332:GLU:HB3	1.73	0.68
37:2:855:LEU:CB	40:5:258:VAL:HA	2.24	0.68
39:4:156:SER:HB2	40:5:110:VAL:HG11	1.76	0.68
39:4:361:ALA:CB	40:5:332:GLU:HB3	2.24	0.68
23:L:51:SER:OG	23:L:55:ARG:NH2	2.26	0.68
37:2:852:GLN:HE22	40:5:257:ILE:HD12	1.58	0.68
39:4:281:ARG:CZ	39:4:283:ILE:HB	2.24	0.68
37:2:710:ILE:C	37:2:714:PHE:HD2	1.97	0.68
37:2:855:LEU:HB3	40:5:258:VAL:HA	1.76	0.68
37:2:855:LEU:HD13	40:5:257:ILE:CG2	2.24	0.68
38:3:7:THR:HA	38:3:10:ILE:HG22	1.76	0.68
40:5:122:SER:HB2	40:5:123:THR:HA	1.76	0.67
37:2:725:PRO:HB3	37:2:734:ARG:HG3	1.76	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:3:351:ILE:HG23	38:3:356:LEU:HD11	1.77	0.67
1:A:379:C:O2	9:J:5:ARG:NH1	2.29	0.66
36:1:526:MET:HB3	40:5:237:ASN:CG	2.20	0.66
36:1:529:VAL:HG23	40:5:233:LEU:HB3	1.77	0.66
37:2:710:ILE:CG1	37:2:714:PHE:CE2	2.78	0.66
37:2:710:ILE:HD12	37:2:714:PHE:CE2	2.31	0.66
39:4:276:CYS:HA	40:5:211:ILE:HG23	1.77	0.66
1:A:818:A:OP1	10:K:80:ARG:NH2	2.29	0.66
36:1:278:LYS:O	36:1:281:THR:OG1	2.09	0.66
37:2:372:VAL:HG11	37:2:419:PHE:HB3	1.78	0.66
39:4:354:LEU:HD22	40:5:339:GLY:HA3	1.78	0.65
27:S:98:VAL:HG21	27:S:117:LEU:HD22	1.78	0.65
36:1:289:ALA:HA	36:1:292:HIS:HB3	1.79	0.65
37:2:862:LYS:HB2	40:5:265:ARG:HD2	1.78	0.65
25:Q:28:MET:HE2	25:Q:33:LEU:HD22	1.79	0.65
40:5:297:PRO:HA	40:5:298:GLU:HB2	1.79	0.65
5:D:127:PHE:CG	5:D:141:LEU:CD2	2.77	0.65
39:4:276:CYS:SG	40:5:215:MET:N	2.70	0.65
39:4:124:ASP:O	40:5:111:ASN:ND2	2.30	0.65
36:1:522:GLN:O	36:1:526:MET:HG3	1.97	0.64
36:1:523:LEU:CA	36:1:526:MET:SD	2.67	0.64
38:3:84:LEU:HD12	38:3:85:GLN:HG2	1.78	0.64
5:D:127:PHE:HD1	5:D:141:LEU:HD21	0.78	0.64
2:0:549:C:O2'	2:0:552:A:N3	2.31	0.64
41:6:142:ILE:HG23	41:6:161:MET:SD	2.37	0.64
37:2:855:LEU:HD13	40:5:257:ILE:HB	1.80	0.64
3:B:16:LEU:HD21	27:S:117:LEU:HD11	1.79	0.63
38:3:30:GLU:N	38:3:62:TYR:OH	2.31	0.63
39:4:116:PRO:CB	40:5:47:LEU:HD13	2.27	0.63
36:1:289:ALA:HB3	36:1:331:ILE:HG21	1.80	0.63
39:4:176:MET:SD	40:5:106:SER:OG	2.57	0.62
1:A:1117:C:O2'	1:A:1119:A:N6	2.32	0.62
13:P:120:ALA:O	18:b:56:VAL:HG11	1.99	0.62
36:1:530:LEU:HD21	40:5:234:ALA:CB	2.26	0.62
43:8:43:ALA:HB1	43:8:47:GLU:HB2	1.80	0.62
36:1:43:TRP:CD1	36:1:74:TYR:HH	2.17	0.62
37:2:855:LEU:HD13	40:5:257:ILE:HG22	1.82	0.62
39:4:336:PRO:HB3	40:5:349:GLU:C	2.24	0.62
41:6:71:LEU:HD11	41:6:134:PHE:CD1	2.35	0.61
1:A:1300:U:H2'	1:A:1300:U:O2	2.00	0.61
2:0:397:G:H2'	2:0:398:U:O4'	1.99	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:146:ARG:HB2	4:C:149:GLN:HB2	1.82	0.61
39:4:354:LEU:HB2	40:5:343:MET:SD	2.40	0.61
36:1:530:LEU:C	40:5:230:LEU:HD11	2.26	0.61
41:6:215:ALA:HB2	43:8:369:LEU:HD12	1.82	0.61
36:1:525:ALA:O	36:1:529:VAL:HG22	2.00	0.61
36:1:530:LEU:HG	40:5:234:ALA:HA	1.81	0.61
39:4:155:PHE:CD2	39:4:176:MET:HG2	2.36	0.61
40:5:79:THR:HG21	40:5:112:ILE:HD11	1.83	0.61
1:A:1693:G:N2	1:A:1834:A:H8	1.99	0.61
36:1:526:MET:HB3	40:5:237:ASN:OD1	2.01	0.61
39:4:279:PRO:HD2	40:5:207:ASN:N	2.15	0.61
39:4:365:GLN:HG3	40:5:329:ASN:CB	2.27	0.61
40:5:257:ILE:HG23	40:5:261:ASN:ND2	2.16	0.61
14:W:16:LYS:HG2	14:W:23:ILE:HG22	1.81	0.60
40:5:340:LYS:HB3	41:6:207:PHE:CE1	2.35	0.60
40:5:350:TYR:C	40:5:350:TYR:CD2	2.79	0.60
42:7:395:GLY:HA2	42:7:398:MET:HE2	1.83	0.60
43:8:115:LYS:CB	43:8:116:ASN:HB3	2.32	0.60
38:3:42:LEU:HD22	38:3:219:LEU:HD22	1.83	0.60
35:h:156:PHE:HE1	35:h:179:LEU:HD21	1.67	0.60
37:2:710:ILE:HG13	37:2:714:PHE:HE2	1.66	0.60
39:4:341:ASP:N	40:5:350:TYR:OH	2.34	0.60
41:6:37:ALA:HB1	41:6:131:ILE:HG12	1.84	0.60
36:1:440:LEU:HD21	36:1:471:ILE:HG23	1.82	0.60
39:4:361:ALA:HB3	40:5:336:GLN:HE21	1.67	0.60
42:7:356:LYS:HD2	42:7:424:VAL:HG13	1.82	0.60
42:7:488:ILE:HG23	42:7:492:VAL:HG23	1.84	0.60
1:A:1075:C:OP1	12:O:107:LYS:NZ	2.34	0.59
1:A:1636:G:H2'	1:A:1636:G:N3	2.16	0.59
16:Y:93:PHE:O	16:Y:140:ARG:NH2	2.35	0.59
41:6:44:LEU:HD21	41:6:84:LEU:HD12	1.82	0.59
2:O:475:A:O2'	2:O:509:G:O6	2.20	0.59
37:2:710:ILE:HD12	37:2:714:PHE:HZ	1.63	0.59
38:3:38:LEU:HA	38:3:249:MET:HG3	1.84	0.59
39:4:243:VAL:HG11	39:4:248:MET:HA	1.83	0.59
38:3:198:ASN:N	38:3:199:ASN:HA	2.17	0.59
39:4:307:LEU:HD22	39:4:324:VAL:HG11	1.83	0.59
1:A:1331:C:H2'	1:A:1331:C:O2	2.03	0.59
36:1:523:LEU:O	36:1:526:MET:HB2	2.02	0.59
37:2:855:LEU:HD12	37:2:856:ALA:N	2.16	0.59
39:4:195:THR:HA	39:4:222:VAL:HB	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:C:H2'	1:A:293:C:O2	2.03	0.59
1:A:694:G:H1	1:A:732:U:H3	1.51	0.59
16:Y:61:GLN:O	16:Y:63:ASN:N	2.36	0.59
36:1:385:PRO:HA	36:1:388:LYS:HB2	1.84	0.59
39:4:152:THR:HG21	40:5:51:LYS:HE3	1.85	0.59
1:A:963:A:H2'	1:A:964:A:O4'	2.03	0.59
37:2:375:LYS:O	37:2:378:ILE:HG22	2.01	0.59
39:4:347:LEU:CD1	40:5:346:ALA:C	2.76	0.58
36:1:530:LEU:O	40:5:230:LEU:HD12	2.03	0.58
39:4:269:VAL:HG22	40:5:47:LEU:CD2	2.33	0.58
43:8:195:ASP:N	43:8:196:ASN:HB2	2.18	0.58
1:A:126:G:H2'	7:H:199:THR:HG21	1.85	0.58
40:5:346:ALA:O	40:5:350:TYR:HB3	2.02	0.58
42:7:245:GLU:HA	42:7:439:PRO:HG2	1.85	0.58
36:1:530:LEU:O	40:5:230:LEU:CD1	2.52	0.58
40:5:333:PHE:HA	40:5:336:GLN:HG3	1.84	0.58
1:A:1734:G:O2'	1:A:1800:A:N6	2.36	0.58
39:4:303:LEU:HD21	39:4:324:VAL:HG21	1.86	0.58
18:b:45:VAL:HG11	18:b:53:ILE:HD13	1.86	0.58
39:4:375:VAL:HG22	40:5:313:ARG:HD2	1.84	0.58
36:1:534:LEU:HB2	40:5:230:LEU:CD1	2.25	0.58
1:A:986:G:C8	13:P:137:SER:O	2.57	0.57
25:Q:37:TYR:OH	25:Q:45:LEU:HD12	2.04	0.57
40:5:211:ILE:HG22	40:5:212:ASN:N	2.19	0.57
39:4:269:VAL:HG22	40:5:47:LEU:HD21	1.86	0.57
8:I:100:ILE:HD11	8:I:122:LEU:HD12	1.85	0.57
38:3:258:THR:O	38:3:262:ILE:HG13	2.04	0.57
39:4:265:GLU:HG2	40:5:50:ILE:HG22	1.86	0.57
43:8:108:ASN:HB2	43:8:114:ASP:HB2	1.86	0.57
1:A:672:A:N6	1:A:1027:A:OP1	2.38	0.57
35:h:24:THR:HB	35:h:71:ILE:HG12	1.85	0.57
39:4:338:ILE:HG13	39:4:340:PRO:HD3	1.87	0.57
35:h:87:LEU:HD21	35:h:108:VAL:HG11	1.87	0.57
40:5:69:GLY:HA2	40:5:78:ILE:HA	1.87	0.57
40:5:80:ASN:HB3	40:5:107:LEU:HD11	1.87	0.57
1:A:1396:A:O2'	1:A:1398:G:N7	2.36	0.57
43:8:292:ILE:HG12	43:8:331:LYS:HB2	1.85	0.57
5:D:127:PHE:HA	5:D:141:LEU:HD23	1.86	0.57
9:J:57:ALA:HB2	9:J:183:GLY:HA2	1.87	0.57
40:5:104:MET:HB2	40:5:114:HIS:HB2	1.85	0.57
43:8:312:VAL:HG11	43:8:325:ILE:HG21	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:15:VAL:HG21	27:S:109:LEU:HG	1.87	0.57
42:7:244:LEU:HD11	42:7:254:GLU:HB3	1.87	0.57
42:7:348:SER:HA	42:7:349:MET:HB3	1.86	0.57
43:8:13:ASP:HA	43:8:14:GLN:C	2.30	0.57
25:Q:75:VAL:HG12	25:Q:93:MET:HB3	1.87	0.57
35:h:256:ILE:HG13	35:h:270:LEU:HB2	1.86	0.57
42:7:379:PRO:HA	42:7:380:MET:HB3	1.87	0.56
39:4:272:ILE:CG1	40:5:43:GLY:HA3	2.35	0.56
36:1:455:LEU:HA	36:1:458:LEU:HB3	1.86	0.56
36:1:526:MET:HE2	40:5:239:LEU:N	2.19	0.56
37:2:594:LEU:O	37:2:598:ILE:HG22	2.06	0.56
38:3:229:ARG:HA	38:3:232:ILE:HG22	1.87	0.56
39:4:285:LEU:HD21	40:5:163:SER:CB	2.36	0.56
43:8:7:ILE:HB	43:8:22:LEU:HA	1.86	0.56
39:4:375:VAL:O	40:5:313:ARG:CD	2.52	0.56
1:A:897:U:H3'	1:A:898:U:H5''	1.87	0.56
1:A:1216:C:N4	1:A:1342:U:OP1	2.36	0.56
39:4:340:PRO:N	40:5:350:TYR:HE1	2.04	0.56
1:A:1016:U:H2'	1:A:1016:U:O2	2.05	0.56
15:X:86:LEU:HD11	15:X:104:LEU:HD21	1.88	0.56
35:h:235:ILE:O	35:h:253:GLY:N	2.39	0.56
39:4:304:SER:O	43:8:348:GLN:NE2	2.38	0.56
40:5:244:GLN:HB3	40:5:247:MET:HB3	1.88	0.56
40:5:257:ILE:O	40:5:261:ASN:HB2	2.06	0.56
43:8:60:VAL:HG11	43:8:99:PRO:HD3	1.88	0.56
37:2:855:LEU:HD13	40:5:257:ILE:CB	2.36	0.56
39:4:324:VAL:O	39:4:328:LEU:N	2.37	0.56
3:B:63:ARG:HG2	3:B:185:MET:HE1	1.87	0.56
37:2:618:ILE:HD11	37:2:677:ILE:HG22	1.88	0.56
2:0:402:C:H3'	2:0:403:G:C5'	2.35	0.56
37:2:627:LYS:HB3	37:2:688:VAL:HG21	1.87	0.56
42:7:353:THR:HG23	42:7:354:THR:HA	1.88	0.55
38:3:60:ASN:HB3	38:3:62:TYR:CE2	2.41	0.55
38:3:254:LEU:HD21	38:3:286:TYR:HD2	1.71	0.55
42:7:373:ILE:HG21	42:7:401:MET:HE2	1.88	0.55
1:A:146:G:O2'	1:A:147:A:O5'	2.19	0.55
1:A:688:U:O2	8:I:122:LEU:HD13	2.06	0.55
1:A:1228:A:O2'	1:A:1634:A:N3	2.23	0.55
36:1:372:ASN:HA	36:1:375:VAL:HG12	1.88	0.55
2:0:621:G:OP1	2:0:623:A:N6	2.40	0.55
36:1:208:ILE:HG22	36:1:218:ILE:HG21	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:2:848:GLU:OE2	40:5:251:ASP:HB2	2.06	0.55
37:2:852:GLN:HE22	40:5:257:ILE:CD1	2.19	0.55
42:7:262:ARG:NH1	42:7:282:SER:OG	2.39	0.55
42:7:475:LEU:HD12	42:7:513:PHE:HB2	1.88	0.55
36:1:526:MET:HG2	40:5:237:ASN:HA	1.80	0.55
40:5:340:LYS:HA	40:5:343:MET:HE2	1.89	0.55
43:8:60:VAL:HG12	43:8:63:VAL:HG13	1.88	0.55
1:A:384:U:O4	9:J:5:ARG:NH2	2.39	0.55
1:A:853:C:O4'	1:A:853:C:O2	2.23	0.55
1:A:896:U:H2'	1:A:897:U:O4'	2.07	0.55
1:A:1139:C:O4'	1:A:1139:C:O2	2.25	0.55
1:A:1298:G:N3	1:A:1298:G:H2'	2.21	0.55
39:4:281:ARG:HA	40:5:204:VAL:HG13	1.89	0.55
39:4:328:LEU:HA	39:4:331:LEU:HD12	1.88	0.55
37:2:727:LEU:HB2	37:2:730:PRO:HD2	1.89	0.55
39:4:251:MET:CB	43:8:67:VAL:HG11	2.37	0.55
39:4:372:GLU:OE1	39:4:373:LYS:HG3	2.06	0.55
43:8:128:ILE:HG12	43:8:167:LEU:HD22	1.89	0.55
37:2:727:LEU:O	37:2:731:GLU:HB2	2.06	0.55
38:3:229:ARG:HG2	38:3:256:TYR:HB3	1.88	0.55
39:4:128:ARG:NH2	40:5:70:LEU:HD21	2.22	0.54
2:0:507:U:H3'	2:0:508:A:C5'	2.37	0.54
37:2:870:ASN:CG	39:4:374:LEU:HD22	2.32	0.54
36:1:519:ILE:HA	36:1:523:LEU:CD2	2.36	0.54
37:2:859:LEU:HA	40:5:265:ARG:CZ	2.37	0.54
38:3:17:HIS:CE1	38:3:45:LEU:HD21	2.42	0.54
39:4:220:LEU:HD11	39:4:233:ILE:HG12	1.88	0.54
39:4:375:VAL:O	40:5:313:ARG:NE	2.39	0.54
1:A:1252:C:OP1	30:V:75:LYS:NZ	2.38	0.54
21:E:175:VAL:HG22	21:E:182:LEU:HB2	1.90	0.54
43:8:291:GLU:HA	43:8:330:ARG:HA	1.89	0.54
1:A:1521:C:OP2	28:T:136:THR:OG1	2.26	0.54
2:0:526:A:H2'	2:0:527:C:H5''	1.88	0.54
12:O:60:VAL:HG13	12:O:66:VAL:HG21	1.89	0.54
38:3:405:ILE:HG12	39:4:359:TYR:CE2	2.41	0.54
43:8:115:LYS:HB3	43:8:116:ASN:HB3	1.90	0.54
1:A:1533:A:H2	1:A:1536:G:N3	2.06	0.54
40:5:75:ARG:HH22	40:5:205:ILE:HD12	1.73	0.54
37:2:852:GLN:O	37:2:855:LEU:HD11	2.08	0.54
40:5:192:ILE:O	42:7:548:HIS:CE1	2.61	0.54
1:A:191:A:H3'	1:A:192:C:O4'	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:G:H2'	1:A:407:G:N3	2.23	0.54
1:A:1207:G:O2'	1:A:1837:G:N2	2.40	0.54
39:4:340:PRO:C	40:5:350:TYR:CE1	2.85	0.54
40:5:240:GLY:O	40:5:242:ASN:N	2.41	0.54
36:1:207:GLN:HE22	36:1:216:THR:HB	1.73	0.53
36:1:531:ALA:HB1	39:4:327:PHE:HB3	1.89	0.53
38:3:208:LEU:HD23	38:3:243:LEU:HD23	1.90	0.53
39:4:351:ILE:HA	40:5:343:MET:CE	2.37	0.53
21:E:62:LYS:O	21:E:67:ARG:NH1	2.40	0.53
25:Q:56:LEU:HD22	25:Q:80:LEU:HD13	1.90	0.53
39:4:275:THR:HB	39:4:279:PRO:HG3	1.90	0.53
40:5:79:THR:HG21	40:5:112:ILE:CD1	2.37	0.53
10:K:46:VAL:HG21	10:K:106:LEU:HD13	1.90	0.53
36:1:526:MET:SD	40:5:237:ASN:CA	2.94	0.53
37:2:856:ALA:HA	37:2:859:LEU:HD12	1.90	0.53
2:0:426:U:O2'	2:0:427:U:O2	2.18	0.53
37:2:855:LEU:CB	40:5:258:VAL:CA	2.84	0.53
38:3:261:VAL:HA	38:3:265:LYS:HB3	1.90	0.53
40:5:202:PRO:HB2	40:5:205:ILE:HD11	1.91	0.53
3:B:24:HIS:HB3	3:B:51:LEU:HD21	1.90	0.53
25:Q:45:LEU:HD11	25:Q:86:LEU:HD21	1.91	0.53
36:1:526:MET:SD	40:5:237:ASN:C	2.92	0.53
37:2:464:PRO:HB3	37:2:668:ARG:HG3	1.90	0.53
39:4:152:THR:N	39:4:187:GLU:OE2	2.41	0.53
40:5:190:ALA:HB2	40:5:315:ASP:OD2	2.09	0.53
1:A:1807:C:H2'	1:A:1808:U:O4'	2.09	0.53
2:0:444:C:N4	35:h:182:CYS:SG	2.82	0.53
35:h:296:GLN:NE2	35:h:312:VAL:O	2.41	0.53
37:2:507:ILE:HA	37:2:510:THR:HG22	1.91	0.53
37:2:690:ALA:O	37:2:789:ARG:NH2	2.42	0.53
40:5:350:TYR:CD2	40:5:351:ASN:N	2.77	0.53
42:7:486:PHE:N	42:7:487:ARG:C	2.66	0.53
43:8:71:LEU:CD2	43:8:111:HIS:HB3	2.39	0.53
37:2:714:PHE:O	37:2:718:LEU:HB2	2.09	0.53
39:4:123:VAL:HG21	40:5:44:LEU:CD2	2.37	0.53
39:4:237:VAL:HB	39:4:255:LEU:HD11	1.91	0.53
1:A:1116:C:C2'	1:A:1116:C:O2	2.55	0.53
35:h:156:PHE:CE1	35:h:179:LEU:HD21	2.44	0.53
2:0:387:U:H4'	2:0:388:A:OP1	2.09	0.52
2:0:518:G:H4'	2:0:519:A:OP1	2.09	0.52
2:0:539:U:H2'	2:0:539:U:O2	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:2:738:VAL:HG11	37:2:746:MET:HG2	1.90	0.52
38:3:111:ARG:HG2	38:3:133:ARG:HG2	1.91	0.52
39:4:240:SER:N	39:4:241:MET:HB2	2.24	0.52
39:4:365:GLN:CG	40:5:329:ASN:HB3	2.29	0.52
1:A:897:U:H3'	1:A:898:U:C5'	2.39	0.52
3:B:180:GLN:HB2	3:B:195:TRP:CE3	2.45	0.52
39:4:354:LEU:HD13	40:5:339:GLY:CA	2.39	0.52
41:6:174:MET:HA	41:6:179:TRP:CE3	2.44	0.52
1:A:167:G:OP1	7:H:8:PRO:HB3	2.09	0.52
39:4:318:VAL:HG13	43:8:226:LEU:HB2	1.91	0.52
39:4:358:THR:CA	40:5:336:GLN:HG2	2.37	0.52
40:5:67:LEU:HD22	40:5:78:ILE:CD1	2.38	0.52
37:2:727:LEU:HB2	37:2:730:PRO:CD	2.39	0.52
1:A:533:A:N1	1:A:551:U:C4	2.78	0.52
38:3:127:TYR:OH	38:3:155:ARG:O	2.26	0.52
38:3:375:ILE:HG21	42:7:466:LEU:HD11	1.90	0.52
17:Z:110:ARG:NH2	17:Z:114:MET:SD	2.83	0.52
38:3:304:ASP:HB2	38:3:308:ALA:HB2	1.92	0.52
43:8:250:ALA:HB2	43:8:279:LEU:HD11	1.92	0.52
36:1:528:SER:HA	39:4:331:LEU:HD23	1.91	0.52
40:5:194:PHE:HZ	40:5:319:ILE:HD13	1.74	0.52
42:7:321:PHE:O	42:7:324:LEU:HG	2.10	0.52
42:7:548:HIS:CE1	42:7:552:GLU:HG3	2.44	0.52
43:8:313:ILE:HA	43:8:316:VAL:HG22	1.91	0.52
36:1:526:MET:CG	40:5:237:ASN:CA	2.71	0.52
37:2:856:ALA:HA	37:2:859:LEU:HB2	1.90	0.52
40:5:265:ARG:O	40:5:269:LYS:N	2.43	0.52
43:8:280:LEU:HD22	43:8:301:LEU:HG	1.92	0.52
42:7:274:LEU:HD12	42:7:274:LEU:O	2.10	0.52
37:2:379:ILE:HD11	37:2:447:LEU:HB3	1.92	0.51
39:4:155:PHE:CE1	40:5:106:SER:HB3	2.45	0.51
40:5:134:LEU:HD11	40:5:169:LEU:HD13	1.93	0.51
41:6:155:ARG:HG2	41:6:186:GLN:HA	1.92	0.51
2:0:541:C:H2'	2:0:542:A:H8	1.73	0.51
2:0:608:U:O2'	31:a:76:ARG:NH1	2.37	0.51
39:4:156:SER:OG	40:5:110:VAL:HG21	2.10	0.51
1:A:1834:A:H2	1:A:1837:G:H1	1.56	0.51
37:2:683:GLU:HA	37:2:686:TYR:HB3	1.92	0.51
38:3:214:LEU:O	38:3:232:ILE:HG13	2.10	0.51
42:7:366:GLN:NE2	42:7:416:SER:OG	2.43	0.51
36:1:355:LEU:HD11	37:2:720:VAL:HB	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:1:390:LEU:HD22	36:1:410:VAL:HB	1.92	0.51
13:P:113:GLN:OE1	18:b:45:VAL:HA	2.11	0.51
39:4:358:THR:HG22	40:5:336:GLN:CA	2.32	0.51
37:2:493:LYS:CE	37:2:498:GLU:OE2	2.59	0.51
38:3:114:PHE:HA	38:3:117:LEU:HB2	1.93	0.51
40:5:234:ALA:O	40:5:237:ASN:N	2.44	0.51
42:7:390:LEU:HA	42:7:393:LYS:HB3	1.93	0.51
43:8:147:VAL:HG13	43:8:188:LEU:HD21	1.91	0.51
43:8:196:ASN:HB3	43:8:199:GLN:HB2	1.92	0.51
1:A:581:U:H4'	17:Z:66:GLY:HA3	1.92	0.51
1:A:1207:G:N2	2:0:694:U:OP1	2.43	0.51
3:B:205:ARG:HB3	3:B:210:ILE:HG22	1.93	0.51
36:1:452:PHE:HB2	36:1:489:ARG:HG2	1.92	0.51
37:2:731:GLU:HB3	37:2:755:PHE:CE2	2.45	0.51
37:2:852:GLN:NE2	40:5:257:ILE:HD12	2.24	0.51
43:8:340:ARG:HB3	43:8:344:LYS:HD3	1.93	0.51
36:1:527:SER:HA	36:1:530:LEU:HB2	1.92	0.51
37:2:848:GLU:OE2	40:5:247:MET:HG2	2.11	0.51
38:3:179:MET:HE2	38:3:181:ASN:HD21	1.75	0.51
42:7:229:ASN:OD1	42:7:279:ARG:NH2	2.44	0.51
22:G:73:THR:O	22:G:89:THR:HG21	2.11	0.51
27:S:114:LEU:HB3	27:S:117:LEU:HG	1.94	0.51
36:1:113:LEU:HA	36:1:116:GLU:HB2	1.92	0.51
36:1:452:PHE:CE1	36:1:471:ILE:HD13	2.46	0.51
37:2:870:ASN:HA	40:5:272:GLN:CD	2.36	0.51
39:4:128:ARG:HH21	40:5:70:LEU:HD21	1.76	0.51
39:4:135:ARG:HE	39:4:194:ALA:HB1	1.75	0.51
1:A:547:G:H2'	1:A:549:C:H41	1.76	0.50
1:A:873:G:H2'	1:A:873:G:N3	2.25	0.50
36:1:533:ALA:HB2	40:5:233:LEU:HD12	1.93	0.50
37:2:693:LEU:HD23	37:2:697:TYR:CE2	2.46	0.50
39:4:179:LEU:CD1	40:5:99:TYR:HA	2.41	0.50
5:D:127:PHE:HD1	5:D:141:LEU:CD2	1.70	0.50
29:U:22:LEU:HD13	29:U:28:LEU:HD21	1.93	0.50
36:1:410:VAL:HA	36:1:413:TRP:HB3	1.92	0.50
37:2:691:MET:HE3	37:2:788:LEU:HD11	1.93	0.50
40:5:79:THR:OG1	40:5:112:ILE:HD12	2.10	0.50
43:8:294:PHE:HB2	43:8:328:THR:HA	1.93	0.50
2:0:583:G:HO2'	36:1:3:ALA:N	2.10	0.50
36:1:116:GLU:O	36:1:121:ILE:HD11	2.12	0.50
36:1:384:VAL:HG13	36:1:386:GLU:HB3	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:3:295:PHE:HA	38:3:298:CYS:HB2	1.93	0.50
38:3:405:ILE:HG23	39:4:359:TYR:OH	2.11	0.50
39:4:361:ALA:CA	40:5:332:GLU:HB3	2.42	0.50
42:7:394:TYR:HA	42:7:397:LYS:HB3	1.93	0.50
43:8:100:SER:HA	43:8:103:LEU:HD12	1.93	0.50
36:1:520:ARG:HB2	40:5:241:LYS:O	2.11	0.50
38:3:238:TYR:HE1	38:3:272:GLN:HE22	1.59	0.50
38:3:316:GLU:HA	38:3:319:LEU:HB3	1.92	0.50
39:4:262:TYR:CE2	39:4:264:THR:HG22	2.46	0.50
40:5:196:HIS:CE1	40:5:322:GLN:NE2	2.79	0.50
41:6:207:PHE:CE1	41:6:211:SER:HB3	2.47	0.50
42:7:270:GLY:HA3	42:7:305:TYR:OH	2.12	0.50
1:A:1535:U:O2	1:A:1535:U:C2'	2.59	0.50
2:0:490:A:H1'	36:1:212:HIS:HB3	1.93	0.50
37:2:748:ASP:HA	37:2:778:MET:HE1	1.94	0.50
40:5:276:GLN:O	40:5:280:ARG:N	2.39	0.50
42:7:280:LEU:HD21	42:7:303:SER:HB2	1.93	0.50
11:M:47:PRO:HG2	11:M:116:CYS:SG	2.52	0.50
12:O:55:ARG:NH1	12:O:56:ASP:OD1	2.44	0.50
37:2:598:ILE:O	37:2:598:ILE:HG23	2.11	0.50
1:A:1521:C:OP1	28:T:129:LEU:HD13	2.12	0.50
32:d:17:VAL:HA	32:d:30:VAL:HG12	1.93	0.50
37:2:710:ILE:HB	37:2:714:PHE:CZ	2.41	0.50
1:A:534:G:N2	1:A:551:U:O2	2.34	0.50
1:A:907:G:H2'	1:A:908:A:C8	2.47	0.50
22:G:20:PHE:CZ	22:G:69:VAL:HG21	2.47	0.50
22:G:40:ALA:HB1	22:G:45:TYR:CG	2.46	0.50
39:4:317:LYS:HA	39:4:320:ALA:HB3	1.94	0.50
39:4:351:ILE:HG23	40:5:343:MET:HE3	1.93	0.50
1:A:369:C:O4'	1:A:369:C:O2	2.27	0.50
37:2:445:LEU:HA	37:2:448:VAL:HG22	1.93	0.50
39:4:279:PRO:HA	39:4:280:ASN:CB	2.23	0.50
40:5:332:GLU:O	40:5:336:GLN:HG3	2.12	0.50
1:A:1310:U:O3'	34:g:143:LYS:NZ	2.44	0.49
1:A:1779:G:H3'	1:A:1780:G:H8	1.77	0.49
40:5:173:LEU:HD13	40:5:194:PHE:CZ	2.47	0.49
2:0:517:G:O2'	2:0:518:G:O5'	2.30	0.49
39:4:347:LEU:HD22	40:5:347:LEU:HB2	1.94	0.49
40:5:64:GLN:O	40:5:83:PRO:HA	2.12	0.49
40:5:160:GLY:HA2	40:5:334:THR:HG23	1.94	0.49
42:7:194:PHE:CZ	42:7:235:VAL:HG23	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0:489:C:O2	2:0:489:C:O4'	2.28	0.49
37:2:593:HIS:NE2	38:3:7:THR:HB	2.27	0.49
35:h:90:TRP:CD1	35:h:97:THR:HA	2.47	0.49
36:1:530:LEU:HD23	40:5:230:LEU:HG	1.94	0.49
37:2:379:ILE:HG22	37:2:404:CYS:SG	2.52	0.49
39:4:118:ILE:O	39:4:122:ILE:HG13	2.12	0.49
39:4:170:MET:HG3	39:4:209:TYR:HB3	1.93	0.49
39:4:279:PRO:HB2	40:5:206:LYS:N	2.27	0.49
40:5:243:LEU:O	40:5:245:LEU:HB2	2.12	0.49
2:0:539:U:O2	2:0:539:U:C2'	2.61	0.49
36:1:525:ALA:C	36:1:529:VAL:HG22	2.38	0.49
40:5:41:ILE:CG1	40:5:78:ILE:HD12	2.40	0.49
40:5:153:ASP:HB2	40:5:163:SER:HA	1.95	0.49
40:5:204:VAL:O	40:5:204:VAL:HG22	2.13	0.49
1:A:126:G:N2	1:A:180:G:O2'	2.45	0.49
1:A:531:A:H61	1:A:553:U:H3	1.61	0.49
1:A:534:G:H2'	1:A:535:G:H8	1.77	0.49
7:H:49:VAL:HG22	7:H:115:LYS:HB3	1.94	0.49
7:H:106:LEU:N	7:H:106:LEU:HD23	2.28	0.49
9:J:81:VAL:HG22	9:J:102:VAL:HG12	1.93	0.49
24:N:106:CYS:SG	24:N:107:SER:N	2.85	0.49
28:T:40:TYR:OH	28:T:71:MET:O	2.31	0.49
36:1:533:ALA:CB	40:5:233:LEU:HD12	2.43	0.49
37:2:710:ILE:CD1	37:2:714:PHE:CE2	2.96	0.49
37:2:847:THR:HA	37:2:850:THR:HG22	1.95	0.49
43:8:87:CYS:HA	43:8:90:LEU:HD23	1.95	0.49
16:Y:128:VAL:HG21	16:Y:141:PRO:HD3	1.95	0.49
22:G:30:ILE:HG23	22:G:117:ILE:HD11	1.93	0.49
27:S:99:ASP:O	27:S:102:THR:HB	2.12	0.49
37:2:744:MET:HE2	37:2:806:THR:HA	1.93	0.49
38:3:15:ASP:HA	38:3:208:LEU:HD13	1.93	0.49
43:8:70:LEU:HG	43:8:86:LEU:HD21	1.95	0.49
43:8:104:GLN:HA	43:8:107:SER:HB2	1.94	0.49
1:A:1722:G:O6	1:A:1812:U:O2	2.31	0.49
6:F:51:LYS:N	6:F:51:LYS:CD	2.75	0.49
13:P:85:CYS:SG	13:P:90:ILE:HB	2.52	0.49
35:h:44:LYS:HB2	35:h:56:GLN:HB2	1.94	0.49
35:h:78:ALA:HB2	35:h:92:LEU:HD11	1.94	0.49
39:4:285:LEU:HB2	40:5:161:SER:HA	1.95	0.49
43:8:227:LYS:N	43:8:228:PRO:HD3	2.27	0.49
1:A:64:A:O2'	1:A:66:G:OP2	2.30	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:A:O2'	1:A:534:G:O5'	2.25	0.49
1:A:1512:C:O2'	33:e:7:TYR:O	2.24	0.49
18:b:44:ILE:HD12	18:b:65:PRO:HG2	1.94	0.49
38:3:7:THR:OG1	38:3:244:ASN:ND2	2.46	0.49
39:4:339:VAL:N	39:4:340:PRO:HD3	2.27	0.49
2:0:543:G:C2	2:0:544:U:C4	3.01	0.49
24:N:35:ILE:HG21	34:g:102:VAL:HG21	1.94	0.49
26:R:70:VAL:HG11	26:R:84:ILE:HG22	1.94	0.49
38:3:254:LEU:HD21	38:3:286:TYR:CD2	2.48	0.49
39:4:275:THR:O	39:4:279:PRO:HD3	2.13	0.49
1:A:506:G:OP1	17:Z:108:LYS:NZ	2.46	0.48
4:C:175:GLU:O	4:C:187:LYS:NZ	2.46	0.48
35:h:23:THR:HG22	35:h:31:ILE:HG22	1.95	0.48
35:h:206:LEU:HD12	35:h:218:LEU:HD12	1.95	0.48
40:5:244:GLN:HB2	40:5:248:ASP:HB2	1.94	0.48
1:A:788:G:H2'	1:A:788:G:N3	2.27	0.48
2:0:472:G:H2'	2:0:472:G:N3	2.27	0.48
13:P:39:ASP:N	13:P:69:SER:HB3	2.28	0.48
22:G:35:LEU:HD12	22:G:147:VAL:HG23	1.95	0.48
36:1:375:VAL:HG23	36:1:380:LEU:HB2	1.94	0.48
38:3:241:GLN:O	38:3:242:TYR:HB2	2.13	0.48
38:3:262:ILE:HG12	38:3:267:VAL:HG11	1.94	0.48
2:0:604:C:N4	2:0:677:A:O2'	2.46	0.48
15:X:28:ARG:CB	15:X:29:PRO:HD3	2.43	0.48
22:G:39:ILE:HG23	22:G:68:ILE:HG21	1.94	0.48
43:8:355:ASN:C	43:8:359:GLN:HE21	2.20	0.48
2:0:537:G:OP2	40:5:269:LYS:NZ	2.44	0.48
29:U:63:HIS:CE1	29:U:78:ILE:HD11	2.47	0.48
38:3:148:ALA:HB1	38:3:172:LYS:HD3	1.95	0.48
36:1:390:LEU:HD11	36:1:407:VAL:HA	1.95	0.48
37:2:496:THR:HA	37:2:499:ILE:HG22	1.94	0.48
39:4:183:VAL:HA	40:5:85:PRO:CB	2.43	0.48
39:4:308:GLN:NE2	43:8:345:GLN:O	2.47	0.48
39:4:341:ASP:CA	40:5:350:TYR:OH	2.61	0.48
13:P:113:GLN:NE2	18:b:44:ILE:O	2.36	0.48
36:1:524:THR:O	36:1:525:ALA:C	2.56	0.48
38:3:6:LEU:HD11	38:3:204:PRO:HB3	1.95	0.48
2:0:491:U:O2'	2:0:517:G:O6	2.20	0.48
22:G:50:PRO:HG2	22:G:90:VAL:HG23	1.96	0.48
36:1:448:GLN:HE22	36:1:495:SER:HB2	1.78	0.48
7:H:159:ARG:HG2	7:H:173:ALA:HB2	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:101:ILE:HD12	9:J:190:LEU:HD11	1.96	0.48
38:3:225:HIS:N	38:3:226:PRO:CD	2.77	0.48
39:4:238:SER:OG	39:4:250:VAL:HG12	2.13	0.48
42:7:298:GLU:HA	42:7:301:LYS:HB3	1.96	0.48
1:A:550:C:O2'	1:A:551:U:C5	2.65	0.48
1:A:877:C:H2'	1:A:878:G:O4'	2.14	0.48
2:0:562:U:O2	2:0:562:U:O4'	2.31	0.48
7:H:102:VAL:HG21	7:H:109:LEU:HD11	1.95	0.48
36:1:307:ARG:HH12	36:1:318:MET:HA	1.79	0.48
37:2:855:LEU:HD22	40:5:258:VAL:N	2.28	0.48
38:3:51:VAL:O	38:3:55:MET:HG3	2.14	0.48
39:4:262:TYR:CE2	40:5:53:TYR:CD2	3.02	0.48
39:4:265:GLU:HG2	40:5:50:ILE:O	2.14	0.48
1:A:1397:U:O2	1:A:1397:U:C2'	2.61	0.47
1:A:1520:G:H2'	1:A:1520:G:N3	2.28	0.47
1:A:1761:U:H2'	1:A:1771:G:H1	1.79	0.47
8:I:143:ARG:HD3	8:I:157:HIS:HE2	1.77	0.47
39:4:152:THR:CG2	40:5:51:LYS:HE3	2.44	0.47
39:4:270:ASP:HA	39:4:273:MET:HG2	1.96	0.47
39:4:340:PRO:N	40:5:350:TYR:CE1	2.81	0.47
41:6:171:LYS:HA	41:6:174:MET:HB3	1.97	0.47
1:A:163:U:OP1	7:H:84:TYR:HA	2.15	0.47
10:K:170:PRO:O	10:K:175:ARG:NH1	2.47	0.47
18:b:45:VAL:HG22	18:b:64:LEU:HD11	1.96	0.47
25:Q:80:LEU:HD21	25:Q:83:MET:HB2	1.96	0.47
37:2:480:CYS:HA	37:2:483:ILE:HG22	1.95	0.47
39:4:190:LEU:HB3	39:4:218:ILE:HB	1.96	0.47
39:4:347:LEU:HD23	39:4:351:ILE:HG12	1.95	0.47
42:7:475:LEU:C	42:7:475:LEU:HD23	2.39	0.47
42:7:486:PHE:HB3	42:7:487:ARG:HB3	1.96	0.47
1:A:752:G:H4'	1:A:753:C:OP1	2.13	0.47
2:0:602:U:O2'	2:0:680:A:N7	2.43	0.47
25:Q:18:ARG:NH1	28:T:88:LYS:O	2.47	0.47
36:1:530:LEU:CG	40:5:234:ALA:HA	2.44	0.47
41:6:71:LEU:HD22	41:6:127:LEU:HD23	1.96	0.47
42:7:470:MET:HB3	42:7:474:LYS:HB3	1.96	0.47
1:A:607:U:H3'	1:A:608:C:C5'	2.44	0.47
1:A:1446:A:H5''	30:V:58:THR:HG23	1.96	0.47
11:M:120:VAL:HG12	11:M:145:VAL:HG11	1.96	0.47
27:S:24:LEU:HB2	27:S:58:MET:SD	2.54	0.47
36:1:276:TYR:HA	36:1:279:VAL:HG12	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:3:170:TRP:CZ3	38:3:173:LEU:HD22	2.50	0.47
39:4:354:LEU:HD12	40:5:343:MET:CG	2.44	0.47
1:A:115:U:O2'	1:A:381:C:O2	2.27	0.47
37:2:493:LYS:HE2	37:2:498:GLU:OE2	2.15	0.47
37:2:862:LYS:HB2	40:5:265:ARG:CD	2.45	0.47
39:4:344:GLU:HG3	40:5:350:TYR:CD2	2.50	0.47
43:8:303:ILE:HG22	43:8:304:GLY:H	1.77	0.47
38:3:174:ALA:O	38:3:178:LEU:HG	2.14	0.47
39:4:365:GLN:HA	40:5:329:ASN:OD1	2.14	0.47
1:A:372:U:O2'	11:M:82:MET:HE1	2.15	0.47
1:A:1282:A:H2'	1:A:1283:C:O4'	2.15	0.47
1:A:1298:G:O2'	1:A:1299:A:C8	2.66	0.47
11:M:42:LEU:HD13	11:M:72:ILE:HD11	1.97	0.47
16:Y:63:ASN:HD22	16:Y:114:ASP:HB3	1.79	0.47
21:E:16:ILE:HD11	33:e:36:LEU:HD23	1.96	0.47
36:1:478:CYS:HB3	36:1:502:ARG:HB3	1.97	0.47
37:2:493:LYS:HG3	37:2:498:GLU:OE2	2.09	0.47
37:2:855:LEU:CD1	40:5:257:ILE:HB	2.44	0.47
38:3:212:THR:HG22	38:3:216:HIS:CE1	2.49	0.47
38:3:367:ALA:O	38:3:371:ILE:HG12	2.15	0.47
39:4:128:ARG:HB2	40:5:111:ASN:HA	1.97	0.47
39:4:183:VAL:HA	40:5:85:PRO:HG3	1.96	0.47
39:4:340:PRO:C	40:5:350:TYR:HE1	2.22	0.47
39:4:361:ALA:HA	40:5:332:GLU:HB3	1.95	0.47
40:5:176:VAL:HB	40:5:189:LYS:HE2	1.96	0.47
41:6:70:LEU:HD21	41:6:103:LEU:HD12	1.97	0.47
1:A:1624:U:O2	1:A:1624:U:O4'	2.30	0.47
7:H:159:ARG:HB3	7:H:171:THR:HG22	1.96	0.47
28:T:26:ILE:HG22	28:T:45:LEU:HD11	1.95	0.47
35:h:174:VAL:HB	35:h:188:HIS:HB2	1.97	0.47
36:1:11:ALA:CB	36:1:34:VAL:HG21	2.44	0.47
40:5:154:PRO:HD2	40:5:156:LYS:HE3	1.97	0.47
7:H:49:VAL:HG23	7:H:114:VAL:HB	1.97	0.47
36:1:218:ILE:O	36:1:218:ILE:HG23	2.14	0.47
36:1:526:MET:HE2	40:5:239:LEU:H	1.80	0.47
41:6:70:LEU:HD13	41:6:102:ILE:HB	1.97	0.47
1:A:693:A:H2'	1:A:694:G:H8	1.80	0.47
1:A:1298:G:N3	1:A:1298:G:C2'	2.77	0.47
1:A:1719:A:H62	1:A:1814:G:H21	1.63	0.47
5:D:212:LYS:HA	5:D:215:LEU:HD12	1.97	0.47
25:Q:15:PHE:CZ	25:Q:109:PRO:HB2	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:1:110:GLN:O	36:1:114:ASP:N	2.48	0.47
43:8:50:ASP:OD1	43:8:51:VAL:N	2.47	0.47
39:4:352:ASN:HD21	42:7:523:ILE:HG21	1.80	0.46
