



Full wwPDB EM Validation Report ⓘ

Nov 13, 2022 – 01:16 PM EST

PDB ID : 6W2T
EMDB ID : EMD-21530
Title : Structure of the Cricket Paralysis Virus 5-UTR IRES (CrPV 5-UTR-IRES)
bound to the small ribosomal subunit in the closed state (Class 2)
Authors : Neupane, R.; Pisareva, V.; Rodriguez, C.F.; Pisarev, A.; Fernandez, I.S.
Deposited on : 2020-03-08
Resolution : 3.36 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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

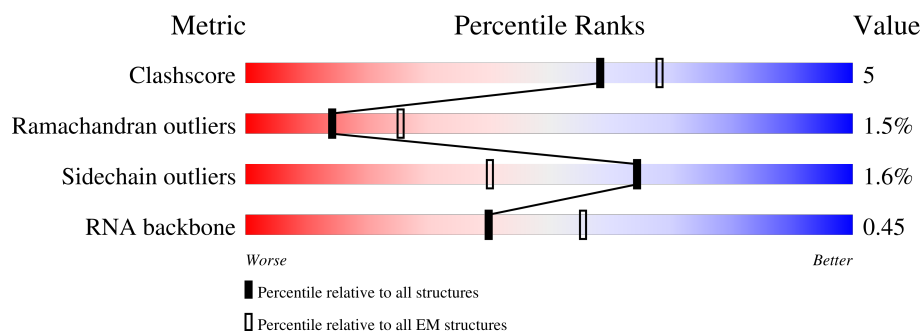
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.36 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.



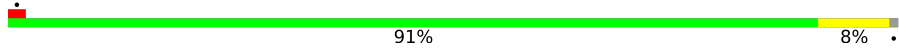


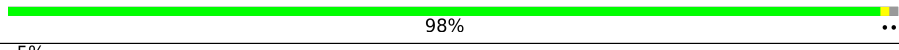


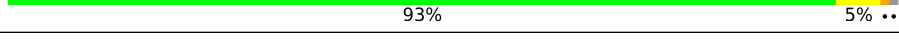
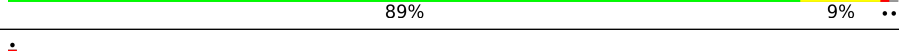
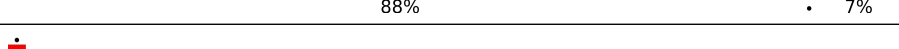
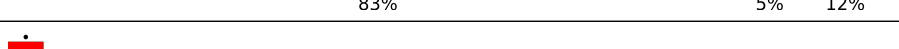
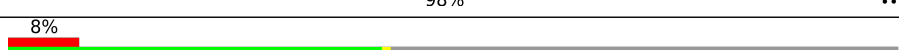

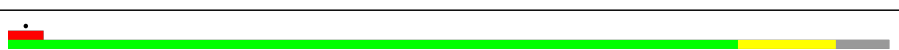







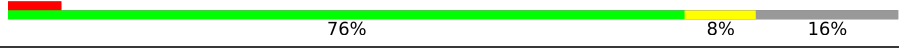
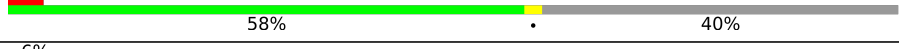

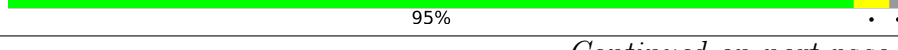

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	B	295	
3	C	264	
4	D	255	
5	F	263	
6	H	249	
7	I	194	

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Mol	Chain	Length	Quality of chain
8	J	208	
9	K	194	
10	M	158	
11	O	151	
12	P	151	
13	W	83	
14	X	130	
15	Y	143	
16	Z	134	
17	b	115	
18	c	84	
19	f	133	
20	E	281	
21	G	204	
22	L	149	
23	N	132	
24	Q	145	
25	R	172	
26	S	135	
27	T	152	
28	U	145	
29	V	119	
30	i	125	
31	d	69	
32	e	56	

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Mol	Chain	Length	Quality of chain
33	g	156	
34	h	317	
35	3	462	
36	4	364	
37	6	218	
38	7	607	
39	8	374	
40	1	1362	
41	2	913	
42	9	558	
43	5	363	
44	A	377	

2 Entry composition [i](#)

There are 46 unique types of molecules in this entry. The entry contains 109778 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 protein called uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	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 3 is a protein called eS1.

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

- Molecule 4 is a protein called uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	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

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

- Molecule 5 is a protein called eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	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 6 is a protein called eS6.

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

- Molecule 7 is a protein called eS7.

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

- Molecule 8 is a protein called eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	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 9 is a protein called uS4.

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

- Molecule 10 is a protein called uS17.

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

- Molecule 11 is a protein called uS15.

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

- Molecule 12 is a protein called uS11.

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

- Molecule 13 is a protein called eS21.

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

- Molecule 14 is a protein called uS8.

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

- Molecule 15 is a protein called uS12.

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

- Molecule 16 is a protein called eS24.

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

- Molecule 17 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	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 18 is a protein called eS27.

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

- Molecule 19 is a protein called eS30.

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

- Molecule 20 is a protein called uS3.

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

- Molecule 21 is a protein called uS7.

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

- Molecule 22 is a protein called eS10.

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

- Molecule 23 is a protein called eS12.

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

- Molecule 24 is a protein called uS19.

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

- Molecule 25 is a protein called uS9.

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

- Molecule 26 is a protein called eS17.

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

- Molecule 27 is a protein called uS13.

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

- Molecule 28 is a protein called eS19.

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

- Molecule 29 is a protein called uS10.

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

- Molecule 30 is a protein called eS25.

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

- Molecule 31 is a protein called eS28.

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

- Molecule 32 is a protein called eS29.

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

- Molecule 33 is a protein called eS31.

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

- Molecule 34 is a protein called RACK1.

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

- Molecule 35 is a protein called Eukaryotic translation initiation factor 3 subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	3	419	Total	C	N	O	S	0	0
			3465	2220	586	639	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	4	272	Total	C	N	O	S	0	0
			2111	1330	359	410	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	6	215	Total	C	N	O	S	0	0
			1737	1109	285	330	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	7	372	Total	C	N	O	S	0	0
			3109	2010	519	563	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	8	365	Total	C	N	O	S	0	0
			2918	1850	493	558	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	1	534	Total	C	N	O	S	0	0
			4377	2770	778	808	21		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	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 42 is a protein called Eukaryotic translation initiation factor 3 subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	9	356	Total	C	N	O	S	0	0
			2867	1804	500	548	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	5	324	Total	C	N	O	S	0	0
			2624	1654	452	503	15		

- Molecule 44 is a RNA chain called CrPV 5'-UTR IRES.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	A	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
A	569	U	C	conflict	GB 8895506
A	570	U	C	conflict	GB 8895506
A	571	U	A	conflict	GB 8895506
A	572	U	C	conflict	GB 8895506
A	574	U	C	conflict	GB 8895506
A	575	U	G	conflict	GB 8895506
A	729	G	-	expression tag	GB 8895506
A	730	G	-	expression tag	GB 8895506
A	731	A	-	expression tag	GB 8895506
A	732	U	-	expression tag	GB 8895506
A	733	C	-	expression tag	GB 8895506

- Molecule 45 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
45	a	1	Total	Mg	0
			1	1	

- Molecule 46 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

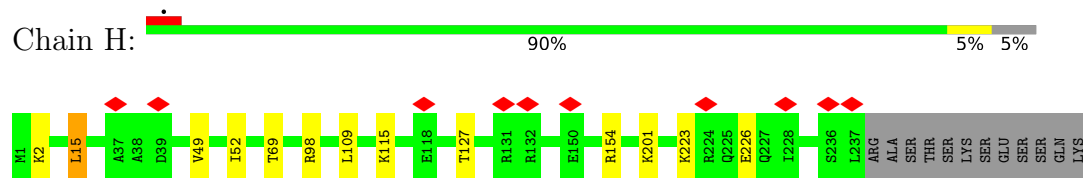
3 Residue-property plots

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.

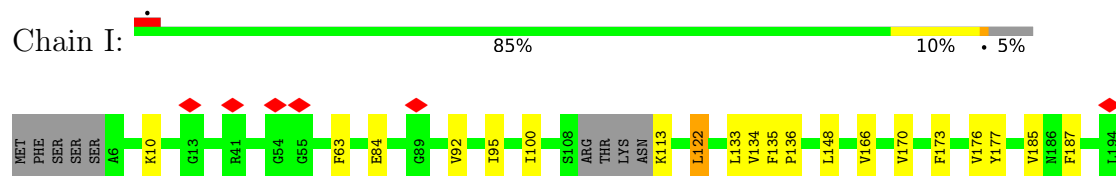
• Molecule 1: 18S rRNA



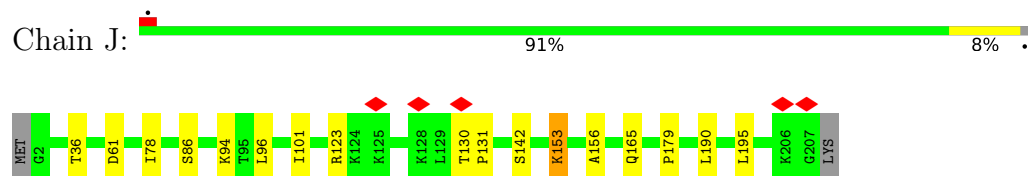
- Molecule 6: eS6



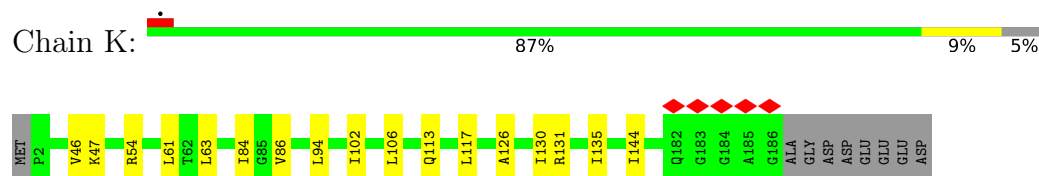
- Molecule 7: eS7



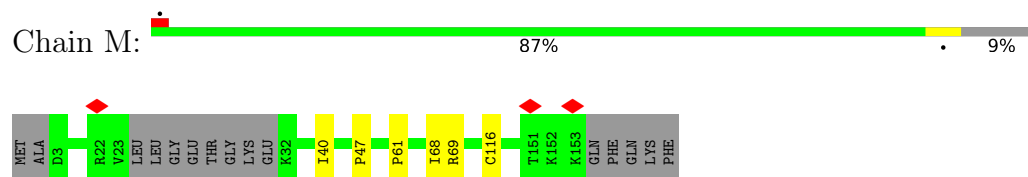
- Molecule 8: eS8



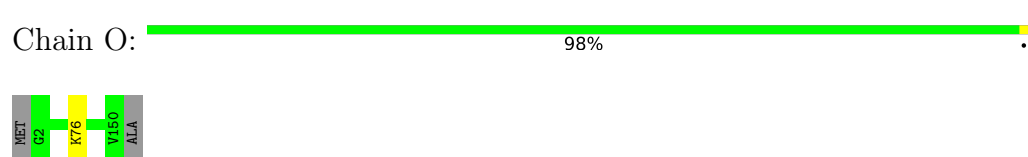
- Molecule 9: uS4



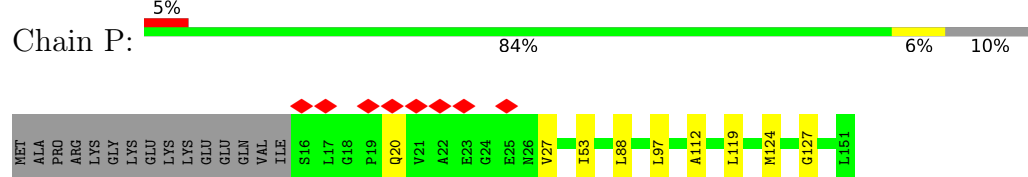
- Molecule 10: uS17



- Molecule 11: uS15



- Molecule 12: uS11




• Molecule 13: eS21

Chain W:  89% 11%


• Molecule 14: uS8

Chain X:  93% 5% ..


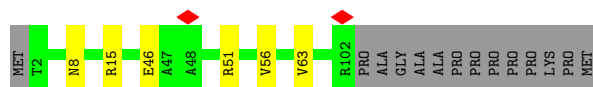
• Molecule 15: uS12

Chain Y:  89% 9% ..

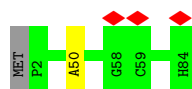
• Molecule 16: eS24

Chain Z:  88% 7% ..

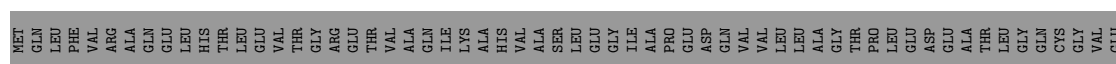
• Molecule 17: eS26

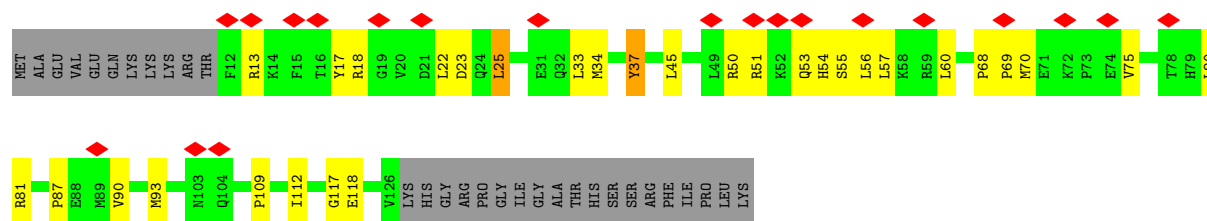
Chain b:  83% 5% 12%

• Molecule 18: eS27

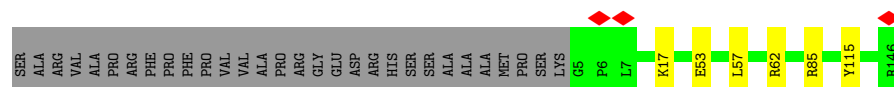
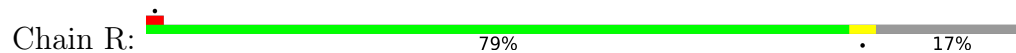
Chain c:  98% ..

• Molecule 19: eS30

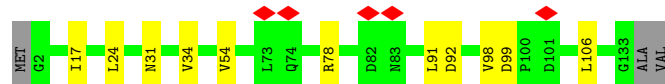
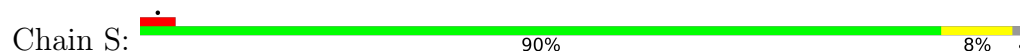
Chain f:  8% 42% 57%



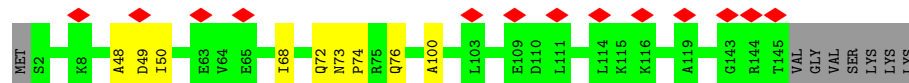
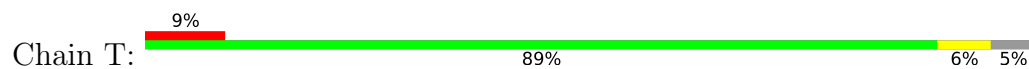
• Molecule 25: uS9



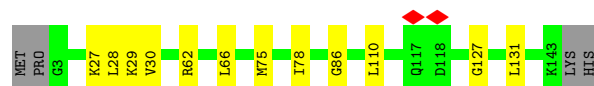
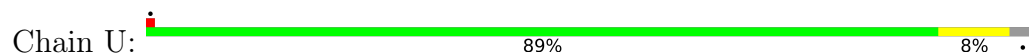
• Molecule 26: eS17



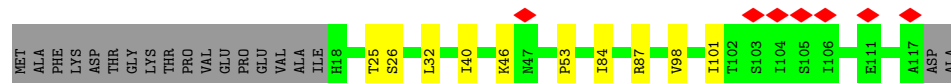
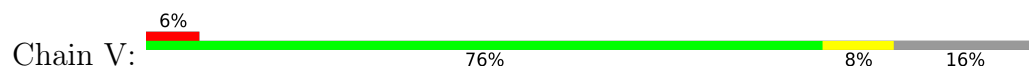
• Molecule 27: uS13



• Molecule 28: eS19



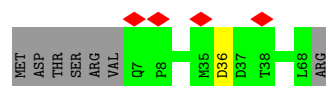
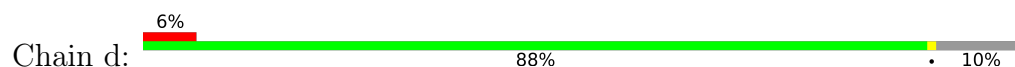
• Molecule 29: uS10



• Molecule 30: eS25



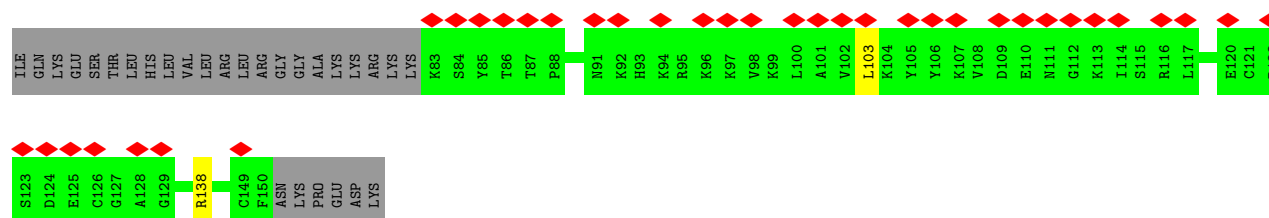
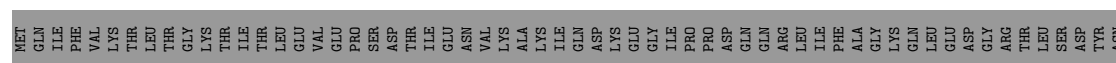
- Molecule 31: eS28