36:1:487:THR:HA	37:2:798:VAL:HG22	1.95	0.46
36:1:526:MET:HA	40:5:236:SER:C	2.40	0.46
37:2:356:LEU:HB3	37:2:360:ILE:HD12	1.96	0.46
43:8:182:SER:O	43:8:186:VAL:HG23	2.16	0.46
12:O:99:ARG:NH2	12:O:119:GLU:OE2	2.48	0.46
35:h:31:ILE:HG13	35:h:43:TRP:CD1	2.51	0.46
36:1:526:MET:CE	40:5:240:GLY:N	2.75	0.46
38:3:254:LEU:HD12	38:3:255:ARG:N	2.30	0.46
42:7:417:CYS:HB3	42:7:418:PRO:HD3	1.97	0.46
36:1:147:THR:HA	36:1:150:VAL:HG22	1.96	0.46
36:1:383:VAL:HG13	36:1:388:LYS:HA	1.98	0.46
37:2:464:PRO:CB	37:2:668:ARG:HG3	2.45	0.46
39:4:354:LEU:C	39:4:358:THR:HG23	2.41	0.46
40:5:49:ILE:HG12	40:5:120:TYR:CE2	2.51	0.46
1:A:1116:C:O2'	1:A:1117:C:C2	2.69	0.46
1:A:1118:C:O4'	1:A:1118:C:O2	2.28	0.46
4:C:149:GLN:HE21	4:C:151:ARG:HB3	1.81	0.46
7:H:116:LYS:HD2	7:H:125:THR:HG21	1.97	0.46
24:N:38:ALA:HB1	24:N:110:VAL:HG21	1.98	0.46
27:S:71:ILE:HB	27:S:74:GLN:HB2	1.96	0.46
39:4:281:ARG:CZ	40:5:202:PRO:HB3	2.46	0.46
39:4:325:GLY:HA2	39:4:328:LEU:HD12	1.98	0.46
1:A:1286:G:O6	24:N:36:ARG:HB3	2.16	0.46
32:d:12:ALA:HB1	32:d:32:VAL:HG12	1.98	0.46
36:1:525:ALA:O	36:1:529:VAL:HG13	2.16	0.46
36:1:530:LEU:HD22	40:5:230:LEU:CD2	2.46	0.46
38:3:134:TYR:O	38:3:138:GLN:HG2	2.15	0.46
41:6:47:ASN:HB3	41:6:69:ILE:HG23	1.98	0.46
43:8:315:ALA:HB1	43:8:320:MET:CE	2.46	0.46
1:A:1542:C:OP1	29:U:62:ARG:NH2	2.49	0.46
5:D:211:LYS:O	5:D:215:LEU:HG	2.16	0.46
35:h:39:THR:HG22	35:h:60:ARG:HG2	1.98	0.46
37:2:850:THR:HA	37:2:853:GLN:HB3	1.97	0.46
40:5:257:ILE:HA	40:5:261:ASN:HD22	1.80	0.46
41:6:124:ASN:HA	41:6:128:LEU:HD22	1.97	0.46
43:8:319:LYS:HG3	43:8:322:TYR:HB2	1.96	0.46
1:A:293:C:O2	1:A:293:C:C2'	2.64	0.46
1:A:380:G:P	9:J:56:ARG:HH22	2.38	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1231:C:O2'	1:A:1253:A:N6	2.48	0.46
2:0:576:U:H3'	2:0:577:A:H5''	1.98	0.46
6:F:44:LEU:HD13	6:F:72:ILE:HD11	1.97	0.46
22:G:141:VAL:HG23	22:G:146:ARG:HG2	1.97	0.46
24:N:58:GLU:HB3	24:N:61:TYR:HB3	1.97	0.46
24:N:62:VAL:HA	24:N:65:VAL:HG12	1.98	0.46
35:h:251:ALA:HA	35:h:256:ILE:HG22	1.97	0.46
37:2:744:MET:HA	37:2:782:LYS:HD2	1.97	0.46
39:4:240:SER:HA	39:4:241:MET:C	2.41	0.46
1:A:536:A:N1	1:A:548:C:N4	2.61	0.46
3:B:185:MET:HE3	14:W:39:VAL:CG2	2.45	0.46
7:H:98:ARG:HE	7:H:106:LEU:HD22	1.80	0.46
36:1:322:VAL:HB	36:1:379:VAL:HG13	1.98	0.46
37:2:443:CYS:HA	37:2:446:THR:HG22	1.98	0.46
38:3:386:SER:HB2	42:7:467:TYR:CZ	2.50	0.46
40:5:349:GLU:O	40:5:350:TYR:C	2.59	0.46
42:7:532:ASP:HA	42:7:535:VAL:HG22	1.97	0.46
21:E:5:ILE:HD12	21:E:10:LYS:HA	1.97	0.46
24:N:69:CYS:O	24:N:74:ILE:HB	2.16	0.46
35:h:32:LEU:HD11	35:h:92:LEU:HD21	1.97	0.46
36:1:78:CYS:SG	36:1:82:ASN:O	2.72	0.46
36:1:534:LEU:N	40:5:230:LEU:HD13	2.31	0.46
40:5:46:VAL:O	40:5:50:ILE:HG13	2.15	0.46
1:A:289:G:H5'	6:F:129:ILE:HD11	1.97	0.45
1:A:628:A:H61	21:E:178:ARG:HB3	1.81	0.45
1:A:823:U:O2	1:A:823:U:O4'	2.34	0.45
36:1:246:TRP:CD2	37:2:723:ARG:HD2	2.51	0.45
37:2:493:LYS:HG3	37:2:497:GLU:OE2	2.16	0.45
38:3:26:LEU:HD22	38:3:53:PHE:CE1	2.51	0.45
39:4:375:VAL:HG22	40:5:313:ARG:CD	2.46	0.45
2:0:574:U:H2'	2:0:575:U:C6	2.51	0.45
10:K:33:GLY:HA3	20:f:111:TYR:CG	2.52	0.45
27:S:31:ASN:HD21	27:S:55:THR:HB	1.81	0.45
37:2:710:ILE:C	37:2:714:PHE:CE2	2.94	0.45
37:2:806:THR:C	37:2:807:LEU:HD23	2.42	0.45
38:3:268:ARG:H	38:3:269:LYS:HB3	1.80	0.45
42:7:376:THR:HA	42:7:379:PRO:HD2	1.98	0.45
1:A:533:A:H2'	1:A:534:G:C8	2.52	0.45
11:M:80:MET:SD	11:M:120:VAL:HG23	2.56	0.45
21:E:1:MET:O	21:E:4:GLN:N	2.50	0.45
35:h:34:ALA:HB1	35:h:66:VAL:HG23	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:3:353:ILE:HG12	38:3:389:GLY:HA3	1.97	0.45
39:4:183:VAL:HA	40:5:85:PRO:HB3	1.97	0.45
1:A:1331:C:O2	1:A:1331:C:C2'	2.64	0.45
37:2:855:LEU:HB2	40:5:258:VAL:HA	1.96	0.45
38:3:138:GLN:HG3	38:3:151:LEU:HD22	1.98	0.45
39:4:375:VAL:HB	40:5:318:LEU:CD2	2.46	0.45
43:8:189:LEU:CD1	43:8:194:GLU:HB3	2.47	0.45
23:L:59:LYS:HB3	23:L:70:TYR:HB2	1.98	0.45
37:2:815:LEU:N	37:2:816:PRO:HD2	2.31	0.45
39:4:340:PRO:CD	40:5:350:TYR:CE1	3.00	0.45
42:7:373:ILE:HG12	42:7:398:MET:HB2	1.98	0.45
43:8:241:LEU:HA	43:8:244:PHE:HB3	1.98	0.45
1:A:1285:G:OP2	24:N:35:ILE:HG22	2.17	0.45
8:I:19:PHE:CZ	8:I:50:GLU:HB2	2.52	0.45
18:b:56:VAL:O	18:b:56:VAL:CG1	2.49	0.45
28:T:68:ILE:HG23	28:T:72:GLN:HE22	1.81	0.45
35:h:121:VAL:HG21	35:h:165:ILE:CD1	2.46	0.45
36:1:331:ILE:C	36:1:434:ASN:HD21	2.25	0.45
38:3:31:ILE:HG22	38:3:32:TYR:H	1.81	0.45
39:4:193:TYR:HB2	39:4:220:LEU:HB3	1.98	0.45
39:4:276:CYS:HA	40:5:211:ILE:CG2	2.45	0.45
39:4:373:LYS:HD2	40:5:322:GLN:NE2	2.32	0.45
41:6:65:VAL:O	41:6:69:ILE:HG12	2.16	0.45
43:8:281:THR:OG1	43:8:320:MET:HE1	2.16	0.45
1:A:550:C:O2'	1:A:551:U:C6	2.69	0.45
35:h:42:MET:HB3	35:h:57:ARG:HB3	1.99	0.45
37:2:692:LEU:HD22	37:2:693:LEU:HD12	1.99	0.45
37:2:862:LYS:O	37:2:866:LEU:HG	2.17	0.45
37:2:869:ASN:ND2	40:5:268:SER:O	2.50	0.45
38:3:49:ASN:HB3	38:3:52:ASP:HB2	1.99	0.45
40:5:239:LEU:HD12	40:5:243:LEU:HD12	1.99	0.45
40:5:318:LEU:O	40:5:322:GLN:N	2.47	0.45
41:6:37:ALA:HA	41:6:131:ILE:HG23	1.99	0.45
43:8:352:ASP:HA	43:8:355:ASN:HD22	1.82	0.45
2:0:541:C:H2'	2:0:542:A:C8	2.51	0.45
24:N:26:LEU:HG	24:N:31:LEU:HD13	1.98	0.45
29:U:28:LEU:HD22	29:U:54:TYR:CD1	2.52	0.45
38:3:374:LEU:HA	38:3:377:ASN:HD22	1.82	0.45
1:A:320:G:N2	1:A:331:C:O2'	2.46	0.45
1:A:1300:U:O2	1:A:1300:U:C2'	2.65	0.45
1:A:1779:G:H2'	1:A:1780:G:O4'	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0:537:G:HI1'	2:0:538:G:C2	2.52	0.45
3:B:134:LEU:CD2	3:B:144:THR:HG21	2.47	0.45
13:P:21:VAL:HG13	13:P:23:GLU:HG2	1.99	0.45
37:2:859:LEU:HD23	40:5:265:ARG:NH1	2.32	0.45
38:3:244:ASN:O	38:3:245:ALA:C	2.60	0.45
39:4:375:VAL:HG21	40:5:318:LEU:HD23	1.98	0.45
2:0:378:C:H2'	2:0:379:U:C6	2.52	0.45
36:1:119:ASP:O	36:1:121:ILE:HD12	2.16	0.45
36:1:225:SER:O	36:1:229:HIS:HB2	2.17	0.45
36:1:449:SER:O	43:8:327:GLN:HB2	2.16	0.45
38:3:402:GLN:HE22	42:7:525:LYS:HB3	1.82	0.45
39:4:347:LEU:CD1	40:5:346:ALA:HB3	2.47	0.45
40:5:237:ASN:C	40:5:238:HIS:CG	2.94	0.45
42:7:296:ASN:HA	42:7:299:LEU:HD12	1.99	0.45
1:A:1535:U:O2	1:A:1535:U:H2'	2.17	0.44
38:3:420:MET:HB3	42:7:347:LYS:HE2	1.99	0.44
39:4:375:VAL:HG11	40:5:318:LEU:HD23	1.98	0.44
42:7:456:GLN:O	42:7:460:ILE:HG12	2.17	0.44
5:D:66:LEU:HD11	5:D:81:ILE:HG12	2.00	0.44
6:F:129:ILE:HG22	6:F:139:LEU:HD23	1.99	0.44
14:W:1:MET:SD	14:W:1:MET:N	2.87	0.44
37:2:445:LEU:HD12	37:2:502:VAL:HG13	1.98	0.44
38:3:38:LEU:HD13	38:3:252:HIS:CE1	2.53	0.44
39:4:281:ARG:HA	40:5:204:VAL:O	2.17	0.44
41:6:117:PHE:O	41:6:121:LEU:HB2	2.17	0.44
1:A:455:A:O2'	1:A:1735:A:N3	2.41	0.44
1:A:1035:A:H2'	1:A:1036:A:O4'	2.17	0.44
35:h:272:GLN:O	35:h:272:GLN:HG2	2.17	0.44
37:2:440:VAL:HA	37:2:443:CYS:HB2	1.99	0.44
37:2:862:LYS:CB	40:5:265:ARG:HD2	2.47	0.44
1:A:321:C:N3	1:A:331:C:O2	2.51	0.44
1:A:1674:G:OP1	22:G:51:HIS:NE2	2.43	0.44
2:0:427:U:HI1'	2:0:428:A:C5	2.52	0.44
24:N:21:VAL:HA	24:N:24:THR:HG22	2.00	0.44
26:R:97:GLN:HB3	26:R:105:LYS:HG3	1.98	0.44
36:1:43:TRP:O	36:1:43:TRP:CE3	2.70	0.44
38:3:143:ASN:N	38:3:144:TYR:HB2	2.33	0.44
22:G:102:LEU:HD11	31:a:100:VAL:HG21	1.98	0.44
36:1:285:LYS:HG2	37:2:724:GLN:HE22	1.83	0.44
37:2:822:ILE:HG21	38:3:303:PHE:CE1	2.53	0.44
38:3:262:ILE:HG12	38:3:267:VAL:CG1	2.46	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:4:374:LEU:HD23	39:4:374:LEU:O	2.18	0.44
1:A:1113:A:C6	1:A:1121:G:C6	3.05	0.44
1:A:1589:A:H2'	1:A:1590:C:O4'	2.17	0.44
1:A:1826:G:H8	1:A:1826:G:OP2	2.01	0.44
2:0:544:U:C4	2:0:545:A:C6	3.06	0.44
24:N:24:THR:HA	24:N:27:ILE:HG12	1.99	0.44
36:1:166:ASN:O	36:1:167:ASN:C	2.60	0.44
36:1:512:GLN:O	36:1:514:MET:N	2.42	0.44
39:4:358:THR:O	39:4:361:ALA:HB3	2.18	0.44
40:5:173:LEU:HD13	40:5:194:PHE:CE2	2.53	0.44
41:6:67:ALA:HB1	41:6:127:LEU:HD22	1.99	0.44
41:6:71:LEU:HD23	41:6:131:ILE:HB	2.00	0.44
6:F:17:HIS:HB2	6:F:108:ARG:HA	2.00	0.44
37:2:445:LEU:HD11	37:2:501:ARG:NE	2.33	0.44
37:2:590:LEU:O	37:2:593:HIS:CD2	2.71	0.44
40:5:66:VAL:HA	40:5:119:TRP:HA	1.99	0.44
43:8:103:LEU:HD11	43:8:130:VAL:HG11	2.00	0.44
9:J:76:THR:HG22	9:J:108:PRO:HG2	1.99	0.44
28:T:31:THR:HG23	28:T:37:GLY:C	2.42	0.44
36:1:323:LEU:HB3	36:1:383:VAL:HG23	1.99	0.44
36:1:495:SER:HA	36:1:496:ASP:HA	1.80	0.44
38:3:214:LEU:HD13	38:3:235:LEU:HD23	2.00	0.44
3:B:38:ILE:HD11	3:B:150:THR:CG2	2.48	0.44
26:R:102:GLU:OE1	26:R:102:GLU:N	2.51	0.44
35:h:101:PHE:CD1	35:h:136:GLY:HA2	2.53	0.44
36:1:161:LEU:HD21	36:1:177:ILE:HB	2.00	0.44
37:2:731:GLU:HB3	37:2:755:PHE:CZ	2.53	0.44
1:A:614:C:H4'	1:A:615:C:H5''	1.99	0.43
1:A:1273:C:O2'	1:A:1506:A:N1	2.40	0.43
1:A:1332:A:N3	21:E:141:LYS:NZ	2.61	0.43
2:0:380:G:H2'	2:0:440:A:N1	2.33	0.43
9:J:130:THR:N	9:J:131:PRO:CD	2.81	0.43
23:L:18:GLU:C	23:L:20:VAL:H	2.26	0.43
43:8:96:GLY:O	43:8:134:CYS:SG	2.76	0.43
1:A:962:A:N1	1:A:1055:A:O2'	2.51	0.43
1:A:1453:C:H2'	1:A:1454:A:H4'	2.01	0.43
23:L:12:TYR:CE1	23:L:52:LEU:HD11	2.53	0.43
23:L:32:HIS:HB2	23:L:45:VAL:HG21	2.00	0.43
27:S:104:GLU:O	27:S:108:LEU:HG	2.18	0.43
36:1:109:GLN:HG2	36:1:113:LEU:HD12	1.99	0.43
36:1:281:THR:O	37:2:723:ARG:NH1	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:1:467:LEU:HD22	36:1:471:ILE:HD11	1.99	0.43
37:2:799:TYR:OH	37:2:837:GLN:HB2	2.18	0.43
38:3:50:MET:HG2	38:3:178:LEU:HD13	2.00	0.43
39:4:220:LEU:HD11	39:4:233:ILE:CG1	2.48	0.43
39:4:340:PRO:CD	40:5:350:TYR:HE1	2.30	0.43
40:5:333:PHE:HA	40:5:336:GLN:CG	2.48	0.43
1:A:73:C:H2'	1:A:74:G:H4'	2.00	0.43
1:A:142:C:O2	1:A:142:C:O4'	2.36	0.43
1:A:1808:U:H2'	1:A:1809:A:C8	2.53	0.43
11:M:33:LEU:HD23	11:M:34:PRO:HD2	2.01	0.43
36:1:452:PHE:HB2	36:1:489:ARG:CG	2.49	0.43
41:6:29:LEU:HD12	41:6:46:ALA:HA	1.99	0.43
42:7:479:LEU:HD23	42:7:482:THR:HB	2.01	0.43
43:8:133:SER:HA	43:8:136:ALA:HB3	1.99	0.43
1:A:1757:G:H2'	1:A:1758:G:H8	1.82	0.43
3:B:160:ALA:N	14:W:66:ASP:OD2	2.48	0.43
9:J:141:ARG:HB3	9:J:145:ILE:HG23	1.99	0.43
36:1:5:PHE:CZ	36:1:30:VAL:HG13	2.54	0.43
37:2:363:GLU:HB2	37:2:366:LEU:HB3	2.00	0.43
39:4:120:ALA:HB3	40:5:48:LYS:HE3	1.99	0.43
39:4:375:VAL:C	40:5:313:ARG:HD2	2.42	0.43
42:7:239:ASN:HA	42:7:242:ARG:HD2	2.00	0.43
42:7:397:LYS:HG3	42:7:408:VAL:CG1	2.48	0.43
1:A:1599:U:O2	1:A:1600:G:N1	2.52	0.43
27:S:83:ASN:HB3	27:S:85:VAL:HG23	2.00	0.43
36:1:484:ILE:O	36:1:491:LEU:HD21	2.18	0.43
37:2:862:LYS:HE2	40:5:265:ARG:HB3	2.01	0.43
39:4:163:GLU:HA	39:4:164:ASP:HA	1.80	0.43
39:4:268:GLY:O	39:4:272:ILE:HG13	2.19	0.43
39:4:339:VAL:N	39:4:340:PRO:CD	2.81	0.43
41:6:88:MET:HE1	42:7:292:LYS:HB3	2.00	0.43
42:7:413:PHE:HB2	42:7:451:VAL:HG21	1.99	0.43
43:8:19:ARG:HD3	43:8:68:VAL:HG12	2.01	0.43
2:0:491:U:O3'	2:0:517:G:C6	2.72	0.43
8:I:69:LEU:HD22	8:I:96:ALA:HB2	2.01	0.43
17:Z:35:VAL:HG23	17:Z:40:ILE:HD11	2.00	0.43
36:1:523:LEU:HD22	40:5:241:LYS:HG3	1.99	0.43
38:3:188:ASP:HA	38:3:191:ARG:HB2	1.99	0.43
39:4:214:ALA:N	39:4:215:PRO:HD3	2.33	0.43
39:4:265:GLU:O	39:4:269:VAL:N	2.44	0.43
39:4:281:ARG:NE	40:5:202:PRO:HA	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:7:241:ASN:HA	42:7:244:LEU:HD12	2.01	0.43
43:8:60:VAL:O	43:8:63:VAL:HG13	2.18	0.43
1:A:441:C:OP2	9:J:2:GLY:N	2.52	0.43
6:F:130:PHE:O	6:F:138:HIS:N	2.45	0.43
35:h:81:GLY:HA2	35:h:87:LEU:HD23	2.01	0.43
40:5:345:GLN:HE21	40:5:349:GLU:CG	2.31	0.43
42:7:252:ASP:N	42:7:253:PRO:CD	2.82	0.43
42:7:379:PRO:HA	42:7:380:MET:CB	2.47	0.43
43:8:323:CYS:SG	43:8:324:LYS:N	2.91	0.43
2:0:396:C:O2	2:0:397:G:N2	2.52	0.43
14:W:30:ALA:O	14:W:60:ARG:HD3	2.18	0.43
36:1:159:GLN:O	36:1:163:LEU:HD23	2.18	0.43
37:2:778:MET:HE2	37:2:782:LYS:HE2	2.01	0.43
39:4:341:ASP:HA	40:5:350:TYR:OH	2.18	0.43
42:7:241:ASN:HD21	42:7:289:GLN:CD	2.26	0.43
43:8:223:LEU:C	43:8:228:PRO:HG2	2.44	0.43
1:A:1611:G:H4'	28:T:86:ARG:NH1	2.33	0.43
2:0:534:U:C4	2:0:535:C:N4	2.86	0.43
37:2:510:THR:HA	37:2:513:LYS:HG2	2.01	0.43
37:2:710:ILE:CD1	37:2:714:PHE:HE2	2.31	0.43
40:5:183:SER:HB3	40:5:184:PRO:HD3	2.01	0.43
41:6:77:LEU:HD23	41:6:141:PHE:CD2	2.54	0.43
41:6:151:GLN:HE21	41:6:192:GLN:HA	1.84	0.43
42:7:376:THR:HG21	42:7:398:MET:HE3	2.00	0.43
42:7:479:LEU:CB	42:7:489:GLN:HE21	2.32	0.43
43:8:103:LEU:HD13	43:8:127:LEU:HA	2.01	0.43
24:N:31:LEU:HD12	24:N:33:ARG:HG3	2.01	0.43
26:R:49:TYR:O	26:R:53:GLU:HG2	2.19	0.43
28:T:124:ARG:HD3	28:T:129:LEU:HD12	2.01	0.43
38:3:26:LEU:HG	38:3:26:LEU:O	2.19	0.43
43:8:186:VAL:HG22	43:8:203:ASP:OD1	2.18	0.43
1:A:427:U:O2	1:A:427:U:O4'	2.37	0.42
1:A:887:U:O2	1:A:887:U:C2'	2.67	0.42
1:A:1315:U:O2	1:A:1315:U:O4'	2.37	0.42
1:A:1563:G:OP1	29:U:121:ARG:NH2	2.52	0.42
2:0:393:U:H2'	2:0:394:C:O4'	2.18	0.42
12:O:84:LEU:HD22	12:O:149:LEU:HD23	2.00	0.42
26:R:94:ALA:HA	26:R:97:GLN:HE21	1.83	0.42
36:1:446:ILE:HG13	36:1:514:MET:HG2	2.01	0.42
36:1:529:VAL:O	40:5:233:LEU:HD13	2.18	0.42
36:1:530:LEU:O	40:5:230:LEU:HD11	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:2:418:ILE:HG23	37:2:441:ARG:HD3	2.00	0.42
37:2:706:ARG:HA	37:2:710:ILE:HD11	2.01	0.42
39:4:285:LEU:HD21	40:5:163:SER:OG	2.18	0.42
42:7:244:LEU:HD21	42:7:254:GLU:HG2	2.01	0.42
43:8:135:GLY:O	43:8:138:GLN:HG2	2.19	0.42
1:A:1261:C:O2	33:e:10:HIS:HE1	2.03	0.42
21:E:191:PRO:O	21:E:199:GLY:HA3	2.19	0.42
36:1:147:THR:N	36:1:148:PRO:CD	2.82	0.42
36:1:285:LYS:HB3	37:2:723:ARG:NE	2.34	0.42
37:2:709:MET:HE3	37:2:736:HIS:CD2	2.55	0.42
39:4:156:SER:CB	40:5:110:VAL:HG11	2.47	0.42
39:4:259:TYR:HE1	40:5:217:GLU:CD	2.27	0.42
39:4:262:TYR:HB3	39:4:265:GLU:HG3	2.01	0.42
39:4:276:CYS:HB3	40:5:215:MET:HB2	2.02	0.42
39:4:329:MET:HG3	43:8:335:SER:O	2.19	0.42
40:5:250:VAL:O	40:5:254:SER:N	2.43	0.42
42:7:265:LEU:HB3	42:7:279:ARG:HD3	2.01	0.42
43:8:126:SER:O	43:8:130:VAL:HG23	2.19	0.42
43:8:316:VAL:HA	43:8:321:VAL:O	2.19	0.42
1:A:191:A:N6	1:A:208:G:O2'	2.51	0.42
28:T:24:ARG:HD3	28:T:29:ALA:HA	2.01	0.42
36:1:63:LYS:HD2	36:1:66:LEU:HD12	2.01	0.42
36:1:410:VAL:HA	36:1:413:TRP:CB	2.49	0.42
37:2:725:PRO:HB2	37:2:731:GLU:HG2	2.00	0.42
39:4:128:ARG:CZ	40:5:112:ILE:HD11	2.49	0.42
40:5:234:ALA:C	40:5:236:SER:N	2.77	0.42
43:8:70:LEU:HD23	43:8:106:LEU:HB2	2.00	0.42
1:A:1113:A:H2'	1:A:1114:U:C6	2.53	0.42
1:A:1620:A:OP1	25:Q:115:TYR:OH	2.34	0.42
3:B:70:ASN:OD1	5:D:274:MET:SD	2.77	0.42
6:F:256:LEU:C	6:F:256:LEU:HD12	2.44	0.42
25:Q:45:LEU:HG	25:Q:84:ILE:HD11	2.01	0.42
27:S:16:ILE:HG23	27:S:38:ILE:HD11	2.02	0.42
36:1:30:VAL:O	36:1:34:VAL:HG23	2.20	0.42
36:1:428:VAL:N	36:1:429:PRO:CD	2.82	0.42
37:2:783:ILE:C	37:2:785:GLU:H	2.28	0.42
38:3:143:ASN:HA	38:3:144:TYR:C	2.44	0.42
39:4:282:VAL:HB	40:5:164:LEU:HD12	2.00	0.42
39:4:375:VAL:O	40:5:313:ARG:CZ	2.68	0.42
40:5:194:PHE:CZ	40:5:319:ILE:HD13	2.54	0.42
42:7:212:ILE:HG23	42:7:271:TYR:HE1	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0:385:A:C6	2:0:386:U:C4	3.07	0.42
3:B:19:LEU:HD13	27:S:102:THR:HG23	2.01	0.42
25:Q:50:ARG:O	25:Q:58:LYS:HG2	2.19	0.42
30:V:33:GLU:OE2	30:V:87:ARG:NE	2.53	0.42
36:1:527:SER:N	40:5:237:ASN:OD1	2.52	0.42
38:3:214:LEU:HA	38:3:217:TRP:NE1	2.34	0.42
39:4:273:MET:HE3	40:5:218:LEU:CA	2.50	0.42
39:4:340:PRO:CA	40:5:350:TYR:HE1	2.32	0.42
1:A:549:C:C5	1:A:550:C:C2	3.08	0.42
1:A:1536:G:H2'	1:A:1537:A:H8	1.85	0.42
36:1:48:GLU:CB	36:1:49:PRO:HD3	2.49	0.42
38:3:274:LEU:HG	38:3:275:LYS:N	2.33	0.42
39:4:347:LEU:HD23	39:4:347:LEU:C	2.44	0.42
39:4:372:GLU:OE2	40:5:318:LEU:HG	2.20	0.42
40:5:148:VAL:HG12	40:5:168:ARG:HB3	2.02	0.42
41:6:136:ASP:O	41:6:140:LYS:N	2.52	0.42
3:B:12:GLU:HA	27:S:111:PHE:CZ	2.54	0.42
4:C:79:VAL:HG13	4:C:81:PHE:CD2	2.54	0.42
27:S:80:ARG:HD2	27:S:83:ASN:HD21	1.84	0.42
36:1:329:ILE:HB	36:1:330:PRO:HD3	2.02	0.42
36:1:452:PHE:CE1	36:1:471:ILE:HG21	2.55	0.42
37:2:739:ALA:O	37:2:789:ARG:NH1	2.51	0.42
37:2:839:THR:HB	37:2:841:THR:HG23	2.01	0.42
37:2:869:ASN:OD1	40:5:269:LYS:O	2.37	0.42
40:5:164:LEU:HB3	40:5:203:ILE:CD1	2.49	0.42
41:6:18:ILE:O	41:6:18:ILE:HG22	2.19	0.42
42:7:475:LEU:CD2	42:7:479:LEU:HD12	2.49	0.42
1:A:533:A:N6	1:A:551:U:O4	2.53	0.42
1:A:536:A:N3	1:A:536:A:H2'	2.35	0.42
2:0:514:U:H2'	2:0:515:G:H1'	2.02	0.42
8:I:38:ALA:HA	8:I:41:ARG:HD3	2.02	0.42
22:G:139:VAL:HG12	32:d:45:ASN:HB2	2.01	0.42
22:G:187:SER:HB3	22:G:190:ILE:HG12	2.02	0.42
39:4:254:PRO:HG3	43:8:110:PHE:CG	2.54	0.42
41:6:67:ALA:HB2	41:6:98:PRO:HG2	2.01	0.42
41:6:179:TRP:CE3	41:6:187:ILE:HG21	2.55	0.42
42:7:369:ALA:O	42:7:373:ILE:HG13	2.19	0.42
43:8:75:GLU:HG3	43:8:76:PRO:HD3	2.02	0.42
43:8:90:LEU:HD12	43:8:130:VAL:HG21	2.02	0.42
25:Q:34:MET:O	25:Q:42:ARG:HG2	2.20	0.42
25:Q:111:MET:SD	25:Q:119:PHE:CZ	3.13	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:6:77:LEU:HD23	41:6:141:PHE:CE2	2.54	0.42
42:7:288:TYR:CE1	42:7:321:PHE:HB3	2.55	0.42
1:A:511:U:O2'	1:A:576:A:N6	2.53	0.42
1:A:1270:G:O2'	1:A:1301:A:N7	2.50	0.42
1:A:1320:G:H2'	1:A:1321:G:O4'	2.20	0.42
2:0:394:C:H2'	2:0:396:C:C4	2.54	0.42
4:C:28:LYS:NZ	13:P:51:GLU:OE1	2.52	0.42
8:I:60:ILE:HB	8:I:92:VAL:HG12	2.02	0.42
23:L:71:LEU:HG	23:L:76:ILE:HG12	2.02	0.42
36:1:300:TYR:CE1	36:1:322:VAL:HG12	2.55	0.42
36:1:436:ILE:O	36:1:440:LEU:HB2	2.20	0.42
39:4:176:MET:HG3	39:4:176:MET:O	2.19	0.42
39:4:279:PRO:HD2	40:5:207:ASN:CA	2.50	0.42
1:A:1334:G:O3'	21:E:183:GLY:HA3	2.20	0.41
3:B:24:HIS:CB	3:B:51:LEU:HD21	2.50	0.41
11:M:10:TYR:OH	11:M:18:GLN:NE2	2.52	0.41
35:h:40:ILE:O	35:h:59:LEU:HB2	2.21	0.41
36:1:338:ILE:HA	36:1:341:LEU:HB2	2.01	0.41
36:1:499:TYR:CE2	36:1:503:GLU:HG2	2.54	0.41
39:4:272:ILE:HG23	40:5:43:GLY:HA3	2.02	0.41
39:4:347:LEU:HD11	40:5:346:ALA:HB3	2.01	0.41
39:4:375:VAL:HB	40:5:318:LEU:HD21	2.01	0.41
43:8:280:LEU:HD21	43:8:300:GLU:HB3	2.02	0.41
2:0:477:G:N2	2:0:478:A:N3	2.67	0.41
2:0:512:C:H3'	2:0:513:U:C5'	2.50	0.41
37:2:449:GLU:HG3	37:2:505:ARG:HD2	2.02	0.41
39:4:350:ASN:C	40:5:343:MET:SD	3.04	0.41
41:6:174:MET:SD	41:6:187:ILE:HG12	2.60	0.41
42:7:284:LEU:HD22	42:7:299:LEU:HD22	2.03	0.41
1:A:190:G:O2'	1:A:209:A:N6	2.53	0.41
1:A:1227:G:C2	1:A:1228:A:C8	3.08	0.41
3:B:63:ARG:CG	3:B:185:MET:HE1	2.51	0.41
6:F:111:VAL:HG23	6:F:111:VAL:O	2.20	0.41
35:h:5:MET:HB3	35:h:270:LEU:HD21	2.01	0.41
38:3:401:TYR:O	38:3:405:ILE:HG13	2.20	0.41
24:N:19:GLN:O	24:N:23:LYS:HG2	2.19	0.41
36:1:90:VAL:HG21	36:1:165:ARG:HH22	1.84	0.41
36:1:526:MET:CB	40:5:237:ASN:OD1	2.66	0.41
38:3:380:LEU:HD12	38:3:393:MET:HE3	2.02	0.41
40:5:218:LEU:O	40:5:222:SER:N	2.54	0.41
42:7:321:PHE:O	42:7:325:MET:HG2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:7:479:LEU:HA	42:7:482:THR:HB	2.01	0.41
43:8:144:LEU:HD21	43:8:184:VAL:HG11	2.02	0.41
1:A:30:C:O2'	1:A:596:U:OP1	2.37	0.41
1:A:318:A:N6	7:H:186:GLN:OE1	2.54	0.41
1:A:380:G:O6	9:J:178:ARG:NH1	2.50	0.41
2:0:422:U:H3'	2:0:423:G:H4'	2.02	0.41
6:F:191:ARG:HD3	6:F:245:ARG:HB3	2.03	0.41
27:S:76:GLU:O	27:S:80:ARG:HG2	2.21	0.41
38:3:292:ILE:HG21	38:3:318:VAL:HB	2.02	0.41
39:4:269:VAL:CG2	40:5:47:LEU:HD21	2.49	0.41
39:4:347:LEU:HD13	40:5:346:ALA:C	2.45	0.41
42:7:218:ASN:HB3	42:7:219:PRO:HD3	2.03	0.41
42:7:231:LEU:O	42:7:235:VAL:HG22	2.19	0.41
1:A:921:G:C6	15:X:28:ARG:HD2	2.55	0.41
1:A:989:C:O2	18:b:32:LYS:NZ	2.54	0.41
1:A:1623:A:H5''	28:T:133:GLY:HA3	2.03	0.41
2:0:454:C:H2'	2:0:455:U:C6	2.55	0.41
2:0:533:C:H2'	2:0:534:U:C6	2.55	0.41
2:0:603:A:H2'	2:0:604:C:C6	2.56	0.41
5:D:141:LEU:HD11	5:D:238:LYS:HE3	2.02	0.41
11:M:126:VAL:HG12	11:M:128:VAL:HG13	2.02	0.41
27:S:126:MET:HB2	27:S:128:PHE:CD1	2.55	0.41
34:g:119:ARG:NE	34:g:132:MET:SD	2.86	0.41
36:1:163:LEU:HG	36:1:164:LEU:HD22	2.01	0.41
43:8:87:CYS:SG	43:8:126:SER:OG	2.79	0.41
1:A:987:A:N1	4:C:120:MET:HE1	2.36	0.41
1:A:1303:C:H2'	1:A:1304:U:O4'	2.20	0.41
2:0:363:A:N6	2:0:461:A:N1	2.69	0.41
21:E:126:ILE:HG21	21:E:134:CYS:HB3	2.02	0.41
28:T:73:ASN:HB3	28:T:76:GLN:HB2	2.02	0.41
32:d:14:VAL:HG23	32:d:30:VAL:HB	2.02	0.41
36:1:58:CYS:SG	36:1:63:LYS:O	2.78	0.41
36:1:229:HIS:O	36:1:232:THR:HG22	2.21	0.41
36:1:526:MET:HE3	40:5:240:GLY:CA	2.50	0.41
36:1:526:MET:O	36:1:530:LEU:N	2.43	0.41
39:4:163:GLU:HG3	39:4:202:HIS:HE2	1.86	0.41
3:B:38:ILE:HD11	3:B:150:THR:HG22	2.03	0.41
15:X:53:ILE:N	15:X:60:LYS:O	2.52	0.41
19:c:33:MET:HA	19:c:81:ARG:HA	2.02	0.41
35:h:87:LEU:HB2	35:h:101:PHE:HB2	2.03	0.41
35:h:277:THR:HG21	35:h:283:PRO:HB3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:h:286:CYS:HA	35:h:302:TYR:HA	2.03	0.41
36:1:142:ASP:O	36:1:146:LEU:HB3	2.21	0.41
36:1:175:HIS:CD2	36:1:228:MET:HB3	2.56	0.41
36:1:383:VAL:O	36:1:388:LYS:HG3	2.21	0.41
36:1:499:TYR:CZ	40:5:242:ASN:HB3	2.56	0.41
38:3:49:ASN:HA	38:3:50:MET:CB	2.44	0.41
1:A:69:C:OP2	7:H:164:LYS:NZ	2.50	0.41
1:A:295:C:H2'	1:A:296:U:O4'	2.20	0.41
2:0:529:G:O2'	2:0:554:C:O2'	2.35	0.41
3:B:119:PRO:HG2	3:B:142:LEU:HD11	2.02	0.41
18:b:40:VAL:HG21	18:b:71:LEU:HD12	2.02	0.41
21:E:162:ASP:N	21:E:163:PRO:CD	2.83	0.41
25:Q:18:ARG:HD2	28:T:88:LYS:HG2	2.02	0.41
26:R:33:LYS:NZ	26:R:36:GLY:O	2.43	0.41
35:h:17:TRP:HB2	35:h:36:ARG:HG3	2.03	0.41
36:1:331:ILE:CA	36:1:434:ASN:HD21	2.34	0.41
37:2:853:GLN:HA	37:2:856:ALA:HB3	2.01	0.41
39:4:125:SER:CA	40:5:111:ASN:HD21	2.31	0.41
39:4:269:VAL:O	39:4:273:MET:HG2	2.20	0.41
39:4:276:CYS:SG	40:5:211:ILE:HG23	2.61	0.41
39:4:359:TYR:CE2	39:4:363:LEU:HD12	2.55	0.41
39:4:365:GLN:CG	40:5:329:ASN:CB	2.97	0.41
40:5:272:GLN:NE2	40:5:275:HIS:ND1	2.69	0.41
41:6:85:CYS:O	41:6:89:ILE:HG13	2.21	0.41
42:7:200:TYR:O	42:7:204:THR:OG1	2.39	0.41
43:8:285:MET:HE1	43:8:336:HIS:HB3	2.02	0.41
1:A:203:G:H2'	1:A:204:G:C8	2.55	0.41
1:A:628:A:N6	21:E:178:ARG:HB3	2.35	0.41
1:A:1650:A:H2'	1:A:1651:A:O4'	2.21	0.41
2:0:511:C:H2'	2:0:512:C:C6	2.56	0.41
16:Y:51:VAL:HG13	16:Y:70:VAL:HG22	2.02	0.41
28:T:27:ALA:O	28:T:31:THR:OG1	2.39	0.41
28:T:86:ARG:CB	28:T:98:VAL:HG23	2.52	0.41
36:1:204:HIS:O	36:1:208:ILE:HG12	2.21	0.41
36:1:241:ILE:HG21	36:1:282:VAL:HG22	2.03	0.41
36:1:524:THR:HG22	39:4:335:VAL:CG2	2.51	0.41
37:2:549:GLU:HG3	37:2:572:HIS:HB2	2.02	0.41
37:2:870:ASN:HD22	40:5:272:GLN:CD	2.27	0.41
39:4:273:MET:HE3	40:5:218:LEU:HB2	2.03	0.41
41:6:84:LEU:HA	41:6:87:CYS:SG	2.61	0.41
1:A:1724:A:C2	1:A:1811:C:C2	3.09	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:d:46:VAL:HG22	32:d:56:LEU:HD21	2.02	0.40
35:h:245:ARG:HD3	35:h:247:TRP:CE2	2.56	0.40
36:1:526:MET:HA	40:5:237:ASN:N	2.36	0.40
36:1:530:LEU:C	40:5:230:LEU:CD1	2.92	0.40
42:7:244:LEU:HD21	42:7:254:GLU:HB3	2.04	0.40
42:7:341:LEU:HD11	42:7:384:GLU:HB3	2.03	0.40
1:A:166:A:H2'	1:A:167:G:C8	2.56	0.40
1:A:878:G:C6	1:A:879:C:C4	3.10	0.40
2:0:376:G:O2'	2:0:447:A:N6	2.53	0.40
3:B:132:GLN:HB3	3:B:133:PRO:HD3	2.02	0.40
10:K:50:LEU:HD13	10:K:105:PHE:CE2	2.57	0.40
17:Z:23:MET:N	17:Z:23:MET:SD	2.94	0.40
21:E:72:VAL:CG1	23:L:20:VAL:HG22	2.51	0.40
37:2:710:ILE:CB	37:2:714:PHE:HE2	2.08	0.40
37:2:745:LYS:NZ	37:2:807:LEU:HD21	2.36	0.40
39:4:117:VAL:HG21	40:5:51:LYS:HB2	2.03	0.40
39:4:350:ASN:O	40:5:343:MET:SD	2.80	0.40
1:A:1149:A:N3	1:A:1149:A:H2'	2.36	0.40
1:A:1240:A:OP1	25:Q:100:LYS:NZ	2.54	0.40
1:A:1700:C:C2	1:A:1834:A:N6	2.90	0.40
2:0:421:A:H2'	2:0:422:U:C4'	2.51	0.40
6:F:256:LEU:HA	6:F:259:LYS:HB3	2.03	0.40
9:J:38:ILE:HD11	9:J:81:VAL:HG23	2.03	0.40
24:N:51:VAL:HB	24:N:77:ILE:HB	2.02	0.40
34:g:107:LYS:HB3	34:g:117:LEU:HD11	2.03	0.40
35:h:11:LEU:HB3	35:h:43:TRP:CZ3	2.57	0.40
36:1:530:LEU:HD23	40:5:230:LEU:O	2.22	0.40
37:2:862:LYS:HE2	40:5:265:ARG:C	2.47	0.40
39:4:251:MET:HB3	43:8:67:VAL:HG11	2.04	0.40
39:4:355:LEU:C	39:4:355:LEU:HD23	2.46	0.40
40:5:185:GLU:HB3	40:5:189:LYS:HE3	2.02	0.40
42:7:353:THR:CG2	42:7:354:THR:HA	2.51	0.40
43:8:83:ILE:O	43:8:87:CYS:SG	2.80	0.40
43:8:251:SER:HB3	43:8:254:LYS:HG2	2.03	0.40
1:A:681:U:H4'	16:Y:9:THR:HG22	2.03	0.40
1:A:905:C:H2'	1:A:906:U:O4'	2.22	0.40
1:A:1162:C:H2'	1:A:1163:C:O4'	2.21	0.40
2:0:537:G:H1'	2:0:538:G:N1	2.37	0.40
27:S:20:TYR:O	27:S:24:LEU:HG	2.20	0.40
31:a:62:VAL:N	31:a:63:PRO:CD	2.84	0.40
36:1:58:CYS:SG	36:1:67:ALA:N	2.95	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:2:722:GLU:C	37:2:734:ARG:HH22	2.29	0.40
38:3:162:ASP:O	38:3:166:LEU:HB2	2.22	0.40
39:4:279:PRO:HG2	40:5:206:LYS:O	2.22	0.40
39:4:295:ALA:O	39:4:299:ILE:HG12	2.21	0.40
41:6:58:PRO:HB3	41:6:93:HIS:NE2	2.37	0.40
42:7:481:LEU:HG	42:7:482:THR:N	2.37	0.40
43:8:115:LYS:HB2	43:8:116:ASN:HB3	2.03	0.40
1:A:193:C:H2'	1:A:194:C:C6	2.57	0.40
1:A:929:G:H2'	1:A:930:C:O4'	2.22	0.40
1:A:1556:A:N3	1:A:1556:A:H2'	2.36	0.40
3:B:30:LEU:HD21	3:B:35:GLU:HG2	2.04	0.40
36:1:452:PHE:HA	36:1:455:LEU:HB3	2.03	0.40
39:4:285:LEU:O	39:4:289:LEU:HG	2.22	0.40
40:5:50:ILE:O	40:5:53:TYR:HD1	2.04	0.40
42:7:397:LYS:O	42:7:408:VAL:HG21	2.21	0.40
42:7:492:VAL:HA	42:7:495:HIS:CD2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	B	215/295 (73%)	201 (94%)	13 (6%)	1 (0%)	24	58
4	C	211/264 (80%)	189 (90%)	21 (10%)	1 (0%)	24	58
5	D	219/255 (86%)	201 (92%)	17 (8%)	1 (0%)	24	58
6	F	260/263 (99%)	248 (95%)	12 (5%)	0	100	100
7	H	235/249 (94%)	216 (92%)	18 (8%)	1 (0%)	30	62
8	I	181/194 (93%)	160 (88%)	20 (11%)	1 (1%)	21	53
9	J	204/208 (98%)	188 (92%)	14 (7%)	2 (1%)	12	44