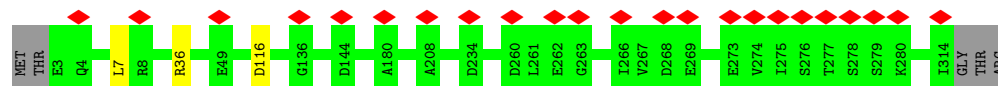
- Molecule 32: eS29



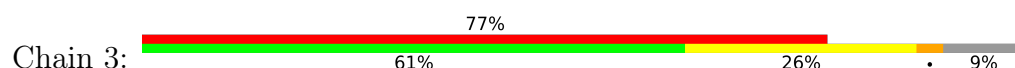
- Molecule 33: eS31

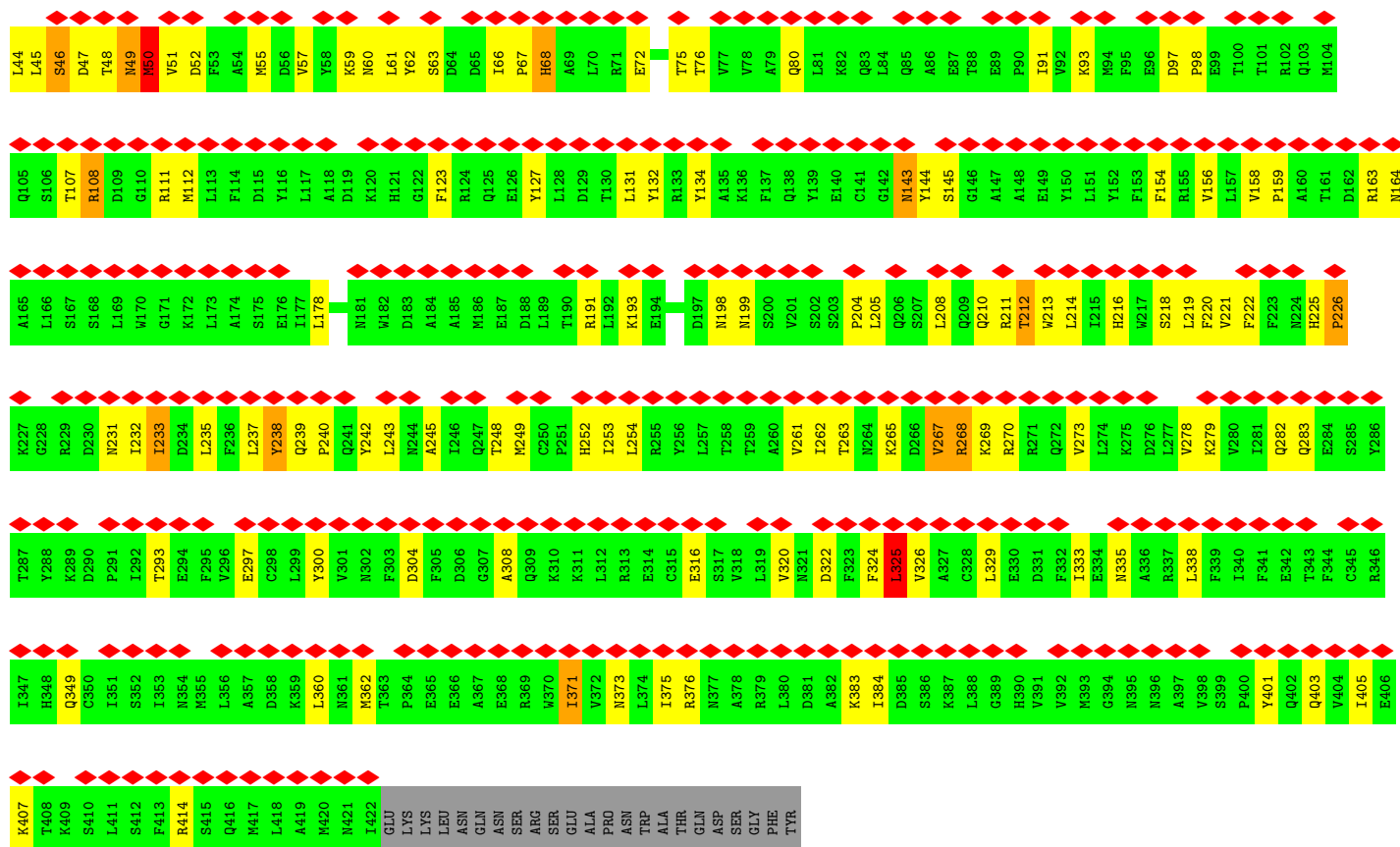


- Molecule 34: RACK1

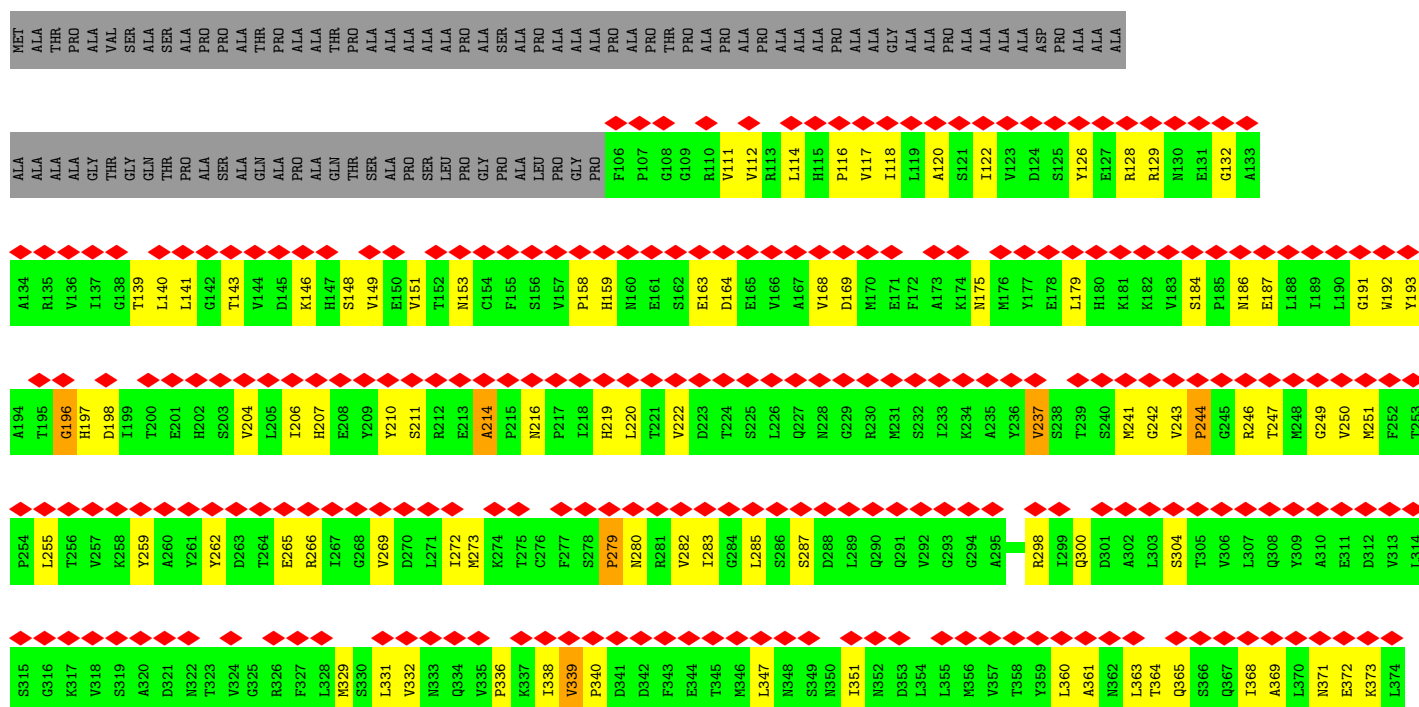


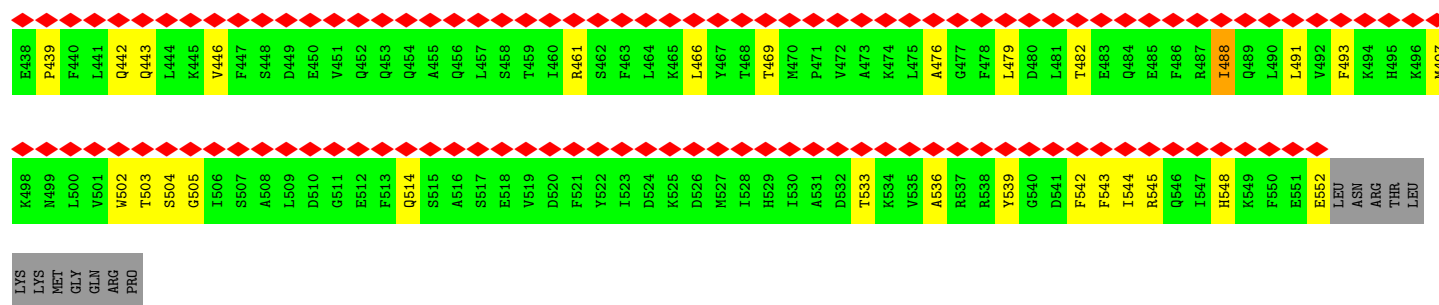
- Molecule 35: Eukaryotic translation initiation factor 3 subunit E