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	K	183/194 (94%)	170 (93%)	13 (7%)	0	100	100
11	M	139/158 (88%)	130 (94%)	9 (6%)	0	100	100
12	O	147/151 (97%)	137 (93%)	9 (6%)	1 (1%)	18	51
13	P	134/151 (89%)	120 (90%)	14 (10%)	0	100	100
14	W	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
15	X	127/130 (98%)	119 (94%)	7 (6%)	1 (1%)	16	49
16	Y	139/143 (97%)	128 (92%)	7 (5%)	4 (3%)	3	26
17	Z	122/134 (91%)	115 (94%)	7 (6%)	0	100	100
18	b	99/115 (86%)	87 (88%)	10 (10%)	2 (2%)	6	32
19	c	81/84 (96%)	75 (93%)	5 (6%)	1 (1%)	10	41
20	f	55/133 (41%)	51 (93%)	4 (7%)	0	100	100
21	E	226/281 (80%)	209 (92%)	17 (8%)	0	100	100
22	G	189/204 (93%)	165 (87%)	21 (11%)	3 (2%)	7	36
23	L	94/149 (63%)	83 (88%)	10 (11%)	1 (1%)	11	42
24	N	115/132 (87%)	96 (84%)	16 (14%)	3 (3%)	4	27
25	Q	113/145 (78%)	92 (81%)	17 (15%)	4 (4%)	3	22
26	R	140/172 (81%)	130 (93%)	9 (6%)	1 (1%)	18	51
27	S	130/135 (96%)	111 (85%)	17 (13%)	2 (2%)	8	37
28	T	142/152 (93%)	132 (93%)	8 (6%)	2 (1%)	9	38
29	U	139/145 (96%)	126 (91%)	12 (9%)	1 (1%)	18	51
30	V	98/119 (82%)	92 (94%)	6 (6%)	0	100	100
31	a	73/125 (58%)	67 (92%)	6 (8%)	0	100	100
32	d	60/69 (87%)	59 (98%)	1 (2%)	0	100	100
33	e	53/56 (95%)	49 (92%)	3 (6%)	1 (2%)	6	32
34	g	66/156 (42%)	54 (82%)	9 (14%)	3 (4%)	2	17
35	h	310/317 (98%)	274 (88%)	34 (11%)	2 (1%)	21	53
36	1	532/1362 (39%)	430 (81%)	85 (16%)	17 (3%)	3	24
37	2	543/913 (60%)	428 (79%)	105 (19%)	10 (2%)	6	33
38	3	417/462 (90%)	333 (80%)	67 (16%)	17 (4%)	2	19
39	4	270/364 (74%)	217 (80%)	45 (17%)	8 (3%)	3	25
40	5	320/363 (88%)	255 (80%)	54 (17%)	11 (3%)	3	23