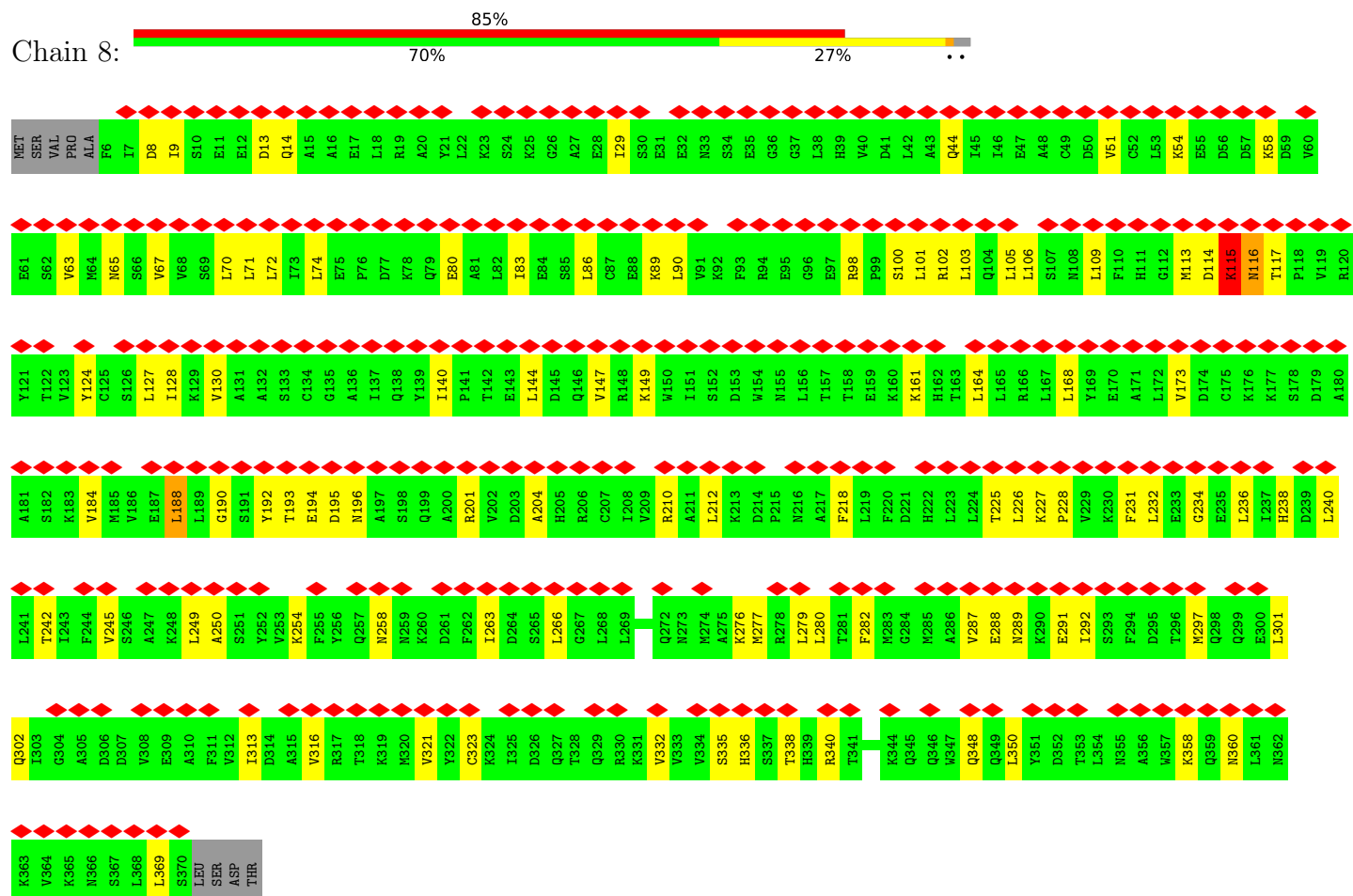


• Molecule 36: Eukaryotic translation initiation factor 3 subunit F

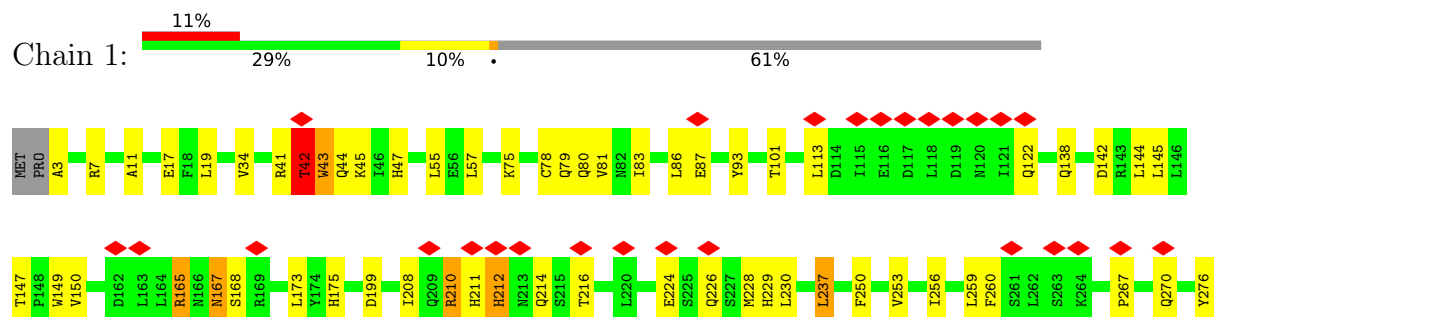


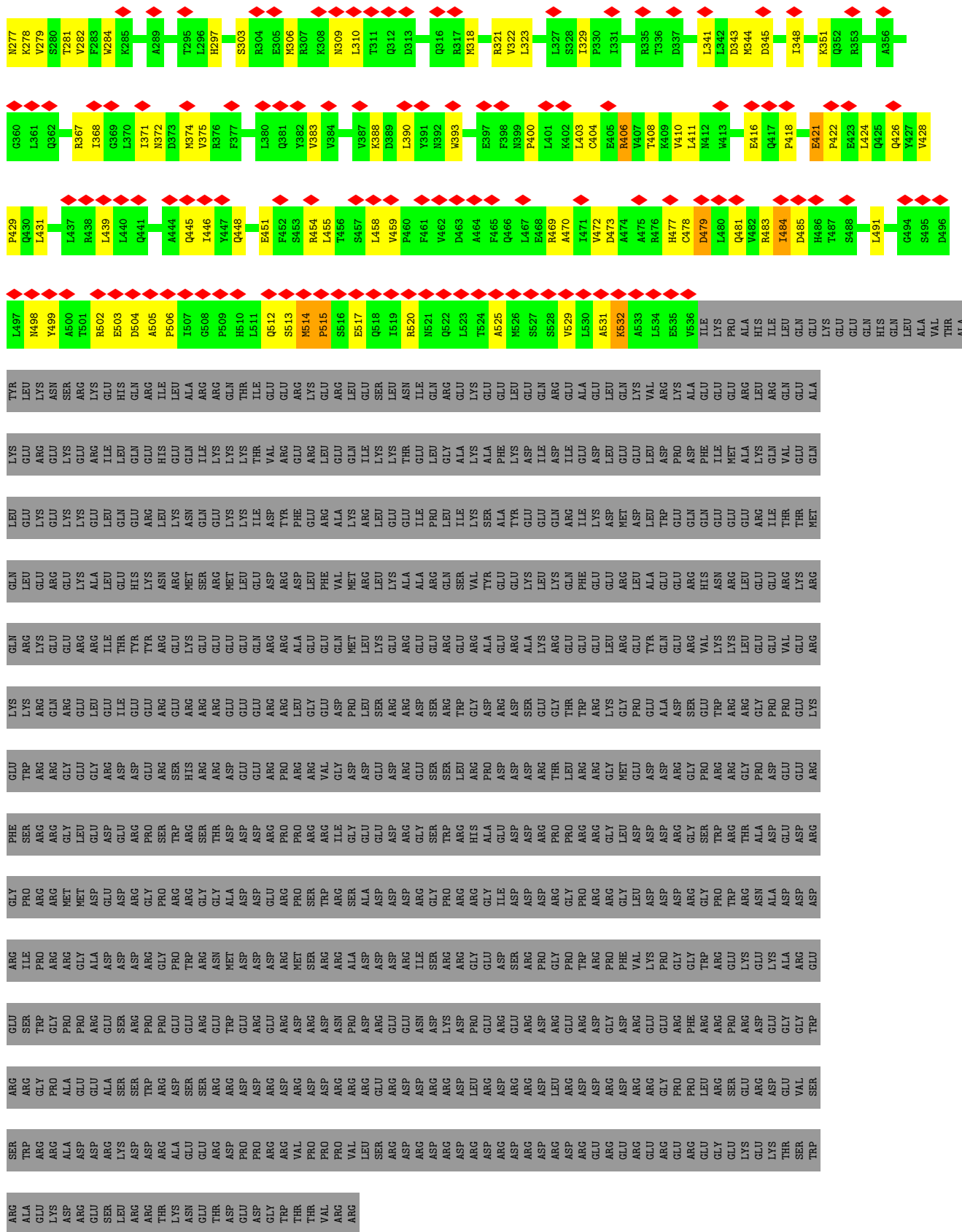


• Molecule 39: Eukaryotic translation initiation factor 3 subunit M

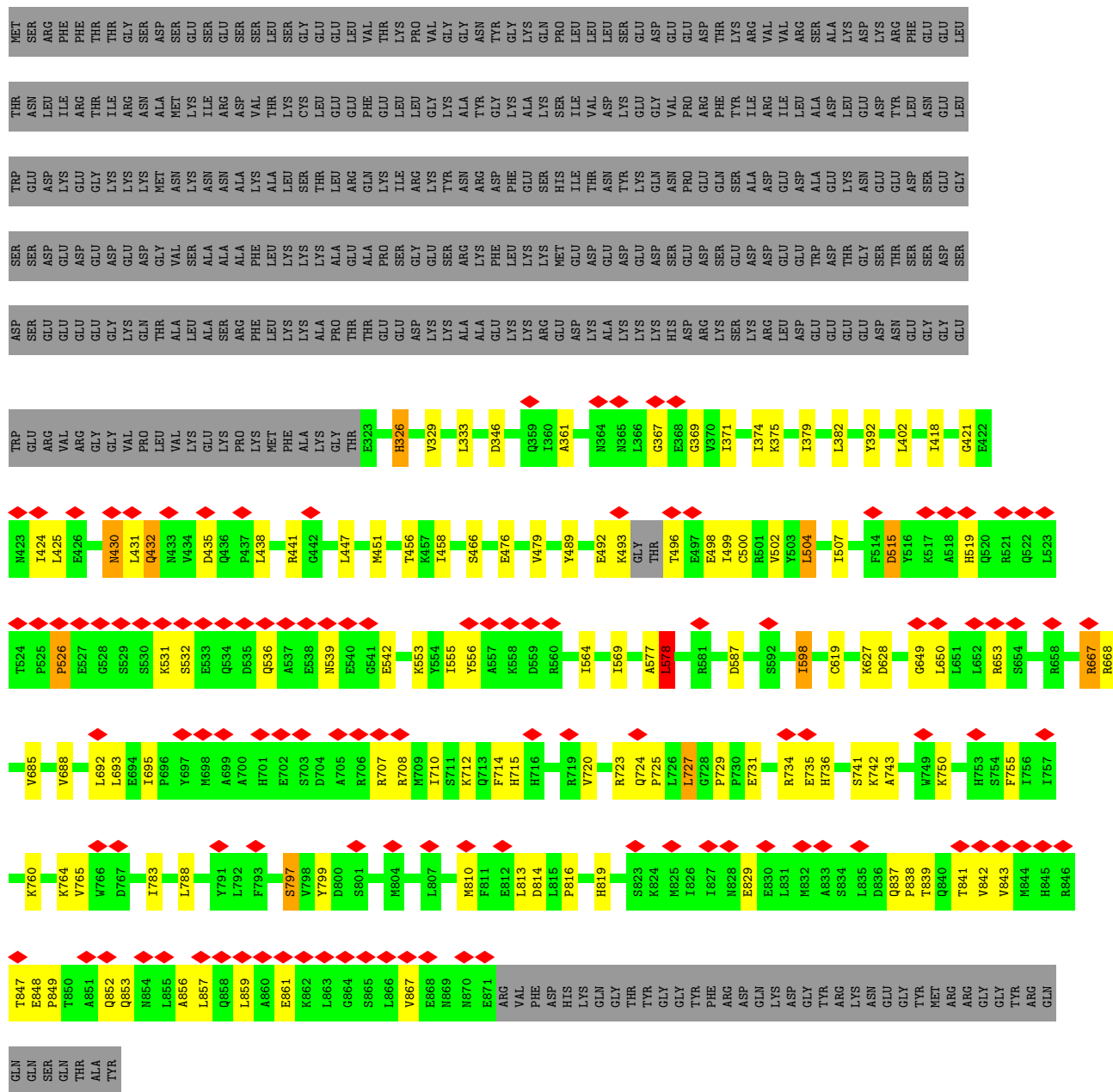


• Molecule 40: Eukaryotic translation initiation factor 3 subunit A

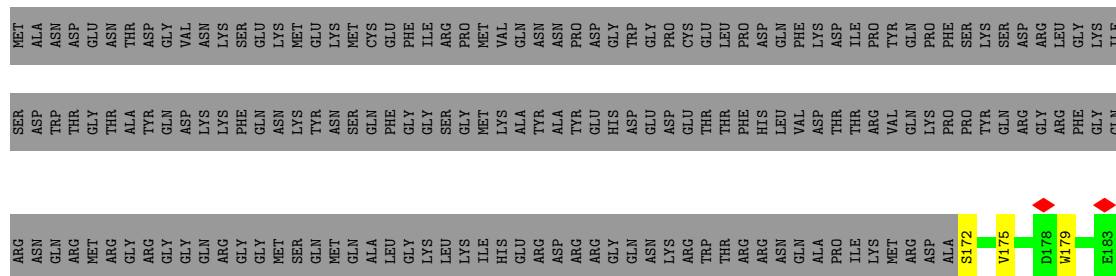


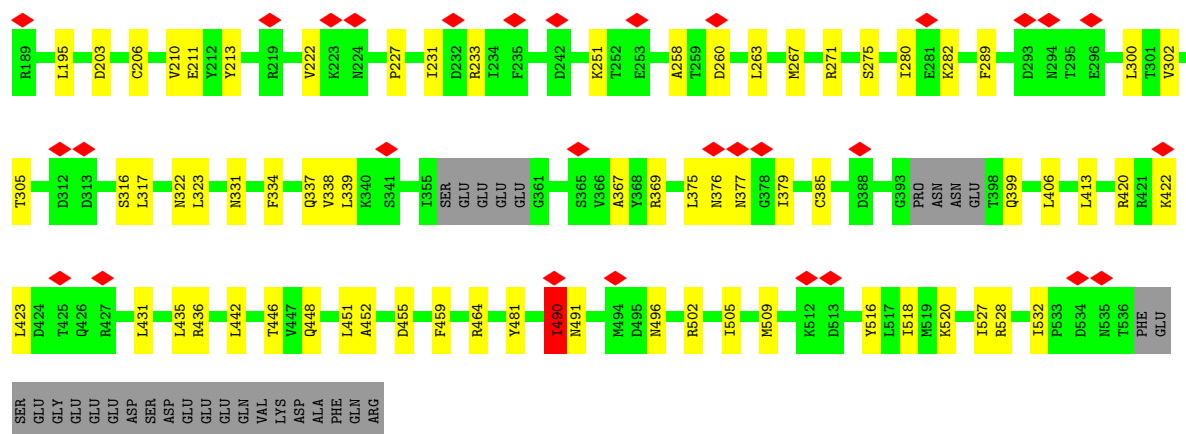


- Molecule 41: Eukaryotic translation initiation factor 3 subunit C

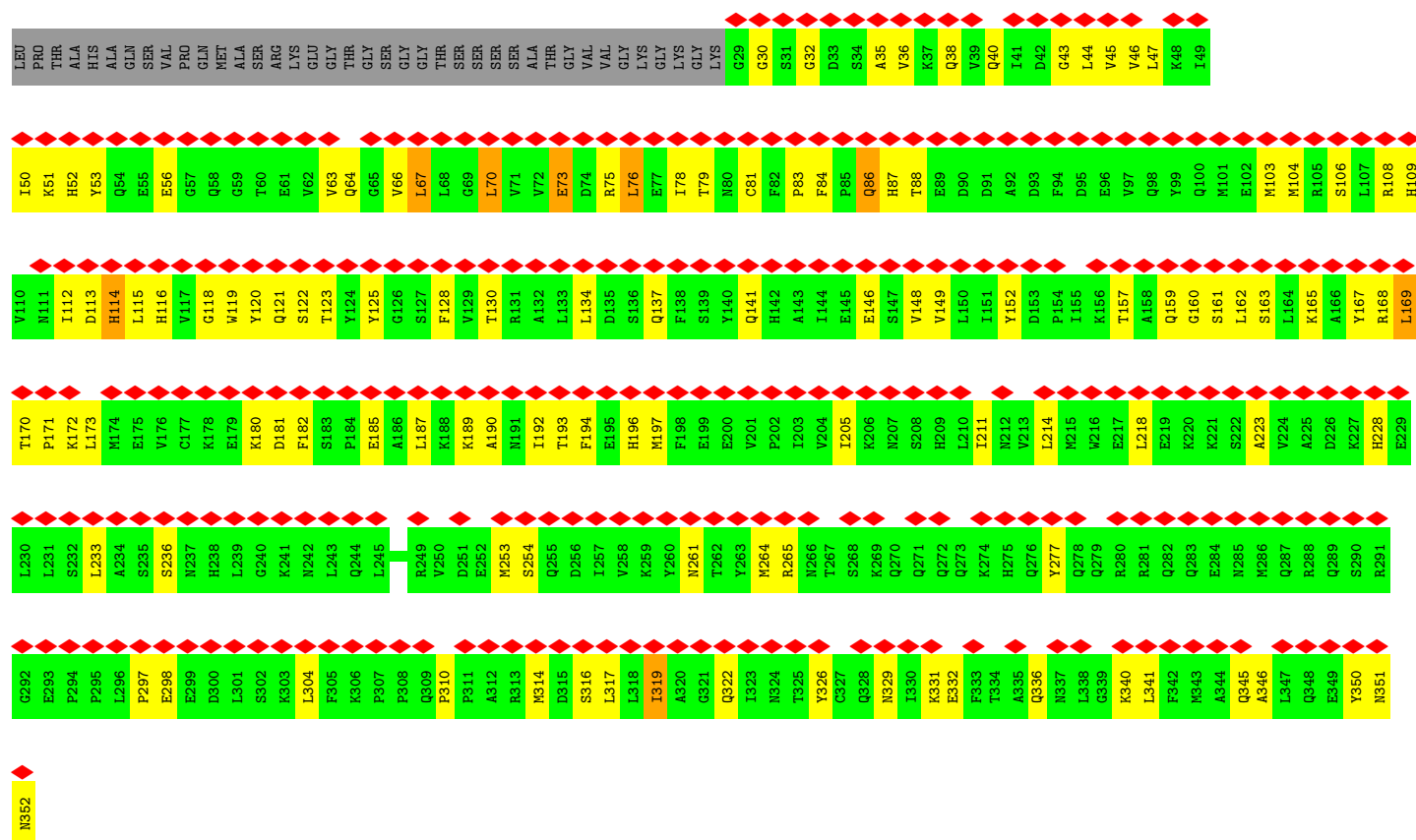
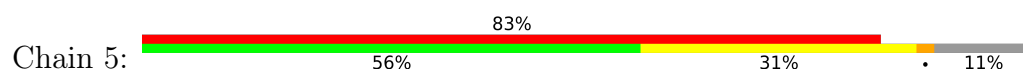


- Molecule 42: Eukaryotic translation initiation factor 3 subunit D

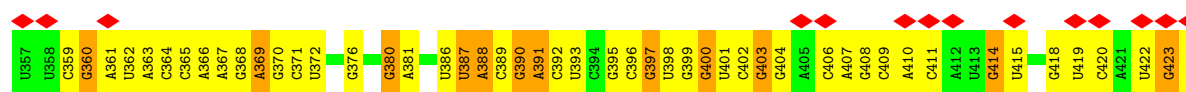




• Molecule 43: Eukaryotic translation initiation factor 3 subunit H



• Molecule 44: CrPV 5'-UTR IRES



A	A633	C556	U491	A425
A	A634	A557	G492	U426
G	A558	A569	A494	U427
U	U635	U560	C496	A428
C	U636	A561	A496	U429
U	G637	U562	C497	G430
U	C638	U562	C498	G431
U	A639	C565	U499	U432
C	C640	U569	G500	G433
A	A	U572	A501	U434
A	U642	U573	U502	U436
C	G643	U574	U503	U435
A	A644	U575	C503	C437
A	A	U576	A504	C438
C	A645	A577	C505	C439
A	A646	G578	U506	A440
A	C647	A579	U507	A443
A	A648	A579	A508	A
G	G	G580	G509	U446
G	A649	A581	C510	U452
A	A	A582	C511	G453
U	C650	G583	C512	C454
U	C651	A584	U513	U455
C	U653	A585	U514	C456
	A654	A586	G515	U457
	G655	A587	U516	A458
	G656	U588	G517	G459
	U657	A590	G518	U460
	C658	G591	A519	A461
	U659	U592	U520	U462
	U660	G593	A521	U463
	C661	G605	A526	G464
	C662	G606	C527	A465
	C663	U607	C530	A466
	U664	U608	C531	C467
	U665	U611	G532	U468
	U666	A615	C533	U469
	G667	A616	U534	U470
	A678	A617	G537	A471
	U679	G618	G538	G472
	A680	G619	A540	U473
	A681	A620	C541	G474
	G685	G621	A542	A475
	U686	A622	G543	U476
	G691	A623	U544	C477
	C695	G624	A545	A478
U	U	G625	G546	G479
U	U	U626	G547	U480
C	C	G627	A550	G481
A	A	A628	U551	U482
A	A	U629	A552	A483
U	U	U630	C553	C484
G	G	U631	C554	U485
U	U	U632	C555	U486
A	A			G487
G	G			C488
A	A			A489
U	U			A490
C	C			

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	23444	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	0.171	Depositor
Minimum map value	-0.101	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	0.21	0/40505	0.68	4/63112 (0.0%)
2	B	0.67	0/1743	0.77	0/2370
3	C	0.67	0/1756	0.78	0/2350
4	D	0.67	0/1754	0.78	0/2370
5	F	0.67	0/2114	0.79	0/2843
6	H	0.68	0/1946	0.83	0/2590
7	I	0.68	0/1510	0.78	0/2022
8	J	0.67	0/1715	0.81	0/2287
9	K	0.67	0/1550	0.82	0/2069
10	M	0.66	0/1195	0.79	0/1597
11	O	0.68	0/1226	0.78	0/1649
12	P	0.69	0/1029	0.83	0/1380
13	W	0.70	0/641	0.82	0/858
14	X	0.67	0/1051	0.80	0/1406
15	Y	0.69	0/1116	0.83	0/1490
16	Z	0.67	0/1028	0.80	0/1366
17	b	0.67	0/830	0.83	0/1112
18	c	0.67	0/665	0.82	0/891
19	f	0.68	0/462	0.83	0/607
20	E	0.69	0/1796	0.82	0/2417
21	G	0.70	0/1521	0.80	0/2046
22	L	0.65	0/834	0.78	0/1125
23	N	0.70	0/918	0.82	0/1233
24	Q	0.67	0/974	0.84	0/1301
25	R	0.69	0/1146	0.81	0/1534
26	S	0.69	0/1082	0.81	0/1452
27	T	0.68	0/1208	0.81	0/1618
28	U	0.69	0/1115	0.80	0/1493
29	V	0.68	0/805	0.81	0/1081
30	i	0.69	0/604	0.83	0/810
31	d	0.70	0/490	0.87	0/656
32	e	0.67	0/470	0.78	0/623

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	g	0.68	0/567	0.81	0/753
34	h	0.69	0/2486	0.81	0/3384
35	3	0.69	0/3538	0.85	2/4786 (0.0%)
36	4	0.71	0/2149	0.85	0/2920
37	6	0.70	0/1772	0.76	1/2396 (0.0%)
38	7	0.69	0/3185	0.78	0/4296
39	8	0.71	0/2963	0.85	3/3998 (0.1%)
40	1	0.68	0/4460	0.81	0/6034
41	2	0.69	0/4522	0.81	1/6102 (0.0%)
42	9	0.68	0/2921	0.79	0/3957
43	5	0.67	0/2675	0.81	0/3609
44	A	0.29	3/8053 (0.0%)	0.76	2/12543 (0.0%)
All	All	0.54	3/116090 (0.0%)	0.76	13/166536 (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
5	F	0	1
14	X	0	1
15	Y	0	1
21	G	0	2
34	h	0	1
35	3	0	12
36	4	0	7
37	6	0	1
39	8	0	3
40	1	0	4
41	2	0	5
42	9	0	2
43	5	0	2
All	All	0	42

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	A	509	G	C1'-N9	-6.20	1.38	1.46
44	A	576	U	C1'-N1	5.45	1.56	1.48
44	A	577	A	C1'-N9	-5.24	1.39	1.46

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	6	131	ILE	CB-CG1-CD1	7.29	134.31	113.90
1	a	688	U	C2'-C3'-O3'	6.84	124.65	113.70
35	3	384	ILE	CB-CG1-CD1	6.39	131.80	113.90
44	A	679	U	C2'-C3'-O3'	6.39	123.92	113.70
35	3	371	ILE	CB-CG1-CD1	6.04	130.80	113.90
39	8	9	ILE	CB-CG1-CD1	5.87	130.35	113.90
1	a	166	A	C2'-C3'-O3'	5.64	122.72	113.70
39	8	140	ILE	CB-CG1-CD1	-5.43	98.70	113.90
41	2	587	ASP	CB-CG-OD2	5.25	123.02	118.30
1	a	1137	U	C2'-C3'-O3'	5.23	122.06	113.70
44	A	485	U	C2'-C3'-O3'	5.21	122.04	113.70
1	a	532	C	C2'-C3'-O3'	5.17	121.98	113.70
39	8	115	LYS	CB-CA-C	5.01	120.42	110.40

There are no chirality outliers.

All (42) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
40	1	165	ARG	Peptide
40	1	416	GLU	Peptide
40	1	477	HIS	Peptide
40	1	514	MET	Peptide
41	2	496	THR	Peptide
41	2	649	GLY	Peptide
41	2	650	LEU	Peptide
41	2	693	LEU	Peptide
41	2	741	SER	Peptide
35	3	143	ASN	Peptide
35	3	22	LEU	Peptide
35	3	23	LEU	Peptide
35	3	237	LEU	Peptide
35	3	249	MET	Peptide
35	3	268	ARG	Peptide
35	3	279	LYS	Peptide
35	3	325	LEU	Peptide
35	3	49	ASN	Peptide
35	3	50	MET	Peptide
35	3	60	ASN	Peptide
35	3	61	LEU	Peptide
36	4	132	GLY	Peptide
36	4	186	ASN	Peptide

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Mol	Chain	Res	Type	Group
36	4	214	ALA	Peptide
36	4	241	MET	Peptide
36	4	242	GLY	Peptide
36	4	243	VAL	Peptide
36	4	279	PRO	Peptide
43	5	169	LEU	Peptide
43	5	304	LEU	Peptide
37	6	204	LYS	Peptide
39	8	115	LYS	Peptide
39	8	117	THR	Peptide
39	8	218	PHE	Peptide
42	9	375	LEU	Peptide
42	9	490	ILE	Peptide
5	F	155	LYS	Peptide
21	G	129	GLY	Peptide
21	G	130	ARG	Peptide
14	X	54	ASP	Peptide
15	Y	61	GLN	Peptide
34	h	36	ARG	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	36229	0	18304	0	0
2	B	1706	0	1698	17	0
3	C	1729	0	1803	7	0
4	D	1717	0	1812	19	0
5	F	2072	0	2175	5	0
6	H	1923	0	2089	4	0
7	I	1488	0	1582	10	0
8	J	1686	0	1772	8	0
9	K	1525	0	1640	9	0
10	M	1175	0	1249	3	0
11	O	1202	0	1289	0	0
12	P	1016	0	1039	4	0
13	W	634	0	629	6	0
14	X	1034	0	1080	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	Y	1098	0	1167	5	0
16	Z	1011	0	1083	3	0
17	b	816	0	867	0	0
18	c	651	0	672	0	0
19	f	457	0	502	0	0
20	E	1768	0	1866	10	0
21	G	1499	0	1540	8	0
22	L	810	0	836	3	0
23	N	908	0	939	7	0
24	Q	956	0	1002	16	0
25	R	1128	0	1195	2	0
26	S	1068	0	1121	7	0
27	T	1190	0	1249	3	0
28	U	1097	0	1130	5	0
29	V	795	0	862	6	0
30	i	598	0	656	0	0
31	d	488	0	514	0	0
32	e	459	0	452	0	0
33	g	555	0	567	0	0
34	h	2429	0	2386	0	0
35	3	3465	0	3446	77	0
36	4	2111	0	2105	73	0
37	6	1737	0	1706	21	0
38	7	3109	0	3084	44	0
39	8	2918	0	2950	59	0
40	1	4377	0	4433	95	0
41	2	4446	0	4446	94	0
42	9	2867	0	2838	43	0
43	5	2624	0	2592	100	0
44	A	7205	0	3626	61	0
45	a	1	0	0	0	0
46	b	1	0	0	0	0
All	All	109778	0	89993	765	0