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	6	213/218 (98%)	179 (84%)	31 (15%)	3 (1%)	9	38
42	7	370/607 (61%)	301 (81%)	57 (15%)	12 (3%)	3	24
43	8	363/374 (97%)	290 (80%)	61 (17%)	12 (3%)	3	23
All	All	7808/10224 (76%)	6786 (87%)	893 (11%)	129 (2%)	9	34

All (129) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	J	94	LYS
15	X	28	ARG
16	Y	61	GLN
22	G	134	VAL
24	N	57	ASP
26	R	17	LYS
27	S	99	ASP
34	g	124	ASP
36	1	167	ASN
36	1	168	SER
36	1	526	MET
36	1	530	LEU
36	1	531	ALA
37	2	651	LEU
38	3	51	VAL
38	3	93	LYS
39	4	338	ILE
40	5	211	ILE
40	5	212	ASN
40	5	241	LYS
42	7	423	PRO
43	8	57	ASP
43	8	335	SER
3	B	44	ASP
4	C	190	PRO
5	D	237	ALA
8	I	88	SER
9	J	123	ARG
22	G	167	LYS
25	Q	17	TYR
25	Q	70	MET
28	T	100	ALA
35	h	275	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	1	416	GLU
36	1	513	SER
37	2	435	ASP
37	2	653	ARG
37	2	742	LYS
37	2	743	ALA
38	3	26	LEU
38	3	48	THR
38	3	50	MET
38	3	62	TYR
38	3	224	ASN
38	3	238	TYR
38	3	242	TYR
38	3	245	ALA
38	3	325	LEU
38	3	328	CYS
39	4	169	ASP
39	4	368	ILE
40	5	87	HIS
40	5	240	GLY
42	7	270	GLY
42	7	381	ARG
42	7	462	SER
43	8	43	ALA
43	8	114	ASP
43	8	116	ASN
7	H	169	PRO
16	Y	62	PRO
16	Y	86	PRO
18	b	47	ALA
27	S	120	THR
35	h	272	GLN
36	1	42	THR
36	1	43	TRP
36	1	223	PRO
36	1	522	GLN
38	3	27	SER
38	3	63	SER
38	3	200	SER
38	3	350	CYS
39	4	133	ALA
39	4	244	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	5	340	LYS
43	8	108	ASN
43	8	225	THR
22	G	51	HIS
24	N	29	ASP
28	T	74	PRO
29	U	115	LYS
33	e	7	TYR
34	g	126	CYS
36	1	221	ASN
36	1	347	ILE
37	2	325	THR
37	2	422	GLU
40	5	73	GLU
40	5	162	LEU
40	5	203	ILE
42	7	221	ILE
42	7	289	GLN
42	7	348	SER
43	8	323	CYS
12	O	83	ASP
19	c	50	ALA
23	L	19	GLY
24	N	33	ARG
25	Q	124	LYS
34	g	86	THR
36	1	209	GLN
36	1	421	GLU
37	2	702	GLU
37	2	869	ASN
40	5	239	LEU
41	6	184	SER
42	7	427	ASN
42	7	489	GLN
43	8	130	VAL
16	Y	60	LYS
39	4	199	ILE
39	4	285	LEU
40	5	339	GLY
42	7	468	THR
43	8	34	SER
43	8	191	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
39	4	116	PRO
41	6	58	PRO
41	6	99	ILE
18	b	56	VAL
25	Q	69	PRO
36	1	436	ILE
42	7	212	ILE
42	7	382	ILE
37	2	564	ILE
38	3	291	PRO
43	8	118	PRO
36	1	506	PRO

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	
3	B	180/246 (73%)	177 (98%)	3 (2%)	53	69
4	C	194/231 (84%)	191 (98%)	3 (2%)	57	71
5	D	186/205 (91%)	184 (99%)	2 (1%)	65	74
6	F	223/224 (100%)	222 (100%)	1 (0%)	84	81
7	H	207/218 (95%)	203 (98%)	4 (2%)	50	67
8	I	165/174 (95%)	164 (99%)	1 (1%)	78	79
9	J	178/180 (99%)	177 (99%)	1 (1%)	78	79
10	K	161/168 (96%)	160 (99%)	1 (1%)	78	79
11	M	130/142 (92%)	129 (99%)	1 (1%)	73	76
12	O	130/131 (99%)	129 (99%)	1 (1%)	73	76
13	P	106/119 (89%)	106 (100%)	0	100	100
14	W	68/68 (100%)	67 (98%)	1 (2%)	57	71
15	X	112/113 (99%)	109 (97%)	3 (3%)	39	62
16	Y	113/114 (99%)	113 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	Z	107/115 (93%)	106 (99%)	1 (1%)	70	75
18	b	89/99 (90%)	89 (100%)	0	100	100
19	c	75/76 (99%)	74 (99%)	1 (1%)	61	72
20	f	47/106 (44%)	47 (100%)	0	100	100
21	E	190/232 (82%)	189 (100%)	1 (0%)	81	80
22	G	158/170 (93%)	156 (99%)	2 (1%)	61	72
23	L	87/125 (70%)	86 (99%)	1 (1%)	65	74
24	N	99/108 (92%)	94 (95%)	5 (5%)	21	48
25	Q	105/130 (81%)	103 (98%)	2 (2%)	50	67
26	R	117/140 (84%)	117 (100%)	0	100	100
27	S	119/121 (98%)	118 (99%)	1 (1%)	73	76
28	T	125/132 (95%)	124 (99%)	1 (1%)	73	76
29	U	111/116 (96%)	110 (99%)	1 (1%)	70	75
30	V	92/107 (86%)	91 (99%)	1 (1%)	65	74
31	a	66/103 (64%)	66 (100%)	0	100	100
32	d	55/62 (89%)	54 (98%)	1 (2%)	51	69
33	e	48/49 (98%)	48 (100%)	0	100	100
34	g	61/140 (44%)	60 (98%)	1 (2%)	55	70
35	h	271/275 (98%)	265 (98%)	6 (2%)	45	65
36	1	490/1245 (39%)	480 (98%)	10 (2%)	48	66
37	2	494/812 (61%)	481 (97%)	13 (3%)	40	63
38	3	384/423 (91%)	375 (98%)	9 (2%)	44	64
39	4	239/282 (85%)	232 (97%)	7 (3%)	37	61
40	5	293/320 (92%)	287 (98%)	6 (2%)	48	66
41	6	190/193 (98%)	188 (99%)	2 (1%)	65	74
42	7	342/544 (63%)	337 (98%)	5 (2%)	57	71
43	8	327/335 (98%)	320 (98%)	7 (2%)	47	66
All	All	6934/8893 (78%)	6828 (98%)	106 (2%)	55	71

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	38	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	B	128	GLN
3	B	142	LEU
4	C	78	GLU
4	C	178	THR
4	C	225	LEU
5	D	213	LEU
5	D	248	TYR
6	F	51	LYS
7	H	106	LEU
7	H	162	LEU
7	H	163	ASN
7	H	171	THR
8	I	82	GLU
9	J	124	LYS
10	K	131	ARG
11	M	40	ILE
12	O	67	THR
14	W	13	VAL
15	X	86	LEU
15	X	103	VAL
15	X	104	LEU
17	Z	10	ARG
19	c	35	VAL
21	E	175	VAL
22	G	104	THR
22	G	142	SER
23	L	3	MET
24	N	18	LEU
24	N	42	LEU
24	N	97	GLU
24	N	110	VAL
24	N	126	GLU
25	Q	37	TYR
25	Q	53	GLN
27	S	102	THR
28	T	114	LEU
29	U	28	LEU
30	V	65	THR
32	d	32	VAL
34	g	144	CYS
35	h	18	VAL
35	h	131	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	h	134	THR
35	h	156	PHE
35	h	164	ILE
35	h	221	LEU
36	1	89	VAL
36	1	163	LEU
36	1	164	LEU
36	1	198	CYS
36	1	301	HIS
36	1	327	LEU
36	1	371	ILE
36	1	387	VAL
36	1	413	TRP
36	1	480	LEU
37	2	346	ASP
37	2	379	ILE
37	2	462	THR
37	2	498	GLU
37	2	513	LYS
37	2	578	LEU
37	2	608	LEU
37	2	616	LEU
37	2	674	HIS
37	2	723	ARG
37	2	738	VAL
37	2	848	GLU
37	2	855	LEU
38	3	7	THR
38	3	75	THR
38	3	84	LEU
38	3	214	LEU
38	3	232	ILE
38	3	233	ILE
38	3	267	VAL
38	3	274	LEU
38	3	418	LEU
39	4	114	LEU
39	4	195	THR
39	4	200	THR
39	4	232	SER
39	4	250	VAL
39	4	264	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
39	4	276	CYS
40	5	70	LEU
40	5	163	SER
40	5	197	MET
40	5	230	LEU
40	5	313	ARG
40	5	352	ASN
41	6	35	THR
41	6	183	GLU
42	7	254	GLU
42	7	294	LEU
42	7	382	ILE
42	7	390	LEU
42	7	481	LEU
43	8	75	GLU
43	8	86	LEU
43	8	165	LEU
43	8	225	THR
43	8	291	GLU
43	8	292	ILE
43	8	350	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (152) such sidechains are listed below:

Mol	Chain	Res	Type
3	B	36	GLN
3	B	110	ASN
3	B	141	ASN
3	B	169	HIS
3	B	193	HIS
4	C	43	ASN
4	C	157	GLN
4	C	160	GLN
4	C	179	ASN
5	D	267	GLN
5	D	272	HIS
6	F	67	GLN
6	F	179	ASN
6	F	214	ASN
7	H	4	ASN
8	I	12	ASN
8	I	114	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	I	168	HIS
9	J	99	ASN
9	J	116	HIS
9	J	155	ASN
9	J	165	GLN
10	K	124	HIS
11	M	11	GLN
11	M	121	GLN
11	M	141	ASN
12	O	49	GLN
12	O	69	ASN
13	P	20	GLN
13	P	26	ASN
13	P	79	GLN
14	W	47	ASN
15	X	16	ASN
15	X	56	HIS
15	X	82	GLN
16	Y	16	HIS
16	Y	61	GLN
16	Y	77	ASN
17	Z	15	ASN
17	Z	94	HIS
17	Z	106	GLN
19	c	26	GLN
19	c	84	HIS
21	E	101	GLN
21	E	226	GLN
22	G	29	GLN
22	G	79	HIS
22	G	82	ASN
22	G	83	ASN
22	G	110	GLN
22	G	118	ASN
22	G	149	GLN
23	L	50	GLN
23	L	61	GLN
24	N	19	GLN
24	N	46	GLN
24	N	55	ASN
25	Q	35	GLN
26	R	80	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	R	97	GLN
27	S	31	ASN
27	S	83	ASN
27	S	116	ASN
27	S	121	GLN
28	T	19	ASN
28	T	72	GLN
28	T	105	ASN
28	T	135	HIS
29	U	63	HIS
29	U	91	HIS
31	a	112	ASN
32	d	45	ASN
33	e	10	HIS
35	h	15	ASN
35	h	196	ASN
35	h	305	ASN
36	1	47	HIS
36	1	167	ASN
36	1	204	HIS
36	1	207	GLN
36	1	226	GLN
36	1	236	GLN
36	1	247	GLN
36	1	288	ASN
36	1	381	GLN
36	1	425	GLN
36	1	432	GLN
36	1	434	ASN
36	1	448	GLN
36	1	498	ASN
37	2	377	ASN
37	2	386	ASN
37	2	460	GLN
37	2	461	ASN
37	2	487	GLN
37	2	715	HIS
37	2	724	GLN
37	2	784	GLN
37	2	840	GLN
37	2	858	GLN
37	2	869	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	2	870	ASN
38	3	181	ASN
38	3	225	HIS
38	3	241	GLN
38	3	244	ASN
38	3	282	GLN
38	3	283	GLN
38	3	321	ASN
38	3	377	ASN
38	3	396	ASN
39	4	153	ASN
39	4	160	ASN
39	4	280	ASN
39	4	308	GLN
39	4	350	ASN
39	4	352	ASN
39	4	371	ASN
40	5	58	GLN
40	5	64	GLN
40	5	111	ASN
40	5	244	GLN
40	5	261	ASN
40	5	272	GLN
40	5	273	GLN
40	5	279	GLN
40	5	285	ASN
40	5	336	GLN
40	5	337	ASN
40	5	345	GLN
40	5	351	ASN
41	6	91	GLN
41	6	101	GLN
41	6	124	ASN
41	6	151	GLN
41	6	186	GLN
42	7	239	ASN
42	7	241	ASN
42	7	243	GLN
42	7	289	GLN
42	7	361	ASN
42	7	443	GLN
42	7	454	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
42	7	489	GLN
42	7	499	ASN
42	7	548	HIS
43	8	33	ASN
43	8	108	ASN
43	8	259	ASN
43	8	272	GLN
43	8	355	ASN
43	8	360	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1683/1697 (99%)	409 (24%)	26 (1%)
2	0	338/377 (89%)	186 (55%)	20 (5%)
All	All	2021/2074 (97%)	595 (29%)	46 (2%)

All (595) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	3	C
1	A	4	C
1	A	17	C
1	A	33	G
1	A	41	G
1	A	44	U
1	A	46	A
1	A	58	C
1	A	64	A
1	A	67	C
1	A	68	A
1	A	73	C
1	A	74	G
1	A	75	G
1	A	77	A
1	A	79	A
1	A	100	U
1	A	103	A
1	A	111	A
1	A	113	G
1	A	115	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	124	U
1	A	126	G
1	A	127	C
1	A	130	G
1	A	142	C
1	A	143	U
1	A	147	A
1	A	160	U
1	A	161	U
1	A	162	C
1	A	163	U
1	A	164	A
1	A	166	A
1	A	167	G
1	A	178	C
1	A	183	G
1	A	184	G
1	A	191	A
1	A	192	C
1	A	201	C
1	A	202	G
1	A	205	G
1	A	206	G
1	A	215	G
1	A	292	A
1	A	307	G
1	A	309	G
1	A	317	C
1	A	319	C
1	A	323	C
1	A	331	C
1	A	332	G
1	A	333	G
1	A	335	G
1	A	347	G
1	A	362	C
1	A	364	A
1	A	367	U
1	A	368	U
1	A	369	C
1	A	370	G
1	A	382	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	385	G
1	A	386	C
1	A	400	C
1	A	407	G
1	A	408	A
1	A	409	C
1	A	417	C
1	A	418	A
1	A	421	G
1	A	429	C
1	A	434	G
1	A	436	G
1	A	441	C
1	A	447	A
1	A	448	A
1	A	449	A
1	A	450	C
1	A	455	A
1	A	463	C
1	A	464	A
1	A	465	A
1	A	466	G
1	A	470	G
1	A	471	G
1	A	472	C
1	A	473	A
1	A	474	G
1	A	482	G
1	A	487	U
1	A	492	C
1	A	493	A
1	A	517	C
1	A	518	G
1	A	525	A
1	A	530	U
1	A	531	A
1	A	532	C
1	A	533	A
1	A	534	G
1	A	536	A
1	A	537	C
1	A	541	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	543	C
1	A	544	G
1	A	547	G
1	A	550	C
1	A	551	U
1	A	554	A
1	A	555	A
1	A	556	U
1	A	559	G
1	A	560	A
1	A	561	A
1	A	562	U
1	A	568	C
1	A	576	A
1	A	583	A
1	A	587	A
1	A	588	G
1	A	589	G
1	A	590	A
1	A	591	U
1	A	593	C
1	A	598	G
1	A	606	G
1	A	607	U
1	A	608	C
1	A	609	U
1	A	614	C
1	A	615	C
1	A	627	U
1	A	628	A
1	A	629	A
1	A	631	U
1	A	643	A
1	A	644	G
1	A	655	A
1	A	658	U
1	A	660	C
1	A	664	A
1	A	668	A
1	A	669	A
1	A	671	A
1	A	672	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	673	G
1	A	675	U
1	A	684	G
1	A	689	U
1	A	690	G
1	A	696	G
1	A	732	U
1	A	734	C
1	A	743	U
1	A	744	G
1	A	745	C
1	A	750	C
1	A	752	G
1	A	753	C
1	A	754	G
1	A	789	G
1	A	810	A
1	A	811	A
1	A	821	G
1	A	822	U
1	A	823	U
1	A	827	A
1	A	830	A
1	A	834	C
1	A	844	U
1	A	847	A
1	A	852	G
1	A	869	A
1	A	870	A
1	A	871	U
1	A	872	A
1	A	873	G
1	A	874	G
1	A	878	G
1	A	881	G
1	A	884	C
1	A	886	A
1	A	888	U
1	A	890	U
1	A	891	G
1	A	892	U
1	A	893	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	894	G
1	A	897	U
1	A	898	U
1	A	912	C
1	A	913	A
1	A	917	U
1	A	918	U
1	A	920	A
1	A	921	G
1	A	922	A
1	A	933	G
1	A	938	A
1	A	943	U
1	A	947	G
1	A	952	G
1	A	956	G
1	A	965	U
1	A	970	G
1	A	971	G
1	A	972	A
1	A	978	G
1	A	988	C
1	A	990	A
1	A	992	A
1	A	999	G
1	A	1002	U
1	A	1008	A
1	A	1017	U
1	A	1023	A
1	A	1045	U
1	A	1050	A
1	A	1060	A
1	A	1061	U
1	A	1062	A
1	A	1083	A
1	A	1085	C
1	A	1087	A
1	A	1088	U
1	A	1100	A
1	A	1114	U
1	A	1115	U
1	A	1116	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1117	C
1	A	1120	U
1	A	1121	G
1	A	1126	G
1	A	1133	A
1	A	1138	C
1	A	1144	A
1	A	1148	A
1	A	1153	C
1	A	1154	U
1	A	1183	A
1	A	1195	A
1	A	1197	G
1	A	1207	G
1	A	1208	A
1	A	1215	C
1	A	1221	G
1	A	1224	G
1	A	1225	U
1	A	1230	C
1	A	1235	G
1	A	1242	U
1	A	1244	U
1	A	1251	A
1	A	1253	A
1	A	1256	G
1	A	1257	G
1	A	1258	A
1	A	1259	A
1	A	1264	C
1	A	1269	G
1	A	1271	C
1	A	1274	G
1	A	1275	G
1	A	1281	G
1	A	1282	A
1	A	1284	A
1	A	1285	G
1	A	1286	G
1	A	1287	A
1	A	1288	U
1	A	1291	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1293	A
1	A	1295	A
1	A	1296	U
1	A	1298	G
1	A	1299	A
1	A	1301	A
1	A	1302	G
1	A	1303	C
1	A	1305	C
1	A	1307	U
1	A	1308	U
1	A	1311	C
1	A	1312	G
1	A	1314	U
1	A	1315	U
1	A	1342	U
1	A	1349	G
1	A	1350	U
1	A	1354	G
1	A	1364	U
1	A	1365	G
1	A	1371	U
1	A	1372	U
1	A	1378	A
1	A	1396	A
1	A	1397	U
1	A	1402	A
1	A	1403	C
1	A	1406	G
1	A	1412	C
1	A	1424	G
1	A	1428	G
1	A	1429	G
1	A	1440	C
1	A	1447	G
1	A	1449	G
1	A	1452	A
1	A	1453	C
1	A	1454	A
1	A	1459	G
1	A	1462	U
1	A	1463	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1466	G
1	A	1475	G
1	A	1478	U
1	A	1479	G
1	A	1480	A
1	A	1489	A
1	A	1490	G
1	A	1494	U
1	A	1495	G
1	A	1498	A
1	A	1506	A
1	A	1507	G
1	A	1508	A
1	A	1509	U
1	A	1512	C
1	A	1519	U
1	A	1520	G
1	A	1521	C
1	A	1533	A
1	A	1536	G
1	A	1543	U
1	A	1544	C
1	A	1548	G
1	A	1552	G
1	A	1553	C
1	A	1554	C
1	A	1556	A
1	A	1557	C
1	A	1560	U
1	A	1564	C
1	A	1573	G
1	A	1574	C
1	A	1575	G
1	A	1580	A
1	A	1588	A
1	A	1593	C
1	A	1600	G
1	A	1601	A
1	A	1604	G
1	A	1606	G
1	A	1619	A
1	A	1621	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1622	U
1	A	1623	A
1	A	1637	A
1	A	1639	G
1	A	1641	A
1	A	1648	G
1	A	1654	G
1	A	1661	A
1	A	1664	A
1	A	1665	G
1	A	1671	G
1	A	1680	G
1	A	1683	C
1	A	1695	A
1	A	1697	A
1	A	1698	C
1	A	1704	C
1	A	1715	A
1	A	1721	U
1	A	1722	G
1	A	1725	U
1	A	1726	G
1	A	1750	C
1	A	1753	C
1	A	1757	G
1	A	1759	G
1	A	1775	U
1	A	1776	G
1	A	1777	G
1	A	1779	G
1	A	1782	G
1	A	1783	C
1	A	1784	G
1	A	1788	A
1	A	1800	A
1	A	1805	G
1	A	1809	A
1	A	1823	A
1	A	1824	A
1	A	1825	A
1	A	1826	G
1	A	1831	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1836	G
1	A	1838	U
1	A	1849	G
1	A	1851	A
1	A	1861	G
1	A	1862	G
1	A	1863	A
1	A	1864	U
1	A	1865	C
1	A	1869	A
2	0	359	C
2	0	360	G
2	0	361	A
2	0	362	U
2	0	363	A
2	0	364	C
2	0	365	C
2	0	366	A
2	0	367	A
2	0	368	G
2	0	370	G
2	0	377	U
2	0	380	G
2	0	381	A
2	0	384	G
2	0	385	A
2	0	386	U
2	0	387	U
2	0	388	A
2	0	391	A
2	0	392	C
2	0	393	U
2	0	395	G
2	0	396	C
2	0	397	G
2	0	400	G
2	0	403	G
2	0	404	G
2	0	406	C
2	0	407	A
2	0	408	G
2	0	409	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	0	410	A
2	0	411	C
2	0	412	A
2	0	417	A
2	0	418	G
2	0	419	U
2	0	420	C
2	0	422	U
2	0	423	G
2	0	425	A
2	0	426	U
2	0	427	U
2	0	428	A
2	0	429	U
2	0	430	G
2	0	431	G
2	0	433	G
2	0	434	U
2	0	435	U
2	0	436	U
2	0	443	A
2	0	446	U
2	0	451	U
2	0	452	U
2	0	453	G
2	0	454	C
2	0	455	U
2	0	457	U
2	0	458	A
2	0	460	U
2	0	461	A
2	0	462	U
2	0	463	U
2	0	464	G
2	0	465	A
2	0	466	A
2	0	467	C
2	0	468	U
2	0	471	A
2	0	472	G
2	0	473	U
2	0	478	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	0	480	U
2	0	481	G
2	0	482	U
2	0	483	A
2	0	484	C
2	0	485	U
2	0	486	U
2	0	487	G
2	0	488	G
2	0	489	C
2	0	490	A
2	0	491	U
2	0	492	G
2	0	493	U
2	0	494	A
2	0	496	A
2	0	497	C
2	0	498	C
2	0	499	U
2	0	500	G
2	0	504	A
2	0	506	U
2	0	507	U
2	0	508	A
2	0	509	G
2	0	513	U
2	0	515	G
2	0	516	U
2	0	518	G
2	0	519	A
2	0	520	U
2	0	526	A
2	0	527	C
2	0	532	G
2	0	534	U
2	0	537	G
2	0	538	G
2	0	539	U
2	0	540	A
2	0	541	C
2	0	542	A
2	0	543	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	0	545	A
2	0	546	G
2	0	550	A
2	0	552	A
2	0	553	C
2	0	557	A
2	0	559	A
2	0	560	U
2	0	561	A
2	0	562	U
2	0	567	U
2	0	568	U
2	0	569	U
2	0	570	U
2	0	572	U
2	0	575	U
2	0	576	U
2	0	577	A
2	0	580	G
2	0	581	A
2	0	582	A
2	0	583	G
2	0	584	A
2	0	586	A
2	0	587	A
2	0	588	U
2	0	590	A
2	0	591	G
2	0	593	G
2	0	603	A
2	0	605	G
2	0	612	G
2	0	614	C
2	0	619	G
2	0	620	A
2	0	621	G
2	0	624	G
2	0	625	G
2	0	626	U
2	0	627	G
2	0	628	A
2	0	633	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	0	637	G
2	0	638	C
2	0	640	C
2	0	641	C
2	0	642	U
2	0	643	G
2	0	644	A
2	0	645	A
2	0	646	G
2	0	647	C
2	0	649	A
2	0	654	A
2	0	656	G
2	0	657	U
2	0	658	C
2	0	659	U
2	0	660	U
2	0	662	C
2	0	663	C
2	0	670	G
2	0	678	A
2	0	679	U
2	0	680	A
2	0	682	G
2	0	684	A
2	0	685	G
2	0	686	U
2	0	692	A

All (46) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	110	U
1	A	166	A
1	A	205	G
1	A	304	C
1	A	407	G
1	A	463	C
1	A	465	A
1	A	500	A
1	A	532	C
1	A	553	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	555	A
1	A	561	A
1	A	606	G
1	A	627	U
1	A	688	U
1	A	752	G
1	A	753	C
1	A	870	A
1	A	887	U
1	A	912	C
1	A	1137	U
1	A	1295	A
1	A	1395	C
1	A	1664	A
1	A	1783	C
1	A	1824	A
2	0	369	A
2	0	387	U
2	0	406	C
2	0	416	U
2	0	425	A
2	0	429	U
2	0	456	C
2	0	480	U
2	0	484	C
2	0	485	U
2	0	496	A
2	0	508	A
2	0	518	G
2	0	526	A
2	0	559	A
2	0	560	U
2	0	581	A
2	0	619	G
2	0	655	G
2	0	656	G

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	15
40	5	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	697:G	O3'	729:C	P	18.10
1	A	834:C	O3'	841:G	P	17.97
1	A	130:G	O3'	141:A	P	17.73
1	A	756:C	O3'	788:G	P	15.69
1	A	323:C	O3'	329:G	P	15.54
1	A	1417:C	O3'	1423:C	P	14.83
1	A	1761:U	O3'	1771:G	P	14.63
1	A	225:G	O3'	287:U	P	8.35
1	A	886:A	O3'	887:U	P	8.27
1	A	745:C	O3'	749:U	P	7.26
1	A	1432:U	O3'	1438:A	P	5.45

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	903:A	O3'	904:A	P	5.12
1	A	798:G	O3'	799:U	P	4.14
1	A	902:G	O3'	903:A	P	3.79
1	A	736:C	O3'	743:U	P	3.40
1	5	243:LEU	C	244:GLN	N	3.13

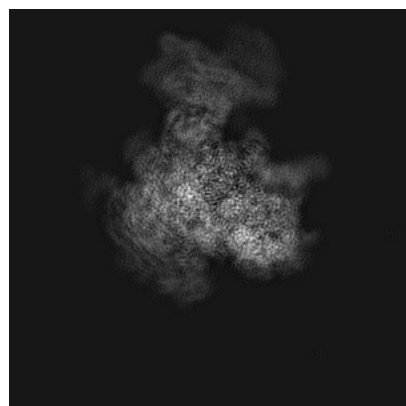
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21529. These allow visual inspection of the internal detail of the map and identification of artifacts.