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

All (765) 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)
40:1:42:THR:CG2	40:1:81:VAL:HG21	1.44	1.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:2:710:ILE:HB	41:2:714:PHE:CE2	1.61	1.35
41:2:438:LEU:CD2	41:2:493:LYS:HD3	1.56	1.35
41:2:438:LEU:HD21	41:2:493:LYS:CD	1.71	1.19
4:D:141:LEU:HD11	4:D:238:LYS:NZ	1.55	1.19
40:1:42:THR:HG21	40:1:81:VAL:HG21	1.18	1.17
41:2:438:LEU:HD21	41:2:493:LYS:HD3	1.10	1.07
40:1:42:THR:HG22	40:1:81:VAL:HG21	1.18	1.06
4:D:141:LEU:CD1	4:D:238:LYS:HZ1	1.70	1.04
40:1:42:THR:HG21	40:1:81:VAL:CG2	1.87	1.04
4:D:141:LEU:CD1	4:D:238:LYS:NZ	2.21	1.03
40:1:42:THR:CG2	40:1:81:VAL:CG2	2.37	1.02
40:1:42:THR:O	42:9:528:ARG:NH2	1.93	1.01
41:2:438:LEU:CG	41:2:493:LYS:HD3	1.90	1.00
41:2:710:ILE:HB	41:2:714:PHE:HE2	1.00	0.98
4:D:141:LEU:HD11	4:D:238:LYS:HZ2	1.26	0.96
41:2:712:LYS:HA	41:2:715:HIS:HD2	1.29	0.95
41:2:438:LEU:CD2	41:2:493:LYS:CD	2.36	0.93
41:2:710:ILE:O	41:2:714:PHE:HD2	1.54	0.90
44:A:365:C:H42	44:A:458:A:H2	1.21	0.85
42:9:435:LEU:HD11	42:9:490:ILE:HG22	1.59	0.85
41:2:492:GLU:O	41:2:493:LYS:HG3	1.82	0.80
41:2:710:ILE:CB	41:2:714:PHE:HE2	1.90	0.79
40:1:322:VAL:HG21	40:1:383:VAL:HA	1.65	0.78
36:4:279:PRO:HA	36:4:280:ASN:HB2	1.66	0.77
40:1:278:LYS:O	40:1:282:VAL:HG23	1.85	0.76
43:5:130:THR:O	43:5:134:LEU:HB2	1.86	0.76
41:2:432:GLN:O	41:2:432:GLN:NE2	2.18	0.75
35:3:268:ARG:N	35:3:269:LYS:HB3	2.03	0.74
40:1:3:ALA:N	44:A:583:G:HO2'	1.85	0.74
40:1:42:THR:HG22	40:1:81:VAL:CG2	2.10	0.73
41:2:438:LEU:HG	41:2:493:LYS:HD3	1.70	0.73
44:A:509:G:C6	44:A:510:C:C5	2.77	0.73
35:3:349:GLN:HB2	41:2:829:GLU:HB3	1.71	0.72
4:D:141:LEU:HD13	4:D:238:LYS:HZ1	1.55	0.71
40:1:277:ASN:O	40:1:281:THR:HG23	1.90	0.71
44:A:365:C:N4	44:A:458:A:H2	1.86	0.71
39:8:292:ILE:HG12	39:8:332:VAL:HG22	1.73	0.71
39:8:358:LYS:HG3	43:5:352:ASN:HD21	1.57	0.70
44:A:576:U:C5	44:A:577:A:H2'	2.27	0.69
35:3:158:VAL:HG22	35:3:159:PRO:HD2	1.73	0.69
41:2:710:ILE:O	41:2:714:PHE:CD2	2.42	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:A:397:G:H2'	44:A:398:U:O4'	1.93	0.68
43:5:66:VAL:HA	43:5:119:TRP:HA	1.76	0.68
40:1:343:ASP:CB	41:2:714:PHE:HE1	2.06	0.68
35:3:335:ASN:HA	35:3:338:LEU:HB3	1.75	0.67
41:2:438:LEU:CD2	41:2:493:LYS:CE	2.72	0.67
24:Q:37:TYR:OH	24:Q:45:LEU:HD12	1.94	0.67
35:3:375:ILE:HG21	38:7:466:LEU:HD21	1.76	0.67
41:2:867:VAL:HG12	41:2:867:VAL:O	1.94	0.67
41:2:438:LEU:CD2	41:2:493:LYS:NZ	2.58	0.67
41:2:710:ILE:CB	41:2:714:PHE:CE2	2.58	0.67
35:3:55:MET:SD	35:3:59:LYS:NZ	2.67	0.67
44:A:360:G:H1	44:A:463:U:H3	1.44	0.66
36:4:168:VAL:HG21	36:4:206:ILE:HG23	1.78	0.66
44:A:509:G:N1	44:A:510:C:C5	2.63	0.66
40:1:343:ASP:OD2	41:2:714:PHE:CZ	2.49	0.65
8:J:101:ILE:HD12	8:J:190:LEU:HD11	1.78	0.65
36:4:373:LYS:HB3	38:7:544:ILE:HG21	1.79	0.65
39:8:212:LEU:HD21	39:8:263:ILE:HG21	1.79	0.65
43:5:44:LEU:HD21	43:5:214:LEU:HD21	1.80	0.64
40:1:237:LEU:HD11	40:1:253:VAL:HG12	1.79	0.64
41:2:685:VAL:HA	41:2:688:VAL:HG12	1.80	0.63
42:9:172:SER:N	42:9:275:SER:HG	1.96	0.63
44:A:493:U:OP1	44:A:516:U:N3	2.31	0.63
35:3:50:MET:O	35:3:52:ASP:N	2.30	0.63
44:A:402:C:H3'	44:A:403:G:H5'	1.80	0.63
43:5:297:PRO:HA	43:5:298:GLU:HB2	1.81	0.63
2:B:65:ILE:HD12	2:B:178:LEU:HD21	1.81	0.62
35:3:268:ARG:H	35:3:269:LYS:HB3	1.63	0.62
38:7:348:SER:HA	38:7:349:MET:CB	2.29	0.62
40:1:42:THR:O	42:9:528:ARG:CZ	2.47	0.62
41:2:432:GLN:HE21	41:2:432:GLN:C	2.01	0.62
40:1:11:ALA:HB2	40:1:34:VAL:HG21	1.80	0.62
40:1:341:LEU:HA	40:1:345:ASP:HB2	1.79	0.62
35:3:218:SER:CB	35:3:232:ILE:HG12	2.29	0.62
35:3:108:ARG:NH2	35:3:134:TYR:OH	2.32	0.62
40:1:19:LEU:HD21	40:1:57:LEU:HD21	1.81	0.62
29:V:46:LYS:HG3	29:V:101:ILE:HD11	1.82	0.62
44:A:492:G:H3'	44:A:516:U:H3	1.64	0.62
35:3:243:LEU:HB2	35:3:248:THR:HG22	1.82	0.61
42:9:271:ARG:NH2	42:9:491:ASN:O	2.34	0.61
43:5:76:LEU:O	43:5:76:LEU:HD12	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:8:124:TYR:CD2	39:8:164:LEU:HD13	2.35	0.61
41:2:438:LEU:HD23	41:2:493:LYS:NZ	2.16	0.61
4:D:211:LYS:O	4:D:215:LEU:HG	2.00	0.61
38:7:240:ILE:HG13	38:7:257:ALA:HB2	1.82	0.61
40:1:403:LEU:HD22	40:1:439:LEU:HD21	1.83	0.61
40:1:529:VAL:HG12	43:5:233:LEU:HD21	1.82	0.61
44:A:365:C:N4	44:A:458:A:C2	2.66	0.61
36:4:159:HIS:CE1	36:4:168:VAL:HG22	2.36	0.60
41:2:712:LYS:HA	41:2:715:HIS:CD2	2.21	0.60
40:1:348:ILE:HA	40:1:351:LYS:HB2	1.84	0.60
41:2:438:LEU:HD23	41:2:493:LYS:CE	2.31	0.60
41:2:438:LEU:HD23	41:2:493:LYS:HZ3	1.66	0.60
36:4:336:PRO:HB3	43:5:350:TYR:O	2.02	0.60
41:2:735:GLU:HB3	41:2:750:LYS:HB3	1.84	0.60
21:G:201:LYS:HA	21:G:204:ARG:HD3	1.84	0.60
35:3:220:PHE:HB2	35:3:325:LEU:HB2	1.84	0.59
35:3:233:ILE:O	35:3:238:TYR:HB2	2.03	0.59
36:4:112:VAL:HG23	36:4:255:LEU:HD13	1.84	0.59
41:2:783:ILE:HD13	41:2:813:LEU:HD22	1.83	0.59
43:5:187:LEU:HA	43:5:190:ALA:HB3	1.84	0.59
21:G:154:LEU:HD13	21:G:177:LEU:HD21	1.84	0.59
39:8:13:ASP:HA	39:8:14:GLN:C	2.23	0.59
41:2:515:ASP:O	41:2:519:HIS:N	2.33	0.59
36:4:126:TYR:O	36:4:129:ARG:NE	2.30	0.59
42:9:406:LEU:HD21	42:9:442:LEU:HD11	1.85	0.59
42:9:435:LEU:HD11	42:9:490:ILE:CG2	2.32	0.59
40:1:479:ASP:HA	40:1:505:ALA:HB2	1.85	0.59
36:4:141:LEU:HB3	36:4:187:GLU:HB3	1.85	0.59
40:1:383:VAL:HG13	40:1:388:LYS:HG2	1.85	0.59
22:L:11:ILE:HD11	22:L:40:VAL:HG11	1.83	0.58
35:3:158:VAL:HG21	35:3:164:ASN:HB3	1.86	0.58
42:9:258:ALA:HB1	42:9:263:LEU:HD13	1.84	0.58
24:Q:81:ARG:NH2	24:Q:117:GLY:O	2.36	0.58
41:2:367:GLY:HA2	41:2:371:ILE:HD11	1.83	0.58
36:4:116:PRO:HG2	36:4:269:VAL:HG21	1.86	0.58
43:5:125:TYR:CD2	43:5:128:PHE:HB2	2.38	0.58
36:4:304:SER:O	39:8:348:GLN:NE2	2.35	0.58
40:1:343:ASP:HB2	41:2:714:PHE:HE1	1.68	0.58
36:4:283:ILE:O	43:5:161:SER:OG	2.22	0.58
44:A:402:C:H3'	44:A:403:G:C5'	2.34	0.58
38:7:348:SER:HA	38:7:349:MET:HB3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:3:131:LEU:HG	35:3:159:PRO:HD3	1.85	0.57
40:1:512:GLN:O	40:1:514:MET:N	2.35	0.57
43:5:108:ARG:HD3	43:5:113:ASP:HA	1.86	0.57
7:I:100:ILE:HD11	7:I:122:LEU:HA	1.86	0.57
36:4:369:ALA:HA	36:4:373:LYS:HE2	1.84	0.57
43:5:180:LYS:HD3	43:5:319:ILE:HD13	1.85	0.57
15:Y:61:GLN:O	15:Y:63:ASN:N	2.37	0.57
41:2:438:LEU:HD21	41:2:493:LYS:CE	2.32	0.57
35:3:49:ASN:HA	35:3:50:MET:HB2	1.87	0.57
43:5:350:TYR:O	43:5:352:ASN:N	2.38	0.57
39:8:242:THR:HG23	39:8:258:ASN:HB3	1.87	0.56
41:2:379:ILE:HD11	41:2:447:LEU:HD13	1.88	0.56
43:5:170:THR:O	43:5:173:LEU:HB2	2.04	0.56
43:5:261:ASN:O	43:5:265:ARG:HG2	2.05	0.56
29:V:32:LEU:HD21	29:V:87:ARG:HG2	1.87	0.56
36:4:269:VAL:HG22	43:5:47:LEU:HD21	1.88	0.56
4:D:141:LEU:CD2	4:D:238:LYS:HZ1	2.17	0.56
41:2:476:GLU:HA	41:2:479:VAL:HG12	1.86	0.56
35:3:263:THR:HG22	35:3:335:ASN:HB2	1.87	0.56
21:G:20:PHE:CZ	21:G:69:VAL:HG11	2.40	0.56
35:3:221:VAL:HG13	35:3:225:HIS:HB2	1.87	0.56
36:4:122:ILE:HG12	36:4:193:TYR:CE1	2.41	0.55
39:8:192:TYR:O	39:8:193:THR:OG1	2.21	0.55
40:1:469:ARG:HA	40:1:472:VAL:HG12	1.88	0.55
42:9:379:ILE:HG21	42:9:505:ILE:HD12	1.87	0.55
36:4:140:LEU:HD22	36:4:220:LEU:CD1	2.36	0.55
40:1:216:THR:HG23	40:1:224:GLU:HB2	1.87	0.55
36:4:365:GLN:HA	43:5:329:ASN:HD21	1.71	0.55
38:7:539:TYR:HA	38:7:542:PHE:CD2	2.41	0.55
40:1:270:GLN:HE22	40:1:309:ASN:HD22	1.54	0.55
35:3:240:PRO:O	35:3:253:ILE:HG12	2.06	0.55
38:7:245:GLU:HA	38:7:439:PRO:HG2	1.88	0.55
16:Z:110:ARG:NH2	16:Z:114:MET:SD	2.79	0.55
36:4:364:THR:O	36:4:368:ILE:HG12	2.06	0.55
43:5:173:LEU:HD21	43:5:180:LYS:NZ	2.22	0.55
38:7:488:ILE:HG22	38:7:491:LEU:HB2	1.87	0.55
4:D:233:LEU:HD12	4:D:233:LEU:O	2.07	0.55
38:7:545:ARG:NH2	43:5:322:GLN:HE22	2.04	0.55
41:2:816:PRO:HA	41:2:819:HIS:HB2	1.88	0.55
42:9:222:VAL:HG21	42:9:422:LYS:O	2.07	0.55
42:9:280:ILE:HB	42:9:516:TYR:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:9:316:SER:O	42:9:322:ASN:ND2	2.39	0.55
38:7:421:LEU:HB3	38:7:443:GLN:HG2	1.89	0.55
42:9:305:THR:OG1	42:9:436:ARG:O	2.23	0.55
43:5:86:GLN:O	43:5:88:THR:OG1	2.23	0.55
42:9:420:ARG:NH2	42:9:464:ARG:O	2.40	0.54
40:1:44:GLN:H	40:1:47:HIS:HD2	1.54	0.54
40:1:229:HIS:HB3	40:1:259:LEU:HD11	1.89	0.54
43:5:141:GLN:HE22	43:5:168:ARG:HA	1.72	0.54
38:7:370:LEU:HA	38:7:412:LEU:HD21	1.90	0.54
40:1:55:LEU:HD13	40:1:93:TYR:HB2	1.89	0.54
41:2:493:LYS:HG3	41:2:498:GLU:OE2	2.06	0.54
36:4:360:LEU:HA	36:4:363:LEU:HB2	1.89	0.54
39:8:80:GLU:HA	39:8:83:ILE:HG22	1.88	0.54
40:1:343:ASP:OD2	41:2:714:PHE:HZ	1.89	0.54
16:Z:35:VAL:HG23	16:Z:40:ILE:HD11	1.89	0.54
2:B:19:LEU:HD11	26:S:106:LEU:HD21	1.89	0.54
37:6:15:LEU:HD13	37:6:45:GLU:HB3	1.89	0.54
35:3:262:ILE:HG12	35:3:267:VAL:HG11	1.90	0.54
37:6:48:LEU:HD13	37:6:84:LEU:HB3	1.89	0.54
10:M:47:PRO:HG2	10:M:116:CYS:SG	2.48	0.53
40:1:210:ARG:HG2	40:1:212:HIS:CD2	2.43	0.53
39:8:44:GLN:HG2	39:8:72:LEU:HD21	1.90	0.53
39:8:201:ARG:NH1	39:8:236:LEU:HD21	2.23	0.53
40:1:42:THR:HB	42:9:528:ARG:HH12	1.74	0.53
43:5:137:GLN:HG3	43:5:169:LEU:HD23	1.90	0.53
3:C:86:LEU:HB3	3:C:98:THR:HB	1.91	0.53
42:9:260:ASP:HB3	42:9:448:GLN:HG2	1.89	0.53
43:5:119:TRP:HE1	43:5:137:GLN:HB3	1.73	0.53
4:D:273:LEU:HA	4:D:276:THR:HG22	1.89	0.53
36:4:158:PRO:HG3	43:5:109:HIS:HB3	1.91	0.53
26:S:98:VAL:HG13	26:S:98:VAL:O	2.08	0.53
43:5:122:SER:HB3	43:5:123:THR:HA	1.90	0.53
5:F:44:LEU:HD13	5:F:72:ILE:HD11	1.91	0.53
36:4:118:ILE:O	36:4:122:ILE:HG13	2.09	0.53
43:5:79:THR:HG21	43:5:112:ILE:HD13	1.91	0.53
6:H:2:LYS:HD3	6:H:15:LEU:HD11	1.90	0.53
25:R:53:GLU:OE1	25:R:85:ARG:NH2	2.42	0.53
41:2:500:CYS:HB3	41:2:555:ILE:HD11	1.91	0.53
43:5:45:VAL:HG21	43:5:78:ILE:HB	1.91	0.53
26:S:31:ASN:HA	26:S:34:VAL:HG12	1.91	0.52
39:8:195:ASP:HA	39:8:196:ASN:C	2.29	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:1:525:ALA:CA	43:5:345:GLN:HE22	2.21	0.52
41:2:326:HIS:HA	41:2:329:VAL:HG22	1.91	0.52
35:3:405:ILE:HG12	36:4:360:LEU:HD11	1.91	0.52
41:2:432:GLN:NE2	41:2:432:GLN:HA	2.24	0.52
43:5:190:ALA:HA	43:5:193:THR:HA	1.92	0.52
39:8:227:LYS:N	39:8:228:PRO:HD3	2.25	0.52
43:5:122:SER:CB	43:5:123:THR:HA	2.40	0.52
35:3:46:SER:HA	35:3:216:HIS:CD2	2.44	0.52
38:7:536:ALA:HA	38:7:539:TYR:HB3	1.92	0.52
39:8:276:LYS:O	39:8:279:LEU:HG	2.10	0.52
44:A:656:G:O2'	44:A:658:C:OP2	2.25	0.52
41:2:418:ILE:HG23	41:2:441:ARG:HD2	1.91	0.52
44:A:560:U:O2'	44:A:561:A:O5'	2.24	0.52
8:J:165:GLN:HE22	8:J:195:LEU:HD11	1.74	0.52
43:5:316:SER:HA	43:5:319:ILE:HD12	1.92	0.52
44:A:536:A:N3	44:A:536:A:H2'	2.71	0.52
38:7:238:SER:HA	38:7:423:PRO:HB2	1.92	0.52
41:2:361:ALA:HB1	41:2:367:GLY:HA2	1.91	0.52
41:2:432:GLN:NE2	41:2:432:GLN:CA	2.73	0.52
44:A:415:U:O2	44:A:430:G:N2	2.43	0.52
39:8:103:LEU:HD13	39:8:127:LEU:HD13	1.92	0.52
40:1:445:GLN:HA	40:1:448:GLN:HE22	1.75	0.52
8:J:61:ASP:O	8:J:78:ILE:N	2.43	0.51
35:3:219:LEU:HD11	35:3:324:PHE:CE1	2.44	0.51
10:M:40:ILE:HD11	10:M:68:ILE:HG12	1.91	0.51
35:3:208:LEU:HD22	35:3:243:LEU:HB3	1.91	0.51
39:8:263:ILE:HG22	39:8:266:LEU:HD22	1.92	0.51
43:5:181:ASP:HB2	43:5:185:GLU:HB2	1.91	0.51
21:G:40:ALA:HB1	21:G:45:TYR:CG	2.46	0.51
36:4:159:HIS:ND1	36:4:168:VAL:HG22	2.26	0.51
44:A:368:G:H2'	44:A:369:A:O4'	2.10	0.51
4:D:144:SER:HB3	4:D:149:THR:HG23	1.92	0.51
38:7:341:LEU:HD22	38:7:343:ILE:HB	1.92	0.51
39:8:212:LEU:CD2	39:8:263:ILE:HG21	2.40	0.51
36:4:347:LEU:HD23	43:5:346:ALA:HB1	1.92	0.51
36:4:339:VAL:N	36:4:340:PRO:HD3	2.26	0.51
41:2:867:VAL:O	41:2:867:VAL:CG1	2.58	0.51
42:9:210:VAL:HG13	42:9:367:ALA:HB2	1.93	0.51
43:5:159:GLN:N	43:5:160:GLY:HA3	2.25	0.51
29:V:40:ILE:HD11	29:V:53:PRO:HD3	1.93	0.51
39:8:51:VAL:O	39:8:89:LYS:NZ	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:9:399:GLN:HE22	42:9:455:ASP:HB3	1.76	0.51
42:9:446:THR:HG21	42:9:490:ILE:HD11	1.93	0.51
42:9:490:ILE:HG13	42:9:491:ASN:H	1.76	0.51
23:N:79:VAL:HG12	23:N:80:ASP:H	1.75	0.51
40:1:80:GLN:O	42:9:175:VAL:HB	2.11	0.51
43:5:103:MET:O	43:5:106:SER:OG	2.27	0.51
44:A:423:G:H2'	44:A:423:G:N3	2.26	0.51
4:D:135:GLY:HA2	4:D:165:VAL:HG22	1.93	0.50
40:1:393:TRP:HB3	40:1:403:LEU:HD11	1.93	0.50
40:1:372:ASN:HA	40:1:375:VAL:HB	1.93	0.50
3:C:62:LEU:HD23	3:C:91:VAL:HG21	1.91	0.50
20:E:115:VAL:HG11	20:E:142:LEU:HD21	1.94	0.50
39:8:204:ALA:HB1	39:8:240:LEU:HD11	1.93	0.50
41:2:492:GLU:O	41:2:493:LYS:CG	2.57	0.50
37:6:87:CYS:HA	38:7:446:VAL:HG13	1.93	0.50
44:A:491:U:H2'	44:A:492:G:O4'	2.11	0.50
42:9:300:LEU:HD11	42:9:331:ASN:HD22	1.76	0.50
29:V:98:VAL:HA	29:V:101:ILE:HD12	1.94	0.50
36:4:114:LEU:HD12	36:4:118:ILE:HB	1.92	0.50
38:7:545:ARG:HH21	43:5:322:GLN:HE22	1.59	0.50
40:1:226:GLN:HA	40:1:230:LEU:HD23	1.93	0.50
40:1:318:MET:O	40:1:322:VAL:HG22	2.11	0.50
39:8:225:THR:HG23	39:8:226:LEU:HG	1.94	0.50
41:2:504:LEU:HA	41:2:507:ILE:HG12	1.94	0.50
44:A:519:A:N6	44:A:575:U:O4	2.45	0.50
35:3:123:PHE:O	35:3:127:TYR:HB2	2.11	0.50
39:8:63:VAL:HG11	39:8:98:ARG:HB3	1.93	0.50
44:A:535:C:H2'	44:A:536:A:H8	1.76	0.50
35:3:19:VAL:HG21	35:3:45:LEU:HA	1.92	0.50
35:3:335:ASN:HA	35:3:338:LEU:CB	2.40	0.50
36:4:372:GLU:O	36:4:375:VAL:HB	2.12	0.50
37:6:165:LEU:HD13	37:6:169:GLN:HB3	1.94	0.50
35:3:320:VAL:HA	35:3:329:LEU:HD11	1.93	0.49
41:2:438:LEU:HD21	41:2:493:LYS:NZ	2.26	0.49
14:X:52:ILE:HG22	14:X:61:ILE:HG12	1.93	0.49
36:4:112:VAL:HG22	36:4:149:VAL:HB	1.94	0.49
43:5:170:THR:HB	43:5:171:PRO:HD2	1.93	0.49
21:G:73:THR:O	21:G:89:THR:HG21	2.11	0.49
35:3:76:THR:O	35:3:80:GLN:HG2	2.12	0.49
37:6:45:GLU:HB2	38:7:294:LEU:HD23	1.92	0.49
38:7:469:THR:HG23	38:7:514:GLN:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:5:162:LEU:HD21	43:5:165:LYS:HB3	1.95	0.49
44:A:581:A:N3	44:A:581:A:H2'	2.28	0.49
43:5:30:GLY:HA3	43:5:38:GLN:HB2	1.94	0.49
43:5:122:SER:HA	43:5:152:TYR:O	2.12	0.49
35:3:97:ASP:N	35:3:98:PRO:HD2	2.27	0.49
20:E:105:LEU:HB2	20:E:122:VAL:HG21	1.94	0.49
40:1:306:MET:O	40:1:310:LEU:N	2.45	0.49
40:1:400:PRO:HB3	40:1:446:ILE:HG21	1.95	0.49
36:4:361:ALA:HB1	43:5:332:GLU:HB2	1.94	0.49
40:1:75:LYS:HG2	40:1:86:LEU:HD11	1.94	0.49
40:1:329:ILE:HG21	40:1:371:ILE:HB	1.94	0.49
43:5:185:GLU:HB3	43:5:189:LYS:HE2	1.94	0.49
22:L:59:LYS:HB3	22:L:70:TYR:HB2	1.95	0.49
25:R:57:LEU:HD11	25:R:115:TYR:CD2	2.48	0.49
35:3:213:TRP:HA	35:3:216:HIS:CD2	2.48	0.49
36:4:140:LEU:HD22	36:4:220:LEU:HD11	1.94	0.49
43:5:50:ILE:HG12	43:5:152:TYR:CE2	2.48	0.49
5:F:183:VAL:HG11	5:F:220:THR:HG21	1.95	0.49
24:Q:51:ARG:NH2	24:Q:55:SER:OG	2.45	0.49
23:N:69:CYS:SG	23:N:76:LEU:HD11	2.53	0.48
35:3:225:HIS:N	35:3:226:PRO:HD2	2.29	0.48
40:1:428:VAL:N	40:1:429:PRO:HD2	2.29	0.48
42:9:490:ILE:HG13	42:9:491:ASN:N	2.29	0.48
29:V:25:THR:HG22	29:V:84:ILE:HD11	1.96	0.48
35:3:75:THR:HG21	35:3:143:ASN:HB3	1.95	0.48
43:5:173:LEU:HD11	43:5:180:LYS:HD2	1.94	0.48
2:B:17:LYS:HB3	2:B:173:LEU:HD11	1.95	0.48
24:Q:17:TYR:HB3	24:Q:25:LEU:HD11	1.96	0.48
36:4:204:VAL:HA	36:4:207:HIS:HB2	1.93	0.48
40:1:101:THR:HG22	40:1:149:TRP:HB3	1.94	0.48
43:5:67:LEU:HD12	43:5:78:ILE:HD11	1.96	0.48
39:8:101:LEU:HD12	39:8:102:ARG:N	2.28	0.48
43:5:118:GLY:HA3	43:5:148:VAL:O	2.14	0.48
43:5:167:TYR:OH	43:5:196:HIS:O	2.30	0.48
23:N:31:LEU:C	23:N:31:LEU:HD12	2.34	0.48
35:3:10:ILE:HG13	35:3:204:PRO:HB3	1.96	0.48
36:4:184:SER:HB2	43:5:52:HIS:HE2	1.77	0.48
36:4:272:ILE:HG23	43:5:43:GLY:HA3	1.95	0.48
36:4:287:SER:HA	43:5:341:LEU:HD11	1.95	0.48
41:2:685:VAL:HG13	41:2:708:ARG:HG2	1.96	0.48
44:A:389:C:H2'	44:A:390:G:O4'	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:4:265:GLU:HA	43:5:50:ILE:HG21	1.96	0.48
40:1:484:ILE:HG22	40:1:485:ASP:HB2	1.96	0.48
40:1:451:GLU:O	40:1:454:ARG:HG2	2.14	0.48
42:9:213:TYR:HA	42:9:339:LEU:HD12	1.95	0.48
9:K:61:LEU:HD13	9:K:94:LEU:HB3	1.96	0.48
37:6:11:VAL:HG21	37:6:32:TYR:CG	2.48	0.48
43:5:104:MET:O	43:5:108:ARG:HG2	2.12	0.48
35:3:243:LEU:O	35:3:282:GLN:NE2	2.47	0.48
44:A:574:U:H2'	44:A:575:U:C6	2.48	0.48
10:M:40:ILE:CD1	10:M:61:PRO:HB2	2.44	0.47
28:U:28:LEU:O	28:U:30:VAL:N	2.47	0.47
43:5:172:LYS:HB3	43:5:194:PHE:HA	1.95	0.47
24:Q:50:ARG:HB3	24:Q:54:HIS:HB3	1.96	0.47
35:3:156:VAL:HG11	35:3:191:ARG:CZ	2.43	0.47
29:V:26:SER:OG	29:V:32:LEU:HB2	2.15	0.47
39:8:277:MET:HG3	39:8:301:LEU:HD22	1.96	0.47
40:1:284:TRP:CZ2	40:1:426:GLN:HB3	2.50	0.47
41:2:727:LEU:HB3	41:2:729:PRO:HD2	1.95	0.47
35:3:208:LEU:HA	35:3:243:LEU:HD22	1.96	0.47
38:7:363:GLN:HA	38:7:419:LYS:HD3	1.96	0.47
40:1:43:TRP:CH2	40:1:45:LYS:HD2	2.49	0.47
41:2:598:ILE:O	41:2:598:ILE:HG23	2.15	0.47
41:2:839:THR:HB	41:2:841:THR:HG23	1.96	0.47
42:9:385:CYS:HB3	42:9:452:ALA:HA	1.95	0.47
35:3:212:THR:HG22	35:3:216:HIS:CE1	2.49	0.47
38:7:476:ALA:HA	38:7:479:LEU:HD12	1.96	0.47
36:4:282:VAL:HG13	36:4:285:LEU:HB2	1.95	0.47
43:5:157:THR:HG21	43:5:163:SER:HA	1.97	0.47
2:B:173:LEU:HD12	26:S:91:LEU:HD13	1.97	0.47
20:E:74:GLN:HE22	20:E:81:GLU:HB2	1.80	0.47
38:7:284:LEU:HD13	38:7:299:LEU:HD13	1.97	0.47
38:7:376:THR:O	38:7:461:ARG:NH1	2.48	0.47
40:1:514:MET:N	40:1:515:PRO:CD	2.78	0.47
43:5:197:MET:HE1	43:5:326:TYR:HB3	1.97	0.47
44:A:513:U:O2'	44:A:514:U:O4'	2.29	0.47
2:B:30:LEU:HD13	2:B:38:ILE:CD1	2.45	0.47
28:U:75:MET:HA	28:U:78:ILE:HG22	1.96	0.47
37:6:121:LEU:HD11	37:6:128:LEU:HD11	1.97	0.47
38:7:241:ASN:HB3	38:7:423:PRO:HG3	1.97	0.47
38:7:482:THR:HG21	38:7:493:PHE:HD1	1.79	0.47
44:A:644:A:H2	44:A:661:C:H42	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Y:140:ARG:HD2	15:Y:141:PRO:HD2	1.97	0.47
24:Q:56:LEU:O	24:Q:60:LEU:HG	2.15	0.47
39:8:98:ARG:O	39:8:101:LEU:HG	2.14	0.47
44:A:399:G:C6	44:A:400:G:C6	3.02	0.47
4:D:200:ARG:O	9:K:54:ARG:NH2	2.48	0.47
5:F:188:ASN:HD22	5:F:220:THR:HG23	1.79	0.47
12:P:20:GLN:HG3	12:P:27:VAL:HG22	1.98	0.46
26:S:24:LEU:HD22	26:S:54:VAL:HG11	1.97	0.46
35:3:270:ARG:HD2	35:3:273:VAL:HB	1.97	0.46
41:2:731:GLU:HB3	41:2:755:PHE:CZ	2.49	0.46
43:5:170:THR:OG1	43:5:173:LEU:HD23	2.15	0.46
43:5:180:LYS:CD	43:5:319:ILE:HD13	2.44	0.46
44:A:387:U:H4'	44:A:388:A:OP1	2.15	0.46
44:A:561:A:H2'	44:A:562:U:O4'	2.96	0.46
40:1:87:GLU:HA	40:1:173:LEU:CD1	2.44	0.46
41:2:852:GLN:HE22	43:5:254:SER:HB3	1.81	0.46
35:3:204:PRO:O	35:3:208:LEU:HG	2.16	0.46
40:1:470:ALA:HA	40:1:473:ASP:HB2	1.96	0.46
24:Q:33:LEU:HD21	24:Q:87:PRO:HD2	1.96	0.46
36:4:117:VAL:HG11	43:5:51:LYS:HD3	1.97	0.46
36:4:192:TRP:O	36:4:219:HIS:HA	2.14	0.46
42:9:280:ILE:HD11	42:9:518:ILE:HD11	1.96	0.46
27:T:73:ASN:HB3	27:T:76:GLN:HE21	1.79	0.46
35:3:254:LEU:HD13	35:3:283:GLN:NE2	2.31	0.46
35:3:403:GLN:O	35:3:407:LYS:HB2	2.15	0.46
36:4:266:ARG:NH1	43:5:228:HIS:O	2.49	0.46
37:6:47:ASN:HB3	37:6:69:ILE:HG23	1.96	0.46
39:8:263:ILE:HA	39:8:266:LEU:HB2	1.97	0.46
42:9:435:LEU:CD1	42:9:490:ILE:HG22	2.39	0.46
43:5:36:VAL:HA	43:5:146:GLU:HA	1.98	0.46
43:5:173:LEU:HD21	43:5:180:LYS:HZ1	1.79	0.46
43:5:336:GLN:HE21	43:5:340:LYS:HG3	1.80	0.46
40:1:297:HIS:NE2	40:1:329:ILE:HD11	2.30	0.46
41:2:577:ALA:HB1	41:2:619:CYS:SG	2.55	0.46
43:5:52:HIS:CG	43:5:83:PRO:HG3	2.50	0.46
36:4:273:MET:HB3	43:5:218:LEU:HD13	1.98	0.46
39:8:161:LYS:HA	39:8:164:LEU:HD12	1.96	0.46
43:5:64:GLN:O	43:5:83:PRO:HA	2.16	0.46
44:A:437:C:H2'	44:A:437:C:O2	2.16	0.46
44:A:512:C:H3'	44:A:513:U:H5'	1.96	0.46
43:5:63:VAL:HG13	43:5:119:TRP:CE3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:5:81:CYS:HB2	43:5:120:TYR:CE1	2.51	0.46
43:5:261:ASN:O	43:5:264:MET:HB3	2.15	0.46
39:8:236:LEU:HD23	39:8:238:HIS:CE1	2.51	0.46
40:1:138:GLN:O	40:1:142:ASP:HB2	2.16	0.46
40:1:455:LEU:HA	40:1:458:LEU:HB2	1.98	0.46
40:1:478:CYS:HB3	40:1:502:ARG:HD2	1.97	0.46
41:2:553:LYS:HE2	41:2:569:ILE:HD12	1.98	0.46
8:J:36:THR:HG23	8:J:96:LEU:HB2	1.98	0.46
41:2:430:ASN:N	41:2:430:ASN:HD22	2.14	0.46
42:9:334:PHE:CZ	42:9:338:VAL:HG11	2.51	0.46
44:A:459:G:O2'	44:A:460:U:O4'	2.34	0.46
39:8:86:LEU:O	39:8:102:ARG:NH1	2.49	0.45
41:2:755:PHE:HB3	41:2:760:LYS:HB2	1.97	0.45
4:D:141:LEU:HD13	4:D:238:LYS:NZ	2.19	0.45
7:I:84:GLU:HG3	7:I:92:VAL:HG12	1.98	0.45
37:6:151:GLN:HB2	38:7:505:GLY:HA3	1.98	0.45
38:7:545:ARG:HA	38:7:548:HIS:HB3	1.98	0.45
40:1:424:LEU:HD23	40:1:424:LEU:N	2.31	0.45
41:2:843:VAL:HG22	41:2:847:THR:HB	1.98	0.45
43:5:253:MET:HG2	43:5:331:LYS:HD2	1.97	0.45
28:U:27:LYS:HD2	28:U:110:LEU:HD13	1.99	0.45
35:3:219:LEU:HD11	35:3:324:PHE:CZ	2.51	0.45
36:4:300:GLN:HB2	40:1:532:LYS:HG3	1.98	0.45
39:8:71:LEU:HA	39:8:74:LEU:HD13	1.99	0.45
40:1:256:ILE:O	40:1:260:PHE:HB2	2.16	0.45
40:1:472:VAL:HG23	40:1:484:ILE:HG12	1.97	0.45
42:9:406:LEU:CD2	42:9:442:LEU:HD11	2.45	0.45
5:F:173:ILE:HD11	5:F:235:TRP:CE3	2.51	0.45
8:J:130:THR:N	8:J:131:PRO:CD	2.78	0.45
20:E:134:CYS:SG	20:E:135:GLU:N	2.90	0.45
35:3:41:LYS:HA	35:3:44:LEU:HG	1.98	0.45
35:3:254:LEU:HD11	35:3:293:THR:HG22	1.97	0.45
39:8:287:VAL:HG12	39:8:288:GLU:HB2	1.99	0.45
40:1:210:ARG:HB3	40:1:212:HIS:CG	2.51	0.45
41:2:456:THR:HB	41:2:667:ARG:HD2	1.97	0.45
42:9:179:TRP:CG	42:9:532:ILE:HG22	2.50	0.45
44:A:638:C:O2'	44:A:639:A:N7	2.47	0.45
35:3:38:LEU:HD12	35:3:39:GLN:N	2.31	0.45
35:3:143:ASN:HA	35:3:145:SER:N	2.32	0.45
40:1:303:SER:OG	40:1:321:ARG:NH1	2.50	0.45
42:9:435:LEU:HA	42:9:442:LEU:HD22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:A:386:U:C4	44:A:403:G:N3	2.84	0.45
15:Y:51:VAL:HG13	15:Y:70:VAL:CG2	2.47	0.45
35:3:131:LEU:HD11	35:3:158:VAL:HA	1.98	0.45
35:3:297:GLU:HA	35:3:300:TYR:HB3	1.97	0.45
36:4:191:GLY:HA2	36:4:210:TYR:CE1	2.51	0.45
16:Z:79:LEU:HD21	16:Z:96:LEU:HD21	1.99	0.45
35:3:261:VAL:HA	35:3:265:LYS:HB2	1.98	0.45
38:7:533:THR:HA	38:7:536:ALA:HB3	1.99	0.45
44:A:537:G:O2'	44:A:540:A:N1	2.49	0.45
36:4:111:VAL:HG13	36:4:148:SER:HA	1.98	0.45
36:4:116:PRO:HG3	36:4:259:TYR:CE2	2.52	0.45
35:3:304:ASP:HB3	35:3:308:ALA:HB2	1.98	0.45
36:4:298:ARG:HD3	39:8:360:ASN:OD1	2.17	0.45
39:8:323:CYS:HA	40:1:517:GLU:HB3	1.99	0.45
44:A:454:C:H2'	44:A:455:U:C6	2.51	0.45
21:G:39:ILE:HG23	21:G:68:ILE:HD13	1.99	0.45
36:4:175:ASN:O	36:4:179:LEU:HG	2.16	0.45
36:4:364:THR:HG22	41:2:859:LEU:CD1	2.46	0.45
39:8:184:VAL:O	39:8:188:LEU:HD23	2.16	0.45
41:2:707:ARG:HA	41:2:707:ARG:NE	2.32	0.45
24:Q:54:HIS:HB3	24:Q:57:LEU:HB2	1.98	0.44
24:Q:87:PRO:HA	24:Q:90:VAL:HG23	1.99	0.44
37:6:80:THR:HG21	38:7:326:MET:C	2.37	0.44
39:8:70:LEU:HD13	39:8:105:LEU:HD11	1.97	0.44
42:9:302:VAL:HG11	42:9:323:LEU:HB3	1.97	0.44
40:1:403:LEU:CD2	40:1:439:LEU:HD21	2.46	0.44
41:2:379:ILE:HA	41:2:382:LEU:HD12	1.99	0.44
41:2:688:VAL:HG22	41:2:692:LEU:HD12	2.00	0.44
9:K:47:LYS:HG3	9:K:102:ILE:HD11	2.00	0.44
36:4:273:MET:SD	43:5:218:LEU:HB2	2.58	0.44
40:1:306:MET:O	40:1:309:ASN:N	2.51	0.44
41:2:710:ILE:HB	41:2:714:PHE:CD2	2.36	0.44
42:9:211:GLU:HB2	42:9:339:LEU:HD21	1.99	0.44
43:5:277:TYR:OH	44:A:535:C:OP1	2.27	0.44
35:3:211:ARG:NH1	35:3:242:TYR:O	2.50	0.44
36:4:207:HIS:CE1	36:4:219:HIS:NE2	2.86	0.44
36:4:347:LEU:O	36:4:351:ILE:HG13	2.16	0.44
41:2:504:LEU:HD13	41:2:564:ILE:HG23	1.99	0.44
41:2:536:GLN:HG3	41:2:539:ASN:HB2	1.99	0.44
42:9:282:LYS:HE2	42:9:509:MET:HA	2.00	0.44
2:B:50:ASN:HD22	2:B:53:ARG:HD2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:130:ILE:HG12	9:K:135:ILE:HD11	2.00	0.44
20:E:34:TYR:OH	20:E:37:VAL:HG13	2.18	0.44
35:3:373:ASN:HA	35:3:376:ARG:HG2	2.00	0.44
39:8:90:LEU:HD21	39:8:102:ARG:HD2	1.98	0.44
40:1:323:LEU:CD1	40:1:424:LEU:HD22	2.48	0.44
42:9:267:MET:HE3	42:9:451:LEU:HD11	2.00	0.44
42:9:431:LEU:HD22	42:9:481:TYR:OH	2.17	0.44
2:B:119:PRO:HG2	2:B:142:LEU:HD11	2.00	0.44
40:1:147:THR:HA	40:1:150:VAL:HG22	2.00	0.44
35:3:193:LYS:NZ	35:3:235:LEU:HD21	2.33	0.44
35:3:278:VAL:HA	35:3:283:GLN:HG2	1.99	0.44
41:2:542:GLU:N	41:2:542:GLU:OE1	2.51	0.44
41:2:578:LEU:N	41:2:619:CYS:SG	2.91	0.44
2:B:2:SER:HA	2:B:59:LEU:HD13	2.00	0.44
3:C:190:PRO:HG3	40:1:17:GLU:HB3	2.00	0.44
36:4:336:PRO:HG3	43:5:352:ASN:HB2	1.99	0.44
36:4:371:ASN:HD21	43:5:264:MET:HG2	1.82	0.44
41:2:857:LEU:O	41:2:861:GLU:N	2.36	0.44
35:3:210:GLN:HA	35:3:213:TRP:HB2	2.00	0.44
36:4:369:ALA:O	36:4:373:LYS:HB2	2.18	0.44
38:7:236:ASP:O	38:7:240:ILE:HG12	2.18	0.44
4:D:141:LEU:CD1	4:D:238:LYS:HZ2	2.04	0.43
24:Q:68:PRO:HB2	24:Q:69:PRO:HD2	1.99	0.43
35:3:218:SER:HB2	35:3:232:ILE:HG12	1.99	0.43
36:4:120:ALA:HA	43:5:44:LEU:HD22	1.99	0.43
40:1:78:CYS:SG	40:1:86:LEU:HG	2.58	0.43
43:5:46:VAL:O	43:5:50:ILE:HG13	2.17	0.43
44:A:380:G:C4	44:A:440:A:C2	3.06	0.43
2:B:60:LEU:HD22	2:B:159:ILE:HG21	1.99	0.43
5:F:256:LEU:O	5:F:260:GLN:HG2	2.18	0.43
13:W:1:MET:SD	13:W:1:MET:N	2.88	0.43
35:3:158:VAL:CG2	35:3:159:PRO:HD2	2.44	0.43
38:7:266:TYR:CB	38:7:283:LEU:HD13	2.48	0.43
41:2:810:MET:O	41:2:814:ASP:N	2.45	0.43
43:5:70:LEU:HD13	43:5:115:LEU:HD13	2.00	0.43
24:Q:75:VAL:HG22	24:Q:93:MET:HB3	2.00	0.43
42:9:206:CYS:HA	42:9:369:ARG:HB3	1.99	0.43
43:5:211:ILE:O	43:5:214:LEU:N	2.52	0.43
44:A:462:U:C4	44:A:463:U:C4	3.06	0.43
6:H:49:VAL:CG2	6:H:115:LYS:HB3	2.48	0.43
20:E:59:LEU:HA	20:E:66:ILE:HG12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:4:246:ARG:NH1	36:4:247:THR:OG1	2.51	0.43
37:6:211:SER:HA	37:6:214:MET:HB2	1.99	0.43
40:1:87:GLU:HA	40:1:173:LEU:HD13	2.00	0.43
42:9:195:LEU:HD22	42:9:502:ARG:HD2	2.01	0.43
43:5:40:GLN:HB2	43:5:75:ARG:HD3	2.01	0.43
3:C:62:LEU:HD21	3:C:96:CYS:SG	2.58	0.43