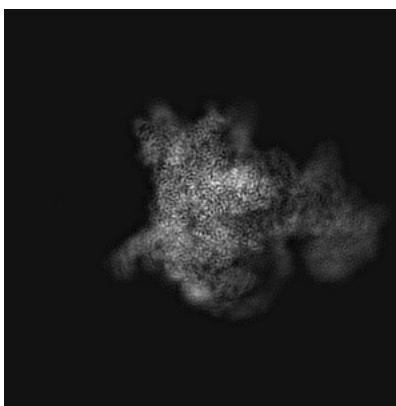
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

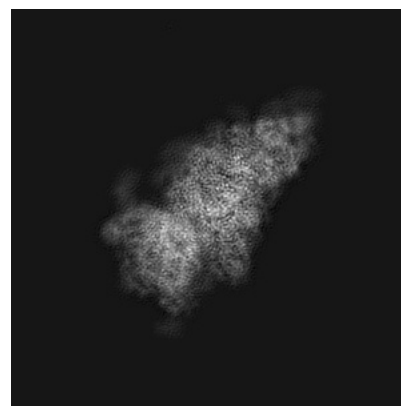
6.1.1 Primary map



X

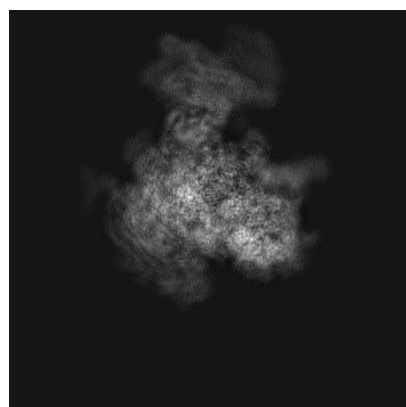


Y

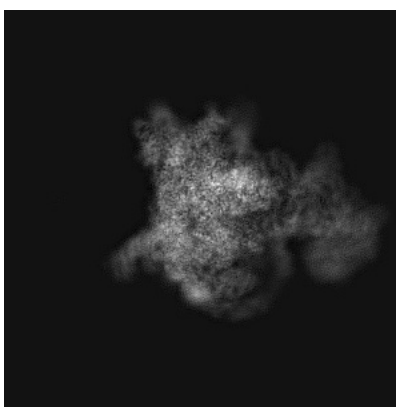


Z

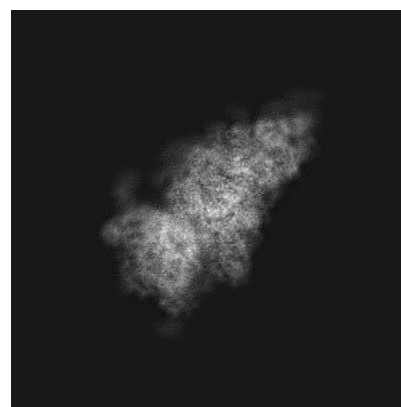
6.1.2 Raw map



X



Y

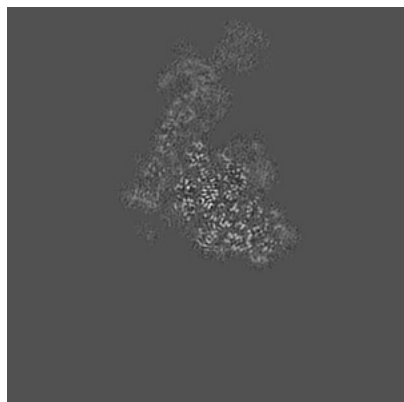


Z

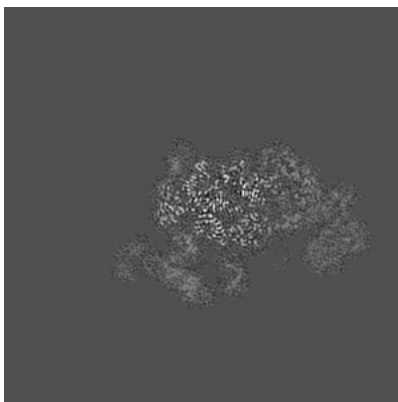
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

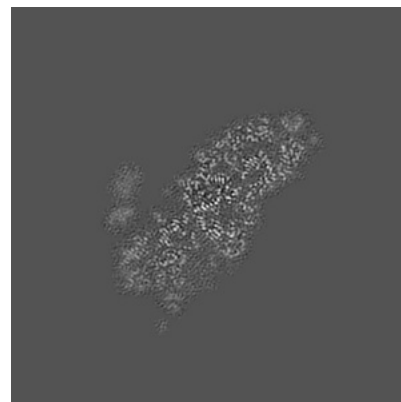
6.2.1 Primary map



X Index: 200

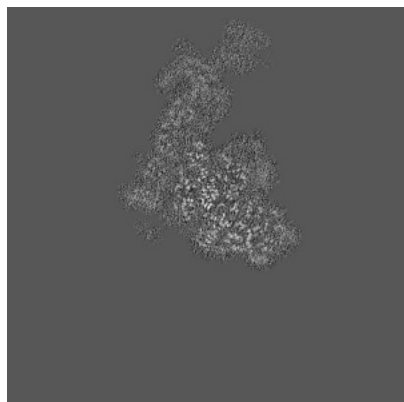


Y Index: 200

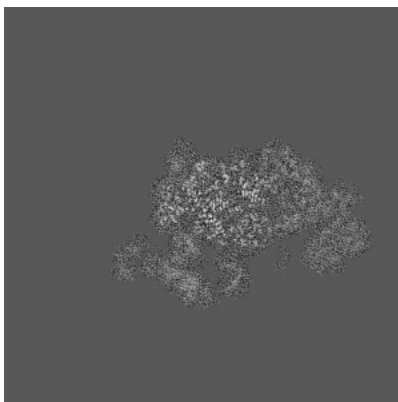


Z Index: 200

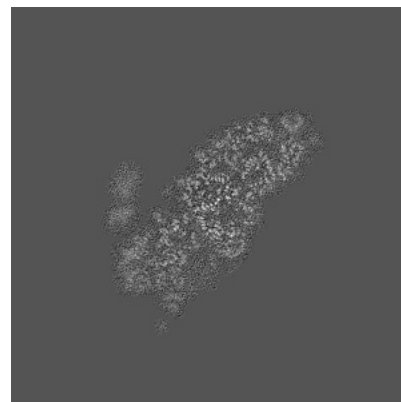
6.2.2 Raw map



X Index: 200



Y Index: 200

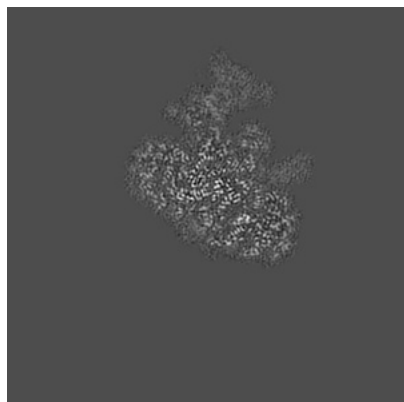


Z Index: 200

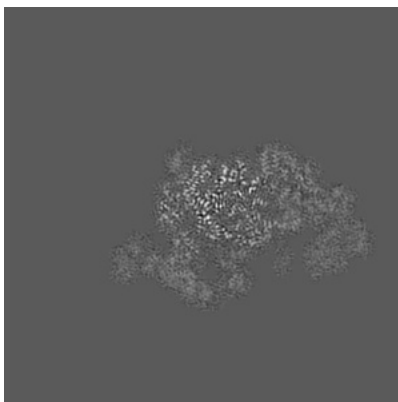
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

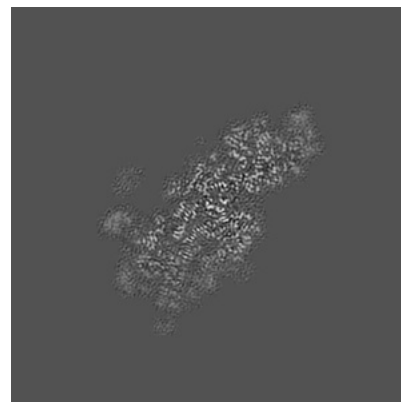
6.3.1 Primary map



X Index: 225

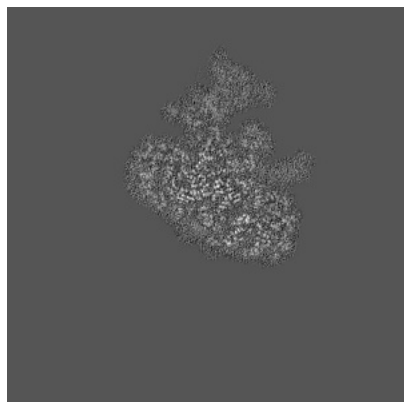


Y Index: 197

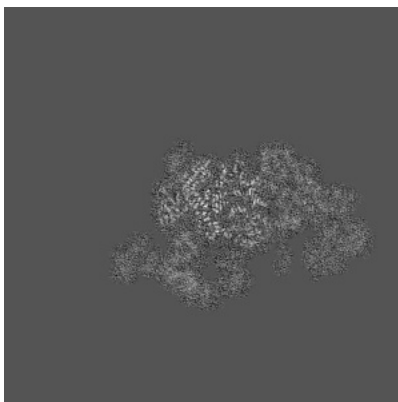


Z Index: 209

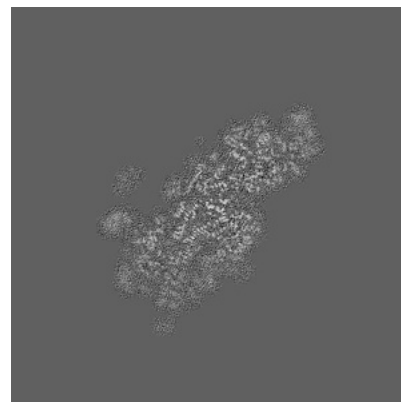
6.3.2 Raw map



X Index: 225



Y Index: 198

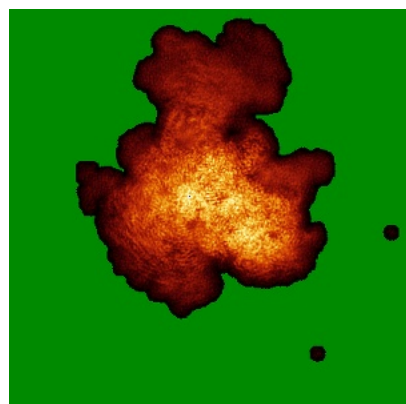


Z Index: 209

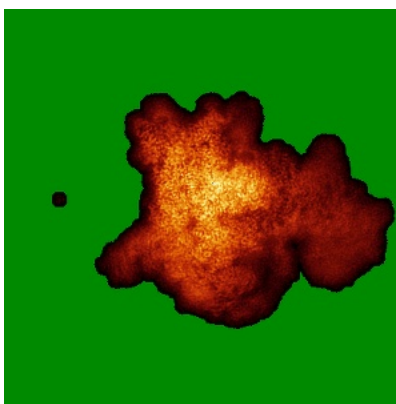
The images above show the largest variance slices of the map in three orthogonal directions.

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

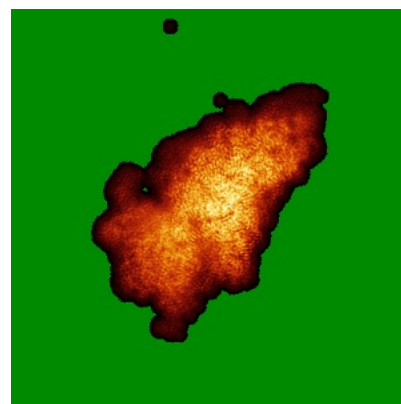
6.4.1 Primary map



X

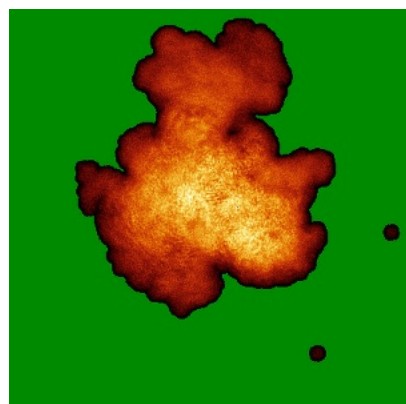


Y

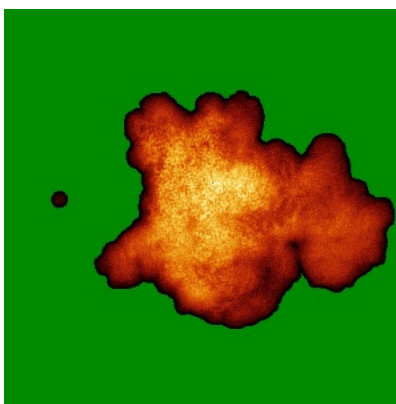


Z

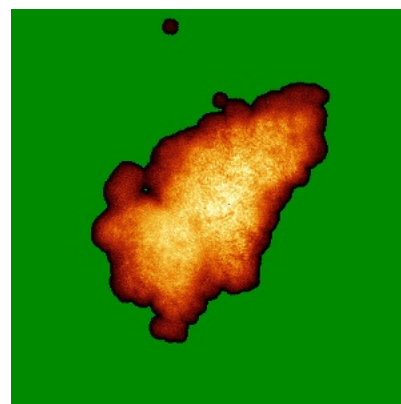
6.4.2 Raw map



X



Y

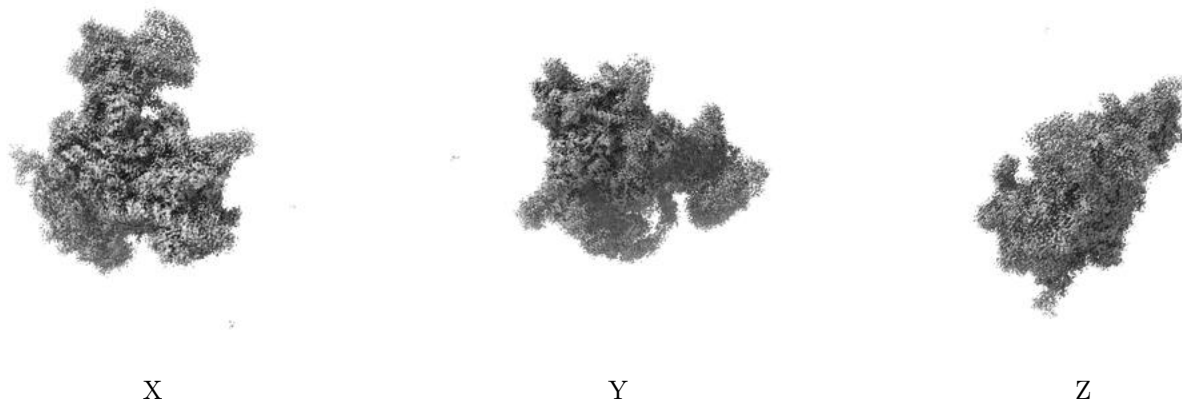


Z

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.

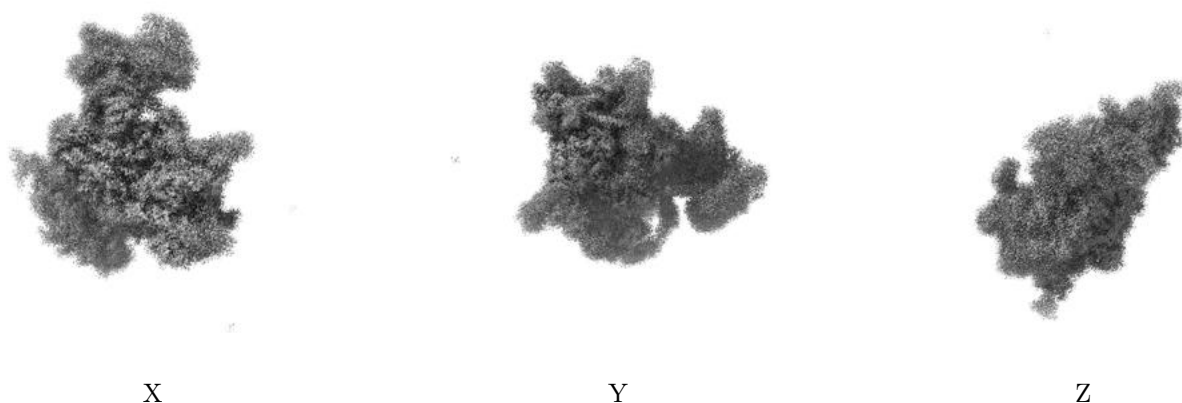
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.018. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

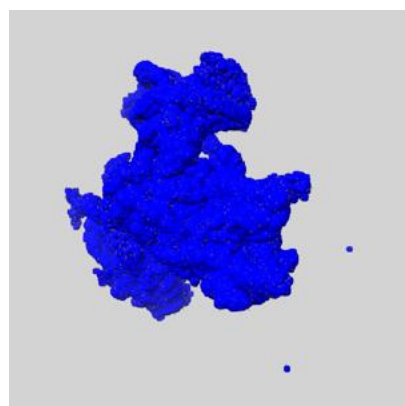
6.6 Mask visualisation [i](#)

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

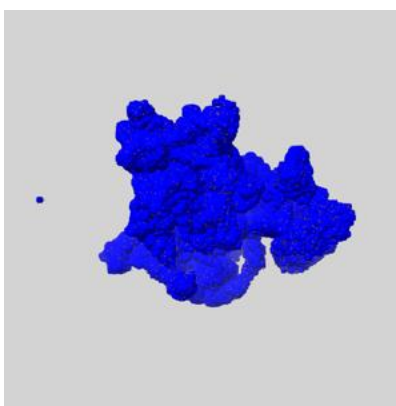
A mask typically either:

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

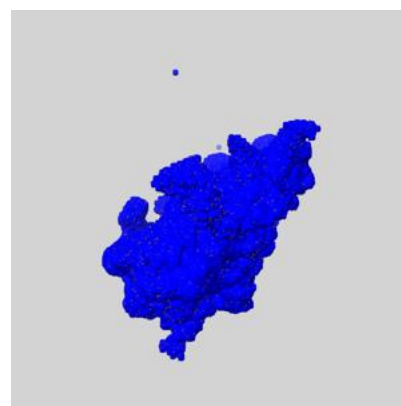
6.6.1 emd_21529_msk_1.map [i](#)



X



Y

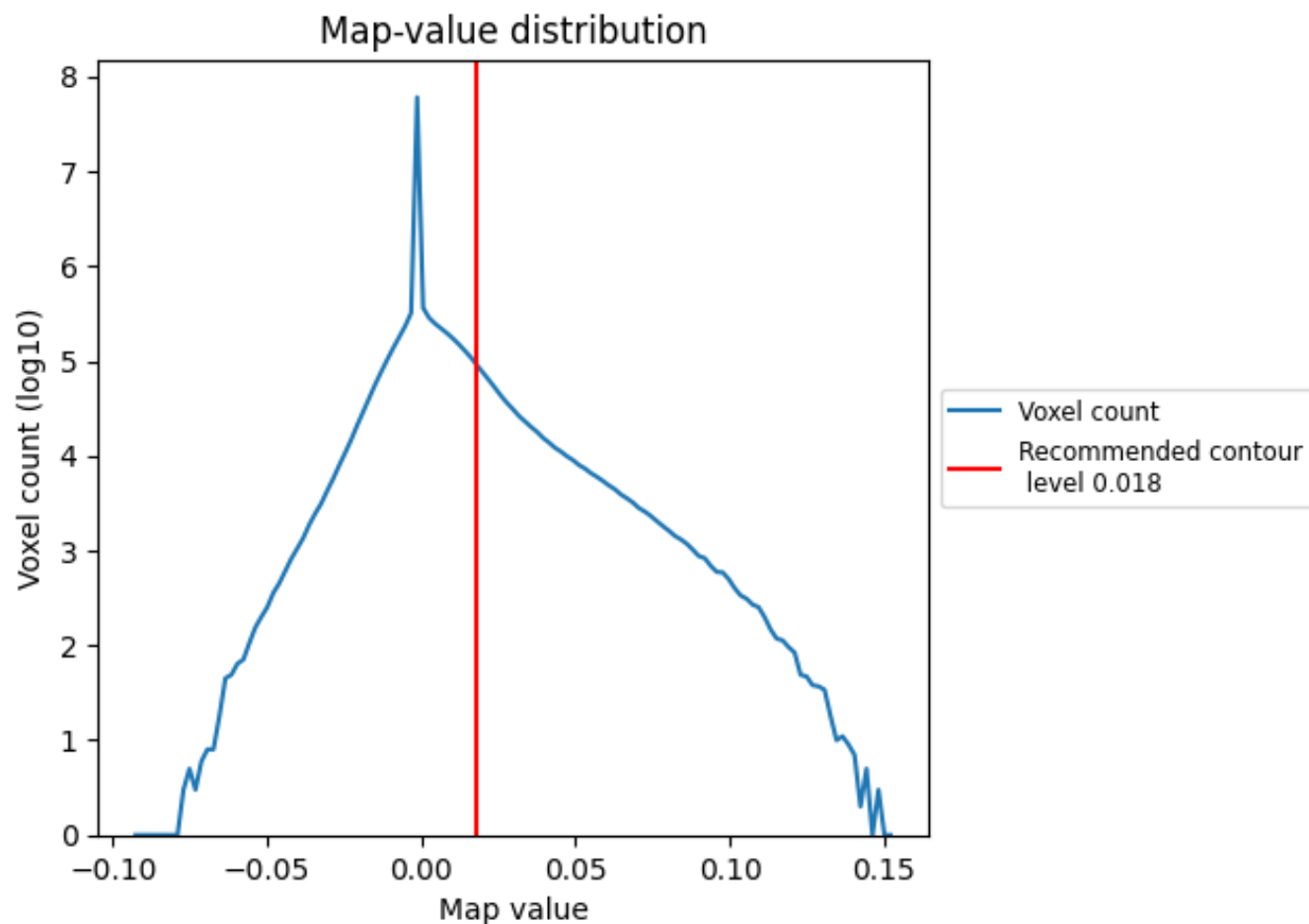


Z

7 Map analysis [i](#)

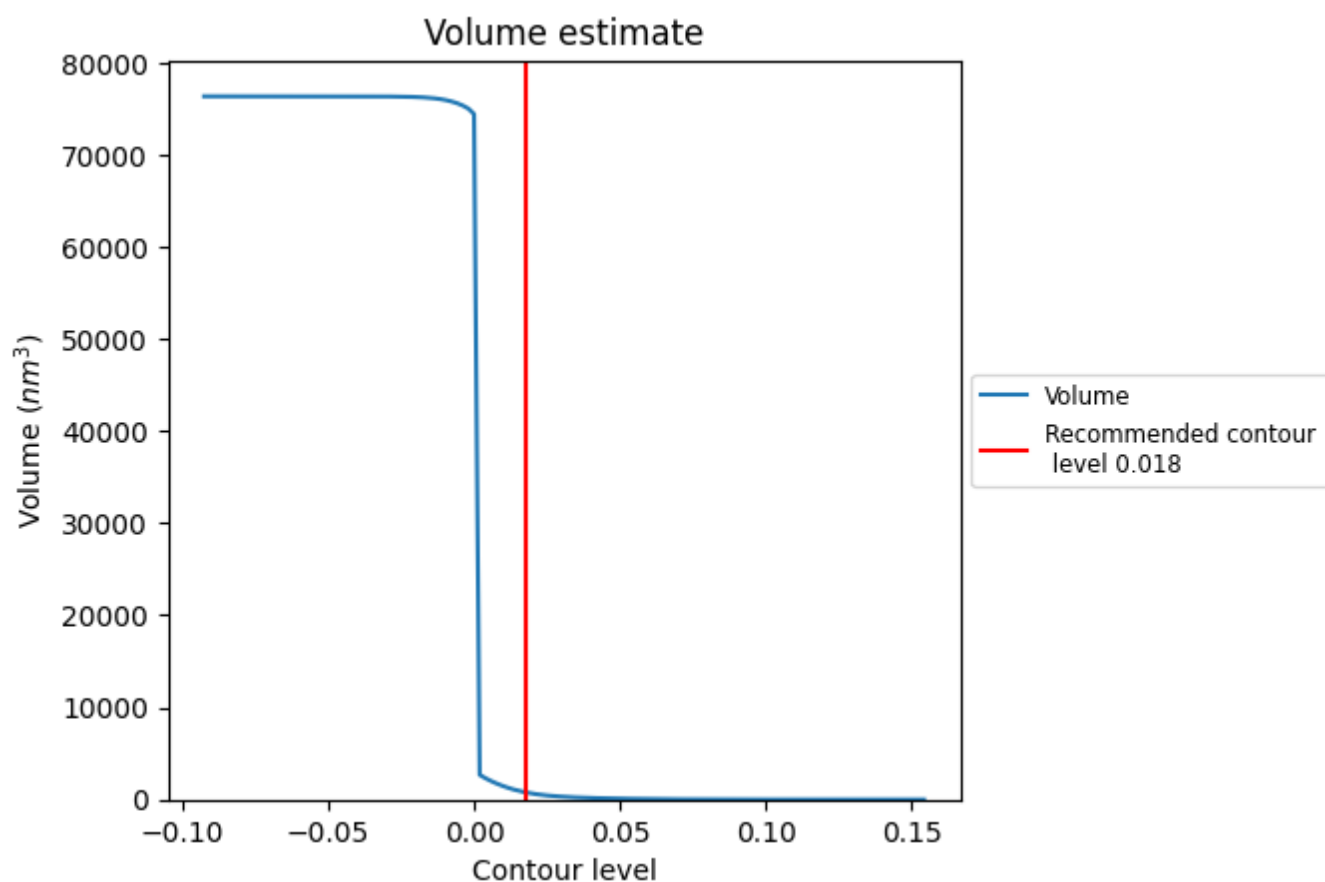
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