4:D:212:LYS:HA	4:D:215:LEU:HD12	1.99	0.43
4:D:250:TYR:N	13:W:23:ILE:HD11	2.33	0.43
14:X:6:VAL:HG12	14:X:34:ILE:HD11	1.99	0.43
37:6:23:PRO:HG2	37:6:57:ASN:HD22	1.84	0.43
43:5:104:MET:HB3	43:5:114:HIS:HB2	2.01	0.43
13:W:72:LEU:O	13:W:75:SER:OG	2.32	0.43
24:Q:22:LEU:HD11	24:Q:109:PRO:HB3	2.00	0.43
38:7:552:GLU:HA	43:5:192:ILE:HA	2.00	0.43
44:A:509:G:O6	44:A:510:C:C5	2.72	0.43
35:3:26:LEU:HB2	35:3:68:HIS:CE1	2.54	0.43
37:6:48:LEU:HD22	37:6:84:LEU:HD13	2.00	0.43
37:6:115:GLN:N	37:6:115:GLN:OE1	2.52	0.43
40:1:403:LEU:HA	40:1:406:ARG:HB3	2.00	0.43
43:5:119:TRP:CZ3	43:5:121:GLN:HB3	2.53	0.43
44:A:464:G:C2	44:A:465:A:C2	3.06	0.43
44:A:526:A:O2'	44:A:527:C:OP1	2.26	0.43
35:3:198:ASN:N	35:3:199:ASN:HA	2.32	0.43
37:6:125:MET:HB3	37:6:128:LEU:HG	2.00	0.43
42:9:520:LYS:HA	42:9:527:ILE:HA	2.01	0.43
43:5:36:VAL:HG11	43:5:168:ARG:CZ	2.49	0.43
3:C:31:TYR:CE2	3:C:49:VAL:HG11	2.54	0.43
44:A:484:C:N4	44:A:491:U:O4	2.52	0.43
44:A:493:U:OP1	44:A:516:U:C4	2.72	0.43
2:B:132:GLN:HB3	2:B:133:PRO:HD3	2.01	0.43
9:K:113:GLN:O	9:K:117:LEU:HB2	2.19	0.43
20:E:137:VAL:HG13	20:E:185:LYS:HB2	2.01	0.43
36:4:139:THR:HA	36:4:192:TRP:HA	1.99	0.43
9:K:46:VAL:HG11	9:K:106:LEU:CD1	2.49	0.42
24:Q:54:HIS:ND1	24:Q:57:LEU:HD13	2.35	0.42
39:8:83:ILE:CG1	39:8:106:LEU:HD21	2.49	0.42
39:8:100:SER:HA	39:8:103:LEU:HD12	2.01	0.42
39:8:109:LEU:HG	39:8:114:ASP:HB3	2.00	0.42
40:1:80:GLN:HA	40:1:83:ILE:HD11	2.02	0.42
41:2:402:LEU:HD23	41:2:402:LEU:HA	1.93	0.42
42:9:227:PRO:O	42:9:337:GLN:NE2	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:124:VAL:HG13	2:B:130:ASP:HB2	2.01	0.42
7:I:135:PHE:HB3	7:I:136:PRO:HD3	2.01	0.42
12:P:119:LEU:O	12:P:124:MET:HB2	2.19	0.42
28:U:62:ARG:NH1	28:U:66:LEU:HD11	2.35	0.42
36:4:216:ASN:HD21	36:4:237:VAL:HG21	1.83	0.42
38:7:284:LEU:HA	38:7:287:TYR:HB3	2.01	0.42
38:7:461:ARG:HA	38:7:502:TRP:HE1	1.84	0.42
41:2:392:TYR:HB2	41:2:458:ILE:HD13	2.00	0.42
41:2:848:GLU:HB3	41:2:849:PRO:HD3	2.01	0.42
9:K:126:ALA:O	9:K:130:ILE:HG13	2.19	0.42
35:3:278:VAL:O	35:3:283:GLN:HB3	2.20	0.42
35:3:371:ILE:O	35:3:375:ILE:HG12	2.19	0.42
39:8:301:LEU:O	39:8:302:GLN:HG3	2.20	0.42
41:2:451:MET:SD	41:2:479:VAL:HG23	2.60	0.42
41:2:723:ARG:HG2	41:2:724:GLN:H	1.82	0.42
43:5:75:ARG:HH12	43:5:205:ILE:HB	1.84	0.42
44:A:541:C:H2'	44:A:542:A:C8	2.53	0.42
44:A:576:U:O2	44:A:576:U:O4'	2.37	0.42
2:B:3:GLY:HA3	13:W:80:SER:HB3	2.00	0.42
23:N:24:THR:HA	23:N:27:ILE:HG12	2.02	0.42
38:7:390:LEU:HD23	38:7:393:LYS:HD2	2.01	0.42
39:8:193:THR:HG22	39:8:194:GLU:HB2	2.00	0.42
40:1:43:TRP:CZ3	40:1:45:LYS:HD2	2.54	0.42
40:1:175:HIS:CD2	40:1:228:MET:HB3	2.55	0.42
41:2:371:ILE:O	41:2:375:LYS:N	2.50	0.42
41:2:421:GLY:HA2	41:2:431:LEU:H	1.84	0.42
41:2:499:ILE:O	41:2:502:VAL:HG12	2.19	0.42
44:A:539:U:O2	44:A:539:U:C2'	2.67	0.42
44:A:647:C:H3'	44:A:648:A:C5'	2.50	0.42
7:I:133:LEU:HD21	7:I:176:VAL:HG11	2.00	0.42
36:4:207:HIS:CE1	36:4:250:VAL:HG11	2.55	0.42
36:4:329:MET:HA	36:4:332:VAL:HG22	2.00	0.42
39:8:254:LYS:O	39:8:258:ASN:ND2	2.53	0.42
39:8:313:ILE:HA	39:8:316:VAL:HG22	2.01	0.42
39:8:350:LEU:C	39:8:350:LEU:HD12	2.40	0.42
40:1:78:CYS:SG	40:1:78:CYS:O	2.78	0.42
40:1:499:TYR:CD1	40:1:503:GLU:HG3	2.55	0.42
41:2:526:PRO:HB2	41:2:531:LYS:HE2	2.01	0.42
41:2:755:PHE:HB3	41:2:760:LYS:CB	2.50	0.42
41:2:799:TYR:CZ	41:2:837:GLN:HB2	2.55	0.42
44:A:662:C:H2'	44:A:663:C:C5	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:6:151:GLN:NE2	37:6:195:SER:HB2	2.34	0.42
39:8:250:ALA:HB1	39:8:280:LEU:HD11	2.01	0.42
44:A:414:G:H2'	44:A:414:G:N3	2.34	0.42
44:A:644:A:H1'	44:A:645:A:C6	2.55	0.42
2:B:57:LYS:HD3	13:W:70:LEU:HD12	2.01	0.42
15:Y:123:VAL:HG12	15:Y:124:LYS:HG3	2.02	0.42
41:2:695:ILE:HD11	41:2:788:LEU:HD22	2.01	0.42
43:5:32:GLY:HA3	43:5:36:VAL:HG13	2.00	0.42
15:Y:68:LYS:HB3	15:Y:91:LEU:HD22	2.02	0.42
21:G:25:THR:HG21	21:G:46:ALA:HB2	2.02	0.42
35:3:42:LEU:CD1	35:3:219:LEU:HD13	2.50	0.42
39:8:63:VAL:HG21	39:8:98:ARG:HB3	2.02	0.42
40:1:421:GLU:O	40:1:424:LEU:HG	2.19	0.42
41:2:424:ILE:HG22	41:2:425:LEU:HD12	2.02	0.42
4:D:141:LEU:HD21	4:D:238:LYS:NZ	2.35	0.42
8:J:153:LYS:HA	8:J:156:ALA:HB2	2.01	0.42
23:N:85:LEU:HA	23:N:88:TRP:CE3	2.55	0.42
23:N:92:CYS:HB2	23:N:103:VAL:HA	2.01	0.42
37:6:195:SER:HA	38:7:503:THR:HG22	2.02	0.42
38:7:421:LEU:HD23	38:7:421:LEU:O	2.19	0.42
43:5:44:LEU:HD23	43:5:47:LEU:HD12	2.02	0.42
12:P:53:ILE:HG23	12:P:88:LEU:HD22	2.02	0.41
36:4:128:ARG:NE	43:5:79:THR:HG22	2.35	0.41
36:4:163:GLU:HA	36:4:164:ASP:HA	1.80	0.41
40:1:483:ARG:HD2	40:1:483:ARG:N	2.34	0.41
35:3:107:THR:O	35:3:111:ARG:HD3	2.20	0.41
36:4:249:GLY:N	39:8:8:ASP:OD1	2.44	0.41
39:8:190:GLY:HA2	39:8:231:PHE:CG	2.55	0.41
39:8:249:LEU:HB3	39:8:254:LYS:HG3	2.03	0.41
39:8:282:PHE:HZ	39:8:340:ARG:HB2	1.84	0.41
40:1:208:ILE:HG13	40:1:211:HIS:NE2	2.35	0.41
44:A:606:G:N3	44:A:606:G:H2'	3.46	0.41
36:4:141:LEU:HB3	36:4:187:GLU:CB	2.50	0.41
38:7:266:TYR:HB2	38:7:283:LEU:HD13	2.01	0.41
39:8:234:GLY:HA2	39:8:240:LEU:HB2	2.03	0.41
39:8:297:MET:O	39:8:301:LEU:HG	2.20	0.41
40:1:250:PHE:CZ	41:2:720:VAL:HG21	2.56	0.41
42:9:231:ILE:HG22	42:9:233:ARG:HG3	2.03	0.41
44:A:427:U:O2	44:A:427:U:O4'	2.75	0.41
6:H:52:ILE:HD11	6:H:109:LEU:HD22	2.02	0.41
8:J:36:THR:HG21	8:J:179:PRO:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:165:GLN:NE2	8:J:195:LEU:HD11	2.36	0.41
24:Q:53:GLN:HE21	24:Q:54:HIS:CD2	2.38	0.41
36:4:331:LEU:HD23	40:1:531:ALA:HB3	2.01	0.41
36:4:363:LEU:HA	38:7:533:THR:HG21	2.01	0.41
41:2:725:PRO:HG3	41:2:734:ARG:HB2	2.01	0.41
42:9:302:VAL:HG11	42:9:323:LEU:CB	2.51	0.41
43:5:64:GLN:O	43:5:120:TYR:CZ	2.73	0.41
43:5:137:GLN:HB2	43:5:149:VAL:HG21	2.02	0.41
9:K:84:ILE:HG13	9:K:86:VAL:HG23	2.02	0.41
44:A:391:A:C2	44:A:401:U:O2	2.74	0.41
2:B:173:LEU:HD12	26:S:91:LEU:CD1	2.50	0.41
14:X:28:ARG:CB	14:X:29:PRO:HD3	2.50	0.41
36:4:140:LEU:HD21	36:4:151:VAL:HG21	2.03	0.41
36:4:153:ASN:N	36:4:187:GLU:OE2	2.49	0.41
36:4:158:PRO:CG	43:5:109:HIS:HB3	2.51	0.41
36:4:196:GLY:N	36:4:222:VAL:O	2.54	0.41
38:7:497:MET:SD	38:7:504:SER:OG	2.76	0.41
40:1:404:CYS:HB2	40:1:459:VAL:HA	2.02	0.41
40:1:408:THR:HA	40:1:411:LEU:HB2	2.02	0.41
41:2:829:GLU:N	41:2:838:PRO:O	2.46	0.41
43:5:134:LEU:HG	43:5:169:LEU:HD11	2.02	0.41
43:5:182:PHE:CE1	43:5:317:LEU:HG	2.56	0.41
20:E:135:GLU:HB3	20:E:187:LYS:HB3	2.03	0.41
26:S:17:ILE:HD11	26:S:54:VAL:HA	2.02	0.41
35:3:108:ARG:NH2	35:3:112:MET:HB3	2.36	0.41
35:3:316:GLU:HB3	35:3:333:ILE:HG23	2.02	0.41
36:4:251:MET:HG3	39:8:67:VAL:HG11	2.02	0.41
39:8:316:VAL:HG12	39:8:321:VAL:O	2.20	0.41
40:1:144:LEU:HD13	41:2:466:SER:HB2	2.03	0.41
40:1:428:VAL:HA	40:1:431:LEU:HD12	2.03	0.41
41:2:783:ILE:CD1	41:2:813:LEU:HD22	2.49	0.41
43:5:50:ILE:HG22	43:5:50:ILE:O	2.20	0.41
44:A:371:C:C4	44:A:372:U:C4	3.09	0.41
44:A:489:C:O2	44:A:489:C:O4'	2.37	0.41
2:B:30:LEU:HD13	2:B:38:ILE:HD12	2.03	0.41
3:C:181:LEU:HA	3:C:184:VAL:HG22	2.02	0.41
20:E:21:LEU:HD11	20:E:48:ILE:HD11	2.03	0.41
24:Q:34:MET:HA	24:Q:37:TYR:CE2	2.56	0.41
28:U:127:GLY:O	28:U:131:LEU:HD23	2.20	0.41
35:3:13:PHE:CE2	35:3:205:LEU:HD23	2.56	0.41
35:3:48:THR:HG21	35:3:72:GLU:HG2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:3:401:TYR:O	35:3:405:ILE:HG13	2.21	0.41
36:4:207:HIS:CE1	36:4:219:HIS:CE1	3.09	0.41
4:D:236:PHE:O	4:D:237:ALA:HB3	2.21	0.41
7:I:63:PHE:HA	7:I:95:ILE:O	2.20	0.41
13:W:56:CYS:SG	13:W:57:GLY:N	2.93	0.41
35:3:50:MET:HG3	35:3:178:LEU:HD13	2.02	0.41
35:3:91:ILE:HG23	35:3:91:ILE:O	2.21	0.41
35:3:231:ASN:O	35:3:235:LEU:HD23	2.21	0.41
37:6:48:LEU:HG	38:7:292:LYS:HG3	2.02	0.41
38:7:376:THR:HA	38:7:379:PRO:HD2	2.03	0.41
39:8:29:ILE:HG13	39:8:54:LYS:HB3	2.03	0.41
40:1:469:ARG:HA	40:1:472:VAL:CG1	2.50	0.41
40:1:485:ASP:HB3	41:2:797:SER:HA	2.01	0.41
41:2:556:TYR:CE1	41:2:564:ILE:HB	2.56	0.41
42:9:175:VAL:HG13	42:9:179:TRP:CE3	2.55	0.41
43:5:73:GLU:O	43:5:73:GLU:HG2	2.20	0.41
43:5:310:PRO:HB3	43:5:314:MET:CG	2.51	0.41
6:H:223:LYS:HA	6:H:226:GLU:HB3	2.02	0.41
35:3:269:LYS:HG3	35:3:269:LYS:O	2.20	0.41
38:7:388:LEU:HA	38:7:391:ARG:HB3	2.02	0.41
39:8:288:GLU:N	39:8:289:ASN:HA	2.36	0.41
41:2:493:LYS:CG	41:2:498:GLU:OE2	2.68	0.41
43:5:67:LEU:HA	43:5:81:CYS:HB3	2.03	0.41
43:5:253:MET:SD	43:5:331:LYS:HB3	2.61	0.41
9:K:63:LEU:HD23	9:K:63:LEU:HA	1.94	0.40
12:P:97:LEU:HD11	12:P:112:ALA:HB1	2.03	0.40
24:Q:90:VAL:HG21	24:Q:112:ILE:HD11	2.03	0.40
35:3:38:LEU:CD1	35:3:252:HIS:HE2	2.33	0.40
35:3:132:TYR:HA	35:3:159:PRO:HG3	2.03	0.40
36:4:210:TYR:O	36:4:214:ALA:N	2.48	0.40
39:8:128:ILE:HG12	39:8:168:LEU:HD21	2.03	0.40
40:1:390:LEU:HD11	40:1:410:VAL:HG13	2.01	0.40
2:B:180:GLN:HB2	2:B:195:TRP:CE3	2.56	0.40
4:D:146:GLU:HB2	4:D:149:THR:HG22	2.01	0.40
7:I:100:ILE:HG23	7:I:100:ILE:O	2.21	0.40
7:I:134:VAL:HG12	7:I:173:PHE:CE2	2.56	0.40
21:G:72:LEU:HD22	21:G:112:LEU:HD11	2.03	0.40
35:3:66:ILE:HB	35:3:67:PRO:HD3	2.03	0.40
36:4:117:VAL:HG22	43:5:47:LEU:HB3	2.02	0.40
39:8:245:VAL:HG12	39:8:258:ASN:HD21	1.86	0.40
40:1:481:GLN:HE22	40:1:498:ASN:C	2.24	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:2:333:LEU:HD22	41:2:374:ILE:HG13	2.03	0.40
43:5:297:PRO:HA	43:5:298:GLU:CB	2.49	0.40
44:A:572:U:C4	44:A:573:U:C4	3.09	0.40
7:I:133:LEU:HD23	7:I:133:LEU:HA	1.97	0.40
7:I:177:TYR:CD2	7:I:185:VAL:HG21	2.57	0.40
20:E:67:ARG:NE	22:L:93:THR:O	2.47	0.40
35:3:143:ASN:N	35:3:144:TYR:HB2	2.36	0.40
37:6:55:GLN:HE21	38:7:442:GLN:HG2	1.87	0.40
37:6:80:THR:HG21	38:7:326:MET:HA	2.02	0.40
37:6:148:ILE:HG22	37:6:149:THR:HG23	2.03	0.40
44:A:560:U:HO2'	44:A:561:A:P	2.44	0.40
2:B:36:GLN:O	2:B:53:ARG:NH1	2.54	0.40
7:I:170:VAL:HG13	7:I:187:PHE:HB2	2.03	0.40
27:T:48:ALA:O	27:T:50:ILE:N	2.55	0.40
40:1:211:HIS:HB2	44:A:490:A:H4'	2.03	0.40
44:A:526:A:H2'	44:A:527:C:H5''	2.03	0.40
3:C:134:LEU:HD23	3:C:218:LEU:HB2	2.04	0.40
23:N:38:ALA:HA	23:N:110:VAL:HB	2.02	0.40
27:T:68:ILE:HG23	27:T:72:GLN:HE22	1.87	0.40
36:4:196:GLY:HA2	36:4:197:HIS:HA	1.92	0.40
39:8:67:VAL:HA	39:8:70:LEU:HD12	2.02	0.40
39:8:144:LEU:HA	39:8:147:VAL:HB	2.03	0.40
40:1:276:TYR:HA	40:1:279:VAL:HG12	2.04	0.40
40:1:454:ARG:HG3	40:1:458:LEU:HD13	2.03	0.40
40:1:483:ARG:O	40:1:491:LEU:HG	2.22	0.40
41:2:853:GLN:HA	41:2:856:ALA:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	215/295 (73%)	206 (96%)	8 (4%)	1 (0%)	29	63
3	C	211/264 (80%)	187 (89%)	23 (11%)	1 (0%)	29	63
4	D	219/255 (86%)	202 (92%)	16 (7%)	1 (0%)	29	63
5	F	260/263 (99%)	240 (92%)	20 (8%)	0	100	100
6	H	235/249 (94%)	219 (93%)	16 (7%)	0	100	100
7	I	181/194 (93%)	165 (91%)	16 (9%)	0	100	100
8	J	204/208 (98%)	188 (92%)	12 (6%)	4 (2%)	7	33
9	K	183/194 (94%)	167 (91%)	16 (9%)	0	100	100
10	M	139/158 (88%)	128 (92%)	11 (8%)	0	100	100
11	O	147/151 (97%)	138 (94%)	9 (6%)	0	100	100
12	P	134/151 (89%)	120 (90%)	13 (10%)	1 (1%)	22	56
13	W	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
14	X	127/130 (98%)	119 (94%)	7 (6%)	1 (1%)	19	53
15	Y	139/143 (97%)	129 (93%)	6 (4%)	4 (3%)	4	26
16	Z	122/134 (91%)	114 (93%)	8 (7%)	0	100	100
17	b	99/115 (86%)	88 (89%)	7 (7%)	4 (4%)	3	20
18	c	81/84 (96%)	74 (91%)	6 (7%)	1 (1%)	13	44
19	f	55/133 (41%)	53 (96%)	2 (4%)	0	100	100
20	E	226/281 (80%)	211 (93%)	14 (6%)	1 (0%)	34	68
21	G	189/204 (93%)	166 (88%)	18 (10%)	5 (3%)	5	28
22	L	94/149 (63%)	86 (92%)	7 (7%)	1 (1%)	14	46
23	N	115/132 (87%)	94 (82%)	19 (16%)	2 (2%)	9	36
24	Q	113/145 (78%)	95 (84%)	15 (13%)	3 (3%)	5	27
25	R	140/172 (81%)	136 (97%)	3 (2%)	1 (1%)	22	56
26	S	130/135 (96%)	110 (85%)	18 (14%)	2 (2%)	10	39
27	T	142/152 (93%)	132 (93%)	7 (5%)	3 (2%)	7	32
28	U	139/145 (96%)	130 (94%)	7 (5%)	2 (1%)	11	40
29	V	98/119 (82%)	88 (90%)	10 (10%)	0	100	100
30	i	73/125 (58%)	70 (96%)	3 (4%)	0	100	100
31	d	60/69 (87%)	54 (90%)	6 (10%)	0	100	100
32	e	53/56 (95%)	48 (91%)	5 (9%)	0	100	100
33	g	66/156 (42%)	52 (79%)	14 (21%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	h	310/317 (98%)	278 (90%)	32 (10%)	0	100	100
35	3	417/462 (90%)	315 (76%)	86 (21%)	16 (4%)	3	21
36	4	270/364 (74%)	219 (81%)	45 (17%)	6 (2%)	6	32
37	6	213/218 (98%)	182 (85%)	31 (15%)	0	100	100
38	7	370/607 (61%)	316 (85%)	52 (14%)	2 (0%)	29	63
39	8	363/374 (97%)	283 (78%)	71 (20%)	9 (2%)	5	29
40	1	532/1362 (39%)	429 (81%)	85 (16%)	18 (3%)	3	23
41	2	543/913 (60%)	424 (78%)	104 (19%)	15 (3%)	5	26
42	9	350/558 (63%)	317 (91%)	28 (8%)	5 (1%)	11	40
43	5	322/363 (89%)	255 (79%)	53 (16%)	14 (4%)	2	18
All	All	8160/10782 (76%)	7106 (87%)	931 (11%)	123 (2%)	14	39

All (123) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	Y	61	GLN
17	b	8	ASN
24	Q	18	ARG
25	R	17	LYS
26	S	99	ASP
27	T	100	ALA
28	U	29	LYS
35	3	26	LEU
35	3	50	MET
35	3	51	VAL
35	3	63	SER
35	3	238	TYR
35	3	245	ALA
35	3	325	LEU
36	4	244	PRO
36	4	338	ILE
39	8	335	SER
39	8	336	HIS
40	1	42	THR
40	1	513	SER
41	2	653	ARG
41	2	742	LYS
41	2	842	VAL

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Mol	Chain	Res	Type
42	9	376	ASN
42	9	490	ILE
43	5	73	GLU
43	5	86	GLN
43	5	351	ASN
2	B	44	ASP
3	C	190	PRO
4	D	237	ALA
14	X	28	ARG
21	G	132	GLY
21	G	134	VAL
24	Q	70	MET
27	T	49	ASP
35	3	28	VAL
35	3	46	SER
35	3	93	LYS
35	3	322	ASP
38	7	423	PRO
39	8	116	ASN
40	1	79	GLN
40	1	122	GLN
41	2	326	HIS
41	2	489	TYR
42	9	203	ASP
42	9	377	ASN
43	5	53	TYR
43	5	76	LEU
43	5	87	HIS
8	J	123	ARG
8	J	142	SER
15	Y	86	PRO
17	b	46	GLU
18	c	50	ALA
21	G	43	GLU
26	S	92	ASP
35	3	62	TYR
36	4	198	ASP
36	4	262	TYR
39	8	113	MET
40	1	167	ASN
40	1	168	SER
40	1	484	ILE

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Mol	Chain	Res	Type
40	1	515	PRO
41	2	435	ASP
41	2	578	LEU
41	2	743	ALA
42	9	289	PHE
43	5	35	ALA
43	5	56	GLU
43	5	114	HIS
43	5	116	HIS
43	5	223	ALA
8	J	86	SER
20	E	43	PRO
35	3	47	ASP
35	3	68	HIS
39	8	58	LYS
39	8	232	LEU
40	1	43	TRP
40	1	344	MET
40	1	421	GLU
8	J	94	LYS
15	Y	60	LYS
17	b	63	VAL
22	L	95	ARG
23	N	101	ARG
35	3	154	PHE
36	4	169	ASP
36	4	196	GLY
40	1	214	GLN
40	1	368	ILE
40	1	506	PRO
41	2	727	LEU
43	5	70	LEU
24	Q	118	GLU
28	U	86	GLY
39	8	115	LYS
39	8	130	VAL
39	8	173	VAL
40	1	418	PRO
41	2	346	ASP
41	2	764	LYS
43	5	319	ILE
23	N	100	PRO

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Mol	Chain	Res	Type
40	1	267	PRO
41	2	369	GLY
41	2	598	ILE
43	5	84	PHE
15	Y	62	PRO
21	G	21	GLY
27	T	74	PRO
35	3	57	VAL
38	7	291	ILE
40	1	7	ARG
41	2	765	VAL
12	P	127	GLY
17	b	56	VAL
21	G	128	ILE
40	1	422	PRO
41	2	526	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	
2	B	180/246 (73%)	178 (99%)	2 (1%)	73	86
3	C	194/231 (84%)	193 (100%)	1 (0%)	88	94
4	D	186/205 (91%)	184 (99%)	2 (1%)	73	86
5	F	223/224 (100%)	222 (100%)	1 (0%)	91	95
6	H	207/218 (95%)	201 (97%)	6 (3%)	42	70
7	I	165/174 (95%)	160 (97%)	5 (3%)	41	69
8	J	178/180 (99%)	177 (99%)	1 (1%)	86	93
9	K	161/168 (96%)	159 (99%)	2 (1%)	71	85
10	M	130/142 (92%)	129 (99%)	1 (1%)	81	91
11	O	130/131 (99%)	129 (99%)	1 (1%)	81	91
12	P	106/119 (89%)	106 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	W	68/68 (100%)	67 (98%)	1 (2%)	65	82
14	X	112/113 (99%)	111 (99%)	1 (1%)	78	89
15	Y	113/114 (99%)	112 (99%)	1 (1%)	78	89
16	Z	107/115 (93%)	107 (100%)	0	100	100
17	b	89/99 (90%)	87 (98%)	2 (2%)	52	76
18	c	75/76 (99%)	75 (100%)	0	100	100
19	f	47/106 (44%)	46 (98%)	1 (2%)	53	77
20	E	190/232 (82%)	186 (98%)	4 (2%)	53	77
21	G	158/170 (93%)	158 (100%)	0	100	100
22	L	87/125 (70%)	86 (99%)	1 (1%)	73	86
23	N	99/108 (92%)	98 (99%)	1 (1%)	76	87
24	Q	105/130 (81%)	100 (95%)	5 (5%)	25	57
25	R	117/140 (84%)	116 (99%)	1 (1%)	78	89
26	S	119/121 (98%)	118 (99%)	1 (1%)	81	91
27	T	125/132 (95%)	125 (100%)	0	100	100
28	U	111/116 (96%)	111 (100%)	0	100	100
29	V	92/107 (86%)	92 (100%)	0	100	100
30	i	66/103 (64%)	64 (97%)	2 (3%)	41	69
31	d	55/62 (89%)	54 (98%)	1 (2%)	59	80
32	e	48/49 (98%)	46 (96%)	2 (4%)	30	60
33	g	61/140 (44%)	59 (97%)	2 (3%)	38	67
34	h	271/275 (98%)	269 (99%)	2 (1%)	84	92
35	3	384/423 (91%)	369 (96%)	15 (4%)	32	62
36	4	239/282 (85%)	233 (98%)	6 (2%)	47	73
37	6	190/193 (98%)	189 (100%)	1 (0%)	88	94
38	7	342/544 (63%)	340 (99%)	2 (1%)	86	93
39	8	327/335 (98%)	319 (98%)	8 (2%)	49	74
40	1	490/1245 (39%)	473 (96%)	17 (4%)	36	66
41	2	494/812 (61%)	482 (98%)	12 (2%)	49	74
42	9	320/496 (64%)	314 (98%)	6 (2%)	57	79
43	5	293/320 (92%)	291 (99%)	2 (1%)	84	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	7254/9389 (77%)	7135 (98%)	119 (2%)	64 81

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	111	GLN
2	B	180	GLN
3	C	209	ASP
4	D	141	LEU
4	D	248	TYR
5	F	246	LEU
6	H	15	LEU
6	H	69	THR
6	H	98	ARG
6	H	127	THR
6	H	154	ARG
6	H	201	LYS
7	I	10	LYS
7	I	113	LYS
7	I	122	LEU
7	I	148	LEU
7	I	166	VAL
8	J	153	LYS
9	K	131	ARG
9	K	144	ILE
10	M	69	ARG
11	O	76	LYS
13	W	51	LYS
14	X	103	VAL
15	Y	142	ARG
17	b	15	ARG
17	b	51	ARG
19	f	99	LYS
20	E	42	THR
20	E	59	LEU
20	E	76	ARG
20	E	148	LYS
22	L	83	LEU
23	N	96	ARG
24	Q	13	ARG
24	Q	23	ASP
24	Q	25	LEU

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Mol	Chain	Res	Type
24	Q	37	TYR
24	Q	80	LEU
25	R	62	ARG
26	S	78	ARG
30	i	58	LEU
30	i	109	TYR
31	d	36	ASP
32	e	14	PHE
32	e	25	SER
33	g	103	LEU
33	g	138	ARG
34	h	7	LEU
34	h	116	ASP
35	3	31	ILE
35	3	108	ARG
35	3	163	ARG
35	3	212	THR
35	3	214	LEU
35	3	222	PHE
35	3	226	PRO
35	3	233	ILE
35	3	239	GLN
35	3	267	VAL
35	3	326	VAL
35	3	360	LEU
35	3	362	MET
35	3	383	LYS
35	3	414	ARG
36	4	143	THR
36	4	146	LYS
36	4	211	SER
36	4	237	VAL
36	4	244	PRO
36	4	339	VAL
37	6	199	LYS
38	7	488	ILE
38	7	543	PHE
39	8	65	ASN
39	8	116	ASN
39	8	149	LYS
39	8	188	LEU
39	8	210	ARG