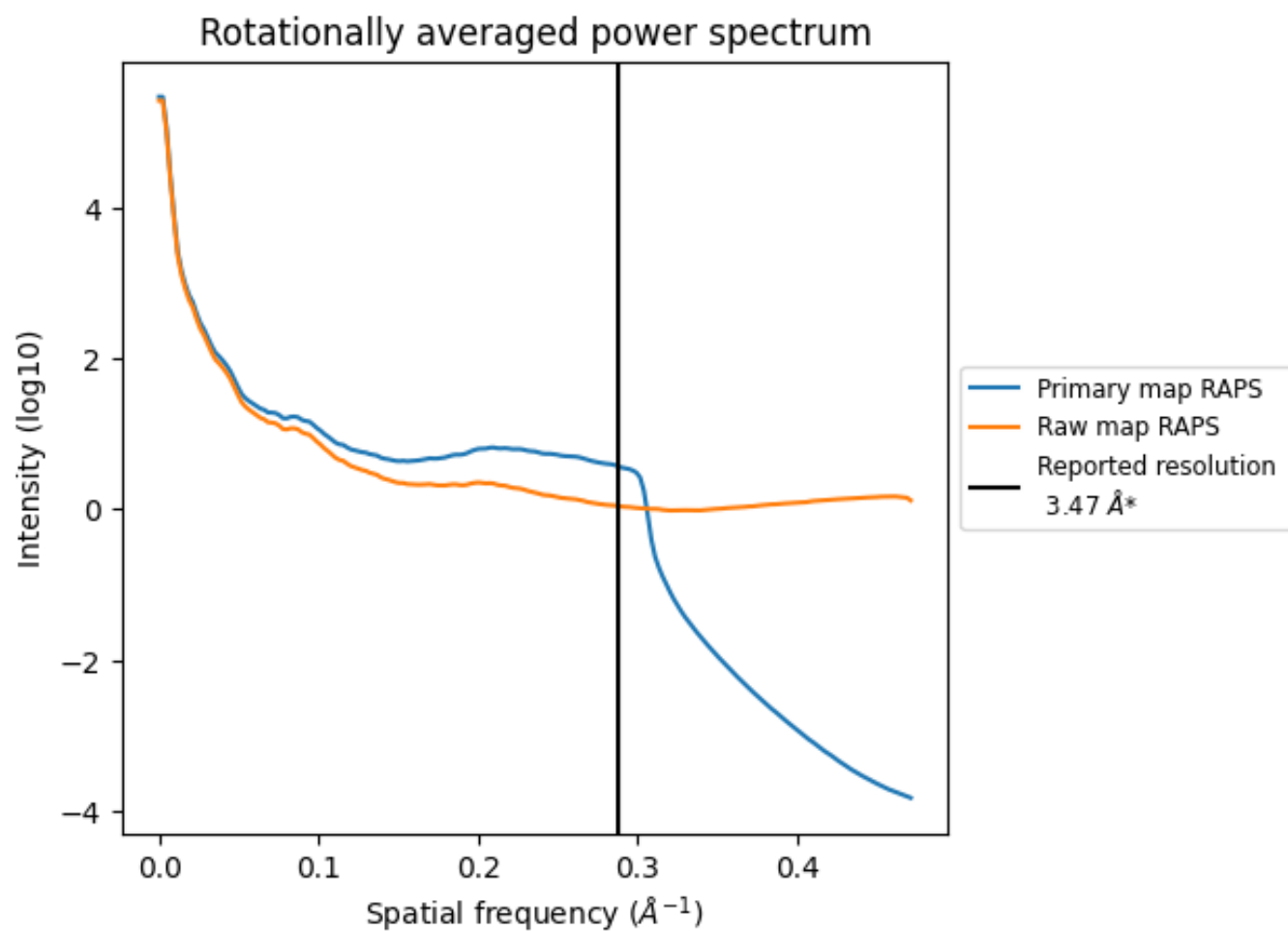
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 758 nm³; this corresponds to an approximate mass of 685 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 ⓘ

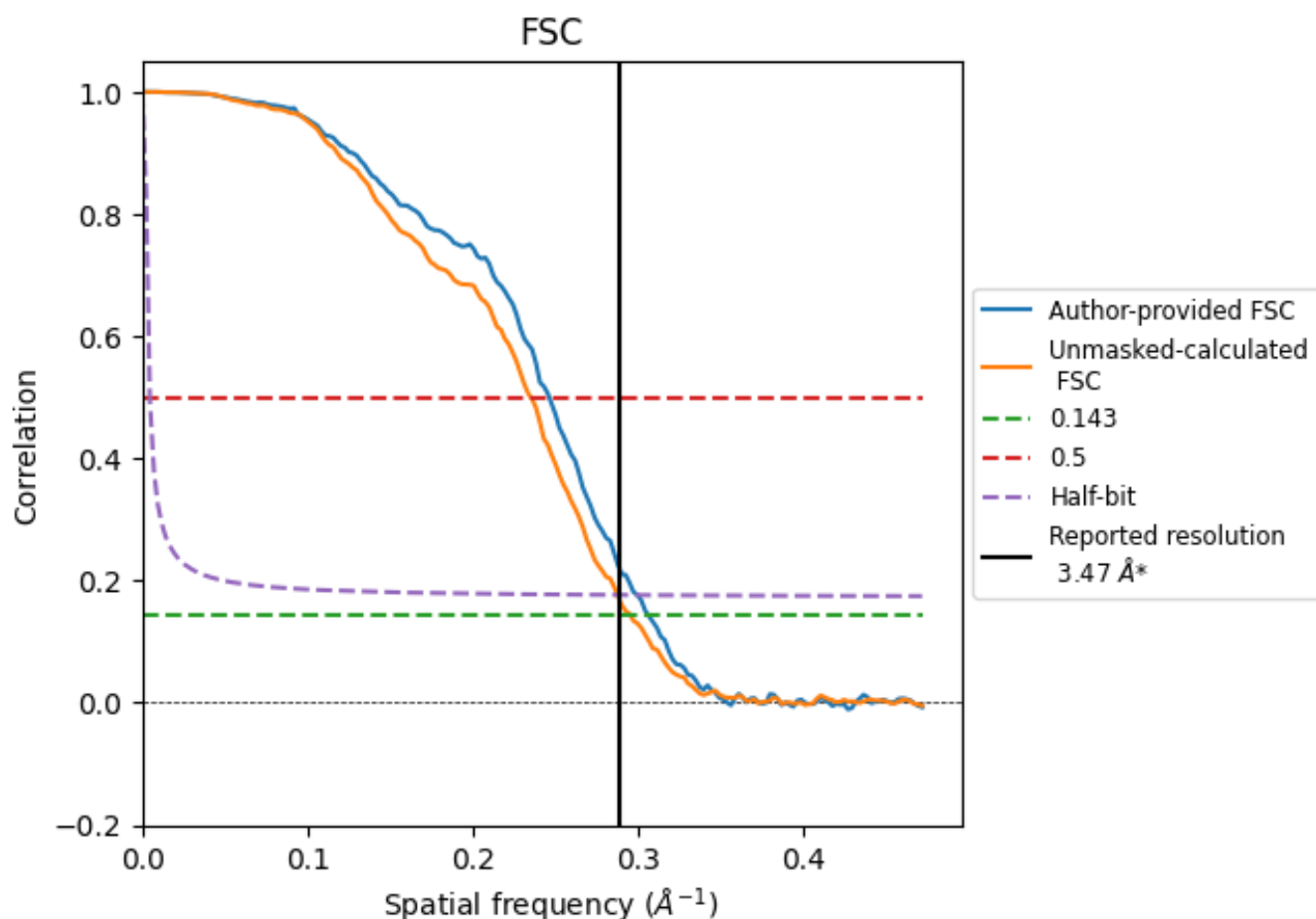


*Reported resolution corresponds to spatial frequency of 0.288 Å⁻¹

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 0.288 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

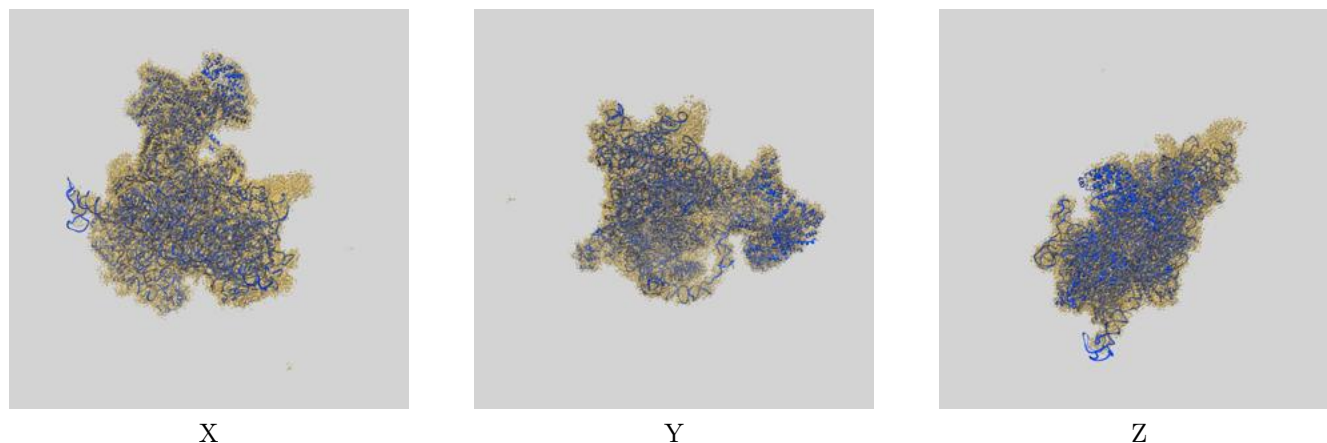
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.47	-	-
Author-provided FSC curve	3.27	4.06	3.34
Unmasked-calculated*	3.39	4.26	3.48

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

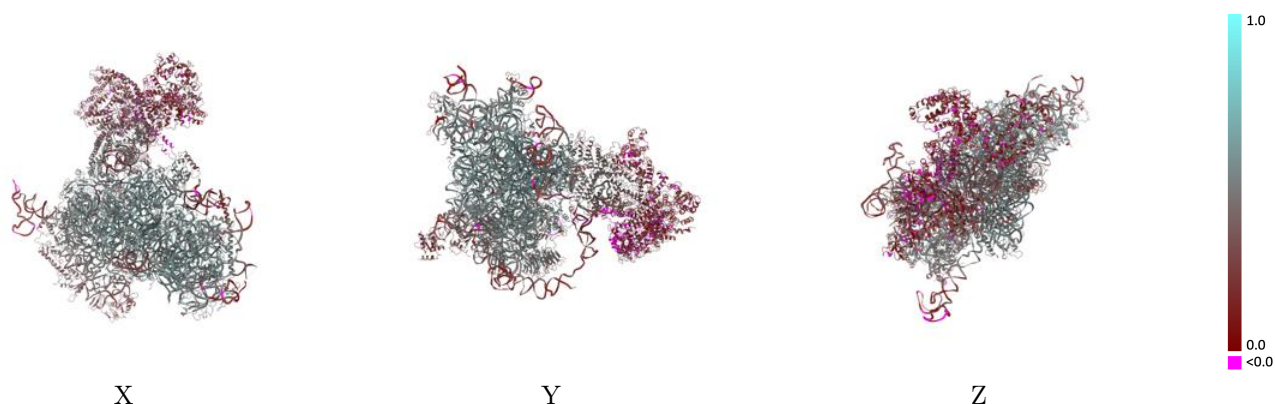
This section contains information regarding the fit between EMDB map EMD-21529 and PDB model 6W2S. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



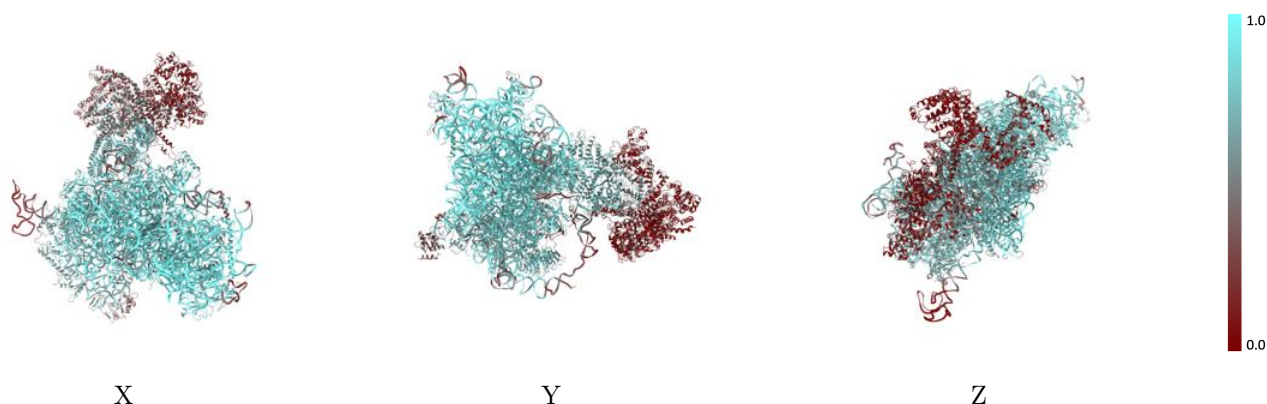
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



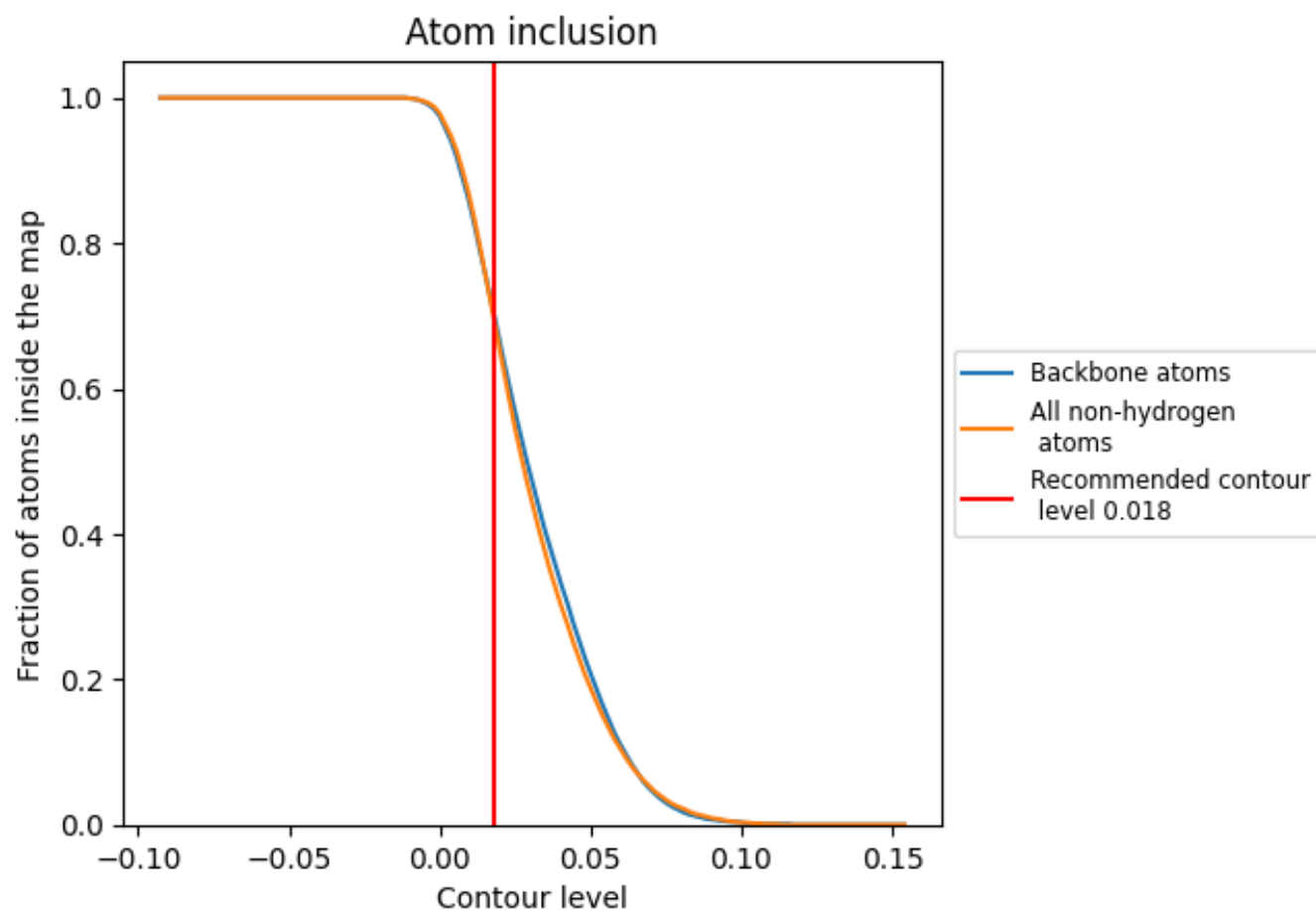
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.018).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 69% 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 (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6930	 0.4150
0	 0.5050	 0.2600
1	 0.5660	 0.3510
2	 0.5910	 0.3680
3	 0.2170	 0.2080
4	 0.1820	 0.2000
5	 0.1130	 0.0170
6	 0.1010	 0.2130
7	 0.0900	 0.1990
8	 0.1990	 0.2230
A	 0.9030	 0.4920
B	 0.8470	 0.5350
C	 0.8270	 0.5230
D	 0.8700	 0.5460
E	 0.7560	 0.4730
F	 0.8630	 0.5440
G	 0.7100	 0.4560
H	 0.7680	 0.4610
I	 0.7800	 0.4770
J	 0.8420	 0.5090
K	 0.8560	 0.5340
L	 0.6890	 0.3860
M	 0.8800	 0.5510
N	 0.3510	 0.2660
O	 0.8660	 0.5370
P	 0.8220	 0.5250
Q	 0.5890	 0.3520
R	 0.7800	 0.4900
S	 0.6170	 0.4090
T	 0.6500	 0.3970
U	 0.7770	 0.4520
V	 0.7730	 0.4750
W	 0.8820	 0.5410
X	 0.9030	 0.5660
Y	 0.8870	 0.5530



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Z	 0.8530	 0.5190
a	 0.6230	 0.4040
b	 0.8300	 0.5350
c	 0.8310	 0.5280
d	 0.6790	 0.4590
e	 0.8460	 0.4960
f	 0.7770	 0.4890
g	 0.4560	 0.3000
h	 0.7320	 0.4350