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Mol	Chain	Res	Type
39	8	291	GLU
39	8	338	THR
39	8	369	LEU
40	1	41	ARG
40	1	42	THR
40	1	113	LEU
40	1	145	LEU
40	1	165	ARG
40	1	167	ASN
40	1	199	ASP
40	1	210	ARG
40	1	212	HIS
40	1	237	LEU
40	1	367	ARG
40	1	374	MET
40	1	406	ARG
40	1	479	ASP
40	1	504	ASP
40	1	520	ARG
40	1	532	LYS
41	2	430	ASN
41	2	432	GLN
41	2	504	LEU
41	2	515	ASP
41	2	532	SER
41	2	578	LEU
41	2	627	LYS
41	2	628	ASP
41	2	667	ARG
41	2	668	ARG
41	2	736	HIS
41	2	797	SER
42	9	251	LYS
42	9	317	LEU
42	9	413	LEU
42	9	423	LEU
42	9	459	PHE
42	9	496	ASN
43	5	67	LEU
43	5	236	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	157	GLN
3	C	179	ASN
8	J	84	ASN
8	J	165	GLN
10	M	100	ASN
11	O	90	HIS
14	X	16	ASN
15	Y	127	ASN
19	f	88	GLN
20	E	74	GLN
21	G	82	ASN
22	L	7	ASN
22	L	32	HIS
24	Q	53	GLN
24	Q	79	HIS
27	T	76	GLN
30	i	64	ASN
32	e	4	GLN
34	h	133	ASN
34	h	178	ASN
35	3	138	GLN
35	3	143	ASN
35	3	216	HIS
35	3	239	GLN
35	3	244	ASN
35	3	282	GLN
35	3	283	GLN
36	4	180	HIS
36	4	186	ASN
36	4	207	HIS
36	4	291	GLN
38	7	199	GLN
38	7	363	GLN
39	8	138	GLN
39	8	258	ASN
39	8	299	GLN
40	1	47	HIS
40	1	80	GLN
40	1	226	GLN
40	1	309	ASN
40	1	442	GLN
40	1	448	GLN
40	1	481	GLN

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Mol	Chain	Res	Type
41	2	430	ASN
41	2	432	GLN
41	2	522	GLN
41	2	715	HIS
41	2	784	GLN
41	2	837	GLN
41	2	852	GLN
42	9	322	ASN
42	9	333	ASN
43	5	111	ASN
43	5	137	GLN
43	5	141	GLN
43	5	255	GLN
43	5	279	GLN
43	5	283	GLN
43	5	322	GLN
43	5	336	GLN
43	5	345	GLN
43	5	352	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1681/1697 (99%)	402 (23%)	0
44	A	338/377 (89%)	175 (51%)	23 (6%)
All	All	2019/2074 (97%)	577 (28%)	23 (1%)

All (577) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	2	A
1	a	3	C
1	a	11	A
1	a	15	U
1	a	17	C
1	a	26	U
1	a	33	G
1	a	41	G
1	a	46	A
1	a	58	C
1	a	61	A

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Mol	Chain	Res	Type
1	a	62	G
1	a	64	A
1	a	67	C
1	a	68	A
1	a	70	G
1	a	73	C
1	a	74	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
1	a	126	G
1	a	127	C
1	a	129	C
1	a	130	G
1	a	143	U
1	a	147	A
1	a	155	G
1	a	159	A
1	a	161	U
1	a	162	C
1	a	163	U
1	a	167	G
1	a	178	C
1	a	180	G
1	a	183	G
1	a	184	G
1	a	191	A
1	a	192	C
1	a	204	G
1	a	205	G
1	a	206	G
1	a	215	G
1	a	292	A
1	a	305	U
1	a	307	G
1	a	308	G
1	a	309	G
1	a	313	A

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Mol	Chain	Res	Type
1	a	314	U
1	a	318	A
1	a	319	C
1	a	323	C
1	a	331	C
1	a	332	G
1	a	347	G
1	a	362	C
1	a	363	A
1	a	364	A
1	a	368	U
1	a	369	C
1	a	370	G
1	a	382	C
1	a	384	U
1	a	385	G
1	a	386	C
1	a	400	C
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	441	C
1	a	447	A
1	a	448	A
1	a	449	A
1	a	450	C
1	a	452	G
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	476	A
1	a	479	C

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Mol	Chain	Res	Type
1	a	482	G
1	a	487	U
1	a	492	C
1	a	493	A
1	a	509	G
1	a	516	A
1	a	517	C
1	a	518	G
1	a	525	A
1	a	528	A
1	a	530	U
1	a	531	A
1	a	532	C
1	a	533	A
1	a	536	A
1	a	538	U
1	a	542	U
1	a	543	C
1	a	544	G
1	a	547	G
1	a	548	C
1	a	550	C
1	a	551	U
1	a	553	U
1	a	554	A
1	a	555	A
1	a	556	U
1	a	559	G
1	a	561	A
1	a	562	U
1	a	567	C
1	a	568	C
1	a	570	C
1	a	576	A
1	a	583	A
1	a	588	G
1	a	589	G
1	a	590	A
1	a	591	U
1	a	592	C
1	a	593	C
1	a	594	A

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Mol	Chain	Res	Type
1	a	598	G
1	a	606	G
1	a	607	U
1	a	608	C
1	a	614	C
1	a	615	C
1	a	617	G
1	a	621	C
1	a	627	U
1	a	628	A
1	a	629	A
1	a	630	U
1	a	643	A
1	a	644	G
1	a	647	U
1	a	654	A
1	a	655	A
1	a	659	G
1	a	660	C
1	a	664	A
1	a	668	A
1	a	669	A
1	a	671	A
1	a	672	A
1	a	684	G
1	a	689	U
1	a	690	G
1	a	734	C
1	a	750	C
1	a	752	G
1	a	753	C
1	a	754	G
1	a	794	A
1	a	797	C
1	a	798	G
1	a	801	U
1	a	810	A
1	a	811	A
1	a	821	G
1	a	822	U
1	a	830	A
1	a	834	C

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Mol	Chain	Res	Type
1	a	844	U
1	a	847	A
1	a	867	G
1	a	868	G
1	a	869	A
1	a	870	A
1	a	871	U
1	a	872	A
1	a	873	G
1	a	878	G
1	a	881	G
1	a	885	U
1	a	888	U
1	a	890	U
1	a	891	G
1	a	892	U
1	a	893	U
1	a	894	G
1	a	897	U
1	a	898	U
1	a	909	G
1	a	910	G
1	a	913	A
1	a	914	U
1	a	920	A
1	a	930	C
1	a	933	G
1	a	943	U
1	a	956	G
1	a	970	G
1	a	971	G
1	a	972	A
1	a	985	G
1	a	989	C
1	a	990	A
1	a	992	A
1	a	999	G
1	a	1017	U
1	a	1023	A
1	a	1045	U
1	a	1051	G
1	a	1052	A

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Mol	Chain	Res	Type
1	a	1053	C
1	a	1060	A
1	a	1061	U
1	a	1062	A
1	a	1070	A
1	a	1081	U
1	a	1083	A
1	a	1085	C
1	a	1087	A
1	a	1115	U
1	a	1116	C
1	a	1117	C
1	a	1121	G
1	a	1126	G
1	a	1133	A
1	a	1138	C
1	a	1143	A
1	a	1144	A
1	a	1148	A
1	a	1149	A
1	a	1153	C
1	a	1154	U
1	a	1166	G
1	a	1170	A
1	a	1181	A
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	1224	G
1	a	1231	C
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	1259	A
1	a	1263	U
1	a	1265	A

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Mol	Chain	Res	Type
1	a	1266	C
1	a	1269	G
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	1287	A
1	a	1288	U
1	a	1291	A
1	a	1292	C
1	a	1295	A
1	a	1298	G
1	a	1299	A
1	a	1301	A
1	a	1302	G
1	a	1303	C
1	a	1306	U
1	a	1308	U
1	a	1309	C
1	a	1310	U
1	a	1311	C
1	a	1312	G
1	a	1313	A
1	a	1314	U
1	a	1318	G
1	a	1320	G
1	a	1341	C
1	a	1342	U
1	a	1348	G
1	a	1350	U
1	a	1355	C
1	a	1364	U
1	a	1371	U
1	a	1372	U
1	a	1373	C
1	a	1374	C
1	a	1375	G
1	a	1378	A
1	a	1382	A
1	a	1396	A

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Mol	Chain	Res	Type
1	a	1397	U
1	a	1402	A
1	a	1404	U
1	a	1406	G
1	a	1409	A
1	a	1424	G
1	a	1428	G
1	a	1429	G
1	a	1453	C
1	a	1454	A
1	a	1462	U
1	a	1463	U
1	a	1464	C
1	a	1466	G
1	a	1476	A
1	a	1480	A
1	a	1487	A
1	a	1489	A
1	a	1490	G
1	a	1494	U
1	a	1498	A
1	a	1499	U
1	a	1507	G
1	a	1519	U
1	a	1520	G
1	a	1521	C
1	a	1522	A
1	a	1523	C
1	a	1533	A
1	a	1535	U
1	a	1536	G
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	1564	C
1	a	1567	G
1	a	1573	G
1	a	1574	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	1575	G
1	a	1578	U
1	a	1580	A
1	a	1585	U
1	a	1588	A
1	a	1601	A
1	a	1604	G
1	a	1606	G
1	a	1619	A
1	a	1621	U
1	a	1622	U
1	a	1623	A
1	a	1637	A
1	a	1638	G
1	a	1639	G
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	1695	A
1	a	1698	C
1	a	1699	A
1	a	1713	C
1	a	1721	U
1	a	1722	G
1	a	1724	A
1	a	1726	G
1	a	1748	G
1	a	1753	C
1	a	1757	G
1	a	1758	G
1	a	1774	C
1	a	1775	U
1	a	1777	G
1	a	1783	C
1	a	1784	G
1	a	1805	G
1	a	1815	A
1	a	1823	A
1	a	1824	A

Continued on next page...

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Mol	Chain	Res	Type
1	a	1825	A
1	a	1831	A
1	a	1836	G
1	a	1837	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
44	A	359	C
44	A	360	G
44	A	361	A
44	A	362	U
44	A	363	A
44	A	364	C
44	A	366	A
44	A	367	A
44	A	369	A
44	A	370	G
44	A	376	G
44	A	380	G
44	A	381	A
44	A	387	U
44	A	388	A
44	A	390	G
44	A	391	A
44	A	392	C
44	A	393	U
44	A	395	G
44	A	396	C
44	A	397	G
44	A	400	G
44	A	403	G
44	A	404	G
44	A	406	C
44	A	407	A
44	A	408	G
44	A	409	C

Continued on next page...

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Mol	Chain	Res	Type
44	A	410	A
44	A	411	C
44	A	414	G
44	A	418	G
44	A	419	U
44	A	420	C
44	A	422	U
44	A	423	G
44	A	424	U
44	A	425	A
44	A	426	U
44	A	427	U
44	A	428	A
44	A	429	U
44	A	430	G
44	A	431	G
44	A	434	U
44	A	435	U
44	A	436	U
44	A	438	C
44	A	440	A
44	A	443	A
44	A	446	U
44	A	452	U
44	A	453	G
44	A	457	U
44	A	458	A
44	A	459	G
44	A	460	U
44	A	462	U
44	A	463	U
44	A	465	A
44	A	466	A
44	A	467	C
44	A	468	U
44	A	472	G
44	A	473	U
44	A	477	G
44	A	478	A
44	A	480	U
44	A	482	U
44	A	483	A

Continued on next page...

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Mol	Chain	Res	Type
44	A	484	C
44	A	485	U
44	A	486	U
44	A	487	G
44	A	488	G
44	A	489	C
44	A	490	A
44	A	491	U
44	A	492	G
44	A	493	U
44	A	494	A
44	A	496	A
44	A	497	C
44	A	498	C
44	A	499	U
44	A	500	G
44	A	504	A
44	A	505	G
44	A	506	U
44	A	507	U
44	A	508	A
44	A	509	G
44	A	510	C
44	A	513	U
44	A	515	G
44	A	516	U
44	A	518	G
44	A	519	A
44	A	521	A
44	A	527	C
44	A	530	C
44	A	532	G
44	A	534	U
44	A	537	G
44	A	538	G
44	A	539	U
44	A	540	A
44	A	541	C
44	A	542	A
44	A	543	G
44	A	544	U
44	A	545	A

Continued on next page...

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Mol	Chain	Res	Type
44	A	546	G
44	A	547	G
44	A	550	A
44	A	552	A
44	A	553	C
44	A	554	C
44	A	556	C
44	A	557	A
44	A	559	A
44	A	560	U
44	A	561	A
44	A	565	G
44	A	569	U
44	A	572	U
44	A	575	U
44	A	576	U
44	A	577	A
44	A	578	G
44	A	579	A
44	A	581	A
44	A	583	G
44	A	584	A
44	A	585	A
44	A	588	U
44	A	590	A
44	A	591	G
44	A	593	G
44	A	605	G
44	A	608	U
44	A	611	U
44	A	615	A
44	A	619	G
44	A	620	A
44	A	621	G
44	A	625	G
44	A	626	U
44	A	627	G
44	A	628	A
44	A	637	G
44	A	638	C
44	A	640	C
44	A	641	C

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Mol	Chain	Res	Type
44	A	642	U
44	A	643	G
44	A	644	A
44	A	646	G
44	A	647	C
44	A	648	A
44	A	649	A
44	A	656	G
44	A	657	U
44	A	658	C
44	A	659	U
44	A	660	U
44	A	662	C
44	A	678	A
44	A	679	U
44	A	680	A
44	A	681	A
44	A	685	G
44	A	686	U
44	A	691	G

All (23) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
44	A	369	A
44	A	387	U
44	A	409	C
44	A	419	U
44	A	425	A
44	A	428	A
44	A	456	C
44	A	465	A
44	A	485	U
44	A	508	A
44	A	518	G
44	A	526	A
44	A	559	A
44	A	561	A
44	A	578	G
44	A	619	G
44	A	626	U
44	A	642	U

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Mol	Chain	Res	Type
44	A	644	A
44	A	655	G
44	A	656	G
44	A	657	U
44	A	679	U

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	a	834:C	O3'	841:G	P	19.31
1	a	697:G	O3'	729:C	P	19.00
1	a	756:C	O3'	788:G	P	16.00
1	a	323:C	O3'	329:G	P	15.98
1	a	130:G	O3'	141:A	P	15.87
1	a	1761:U	O3'	1771:G	P	15.37
1	a	1417:C	O3'	1423:C	P	15.01
1	a	225:G	O3'	287:U	P	7.13
1	a	745:C	O3'	749:U	P	6.54
1	a	1432:U	O3'	1438:A	P	4.95
1	a	886:A	O3'	887:U	P	4.63
1	a	903:A	O3'	904:A	P	4.52
1	a	798:G	O3'	799:U	P	3.46
1	a	902:G	O3'	903:A	P	3.40
1	a	736:C	O3'	743:U	P	3.18

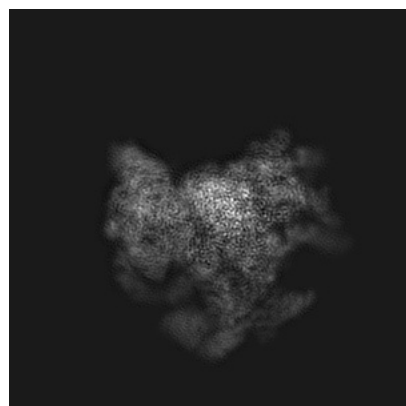
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21530. These allow visual inspection of the internal detail of the map and identification of artifacts.

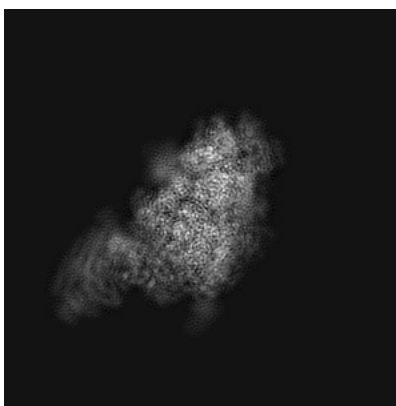
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

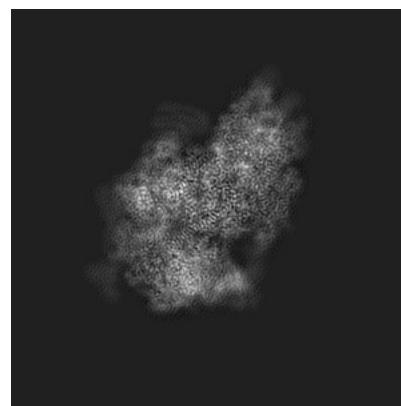
6.1.1 Primary map



X

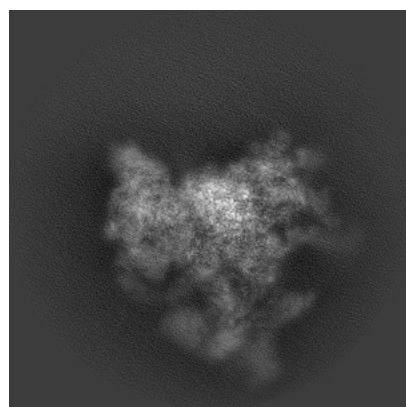


Y

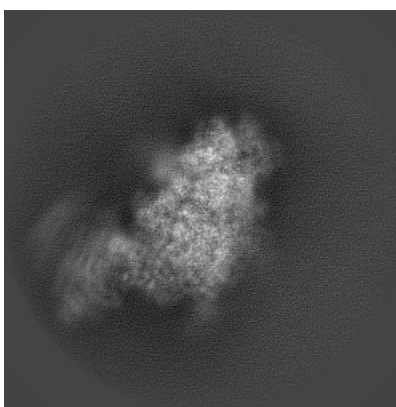


Z

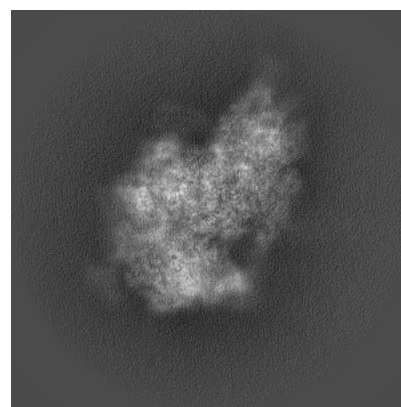
6.1.2 Raw map



X



Y

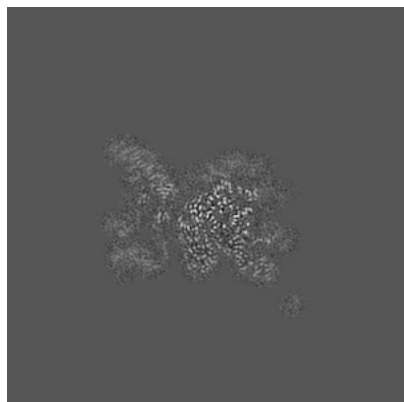


Z

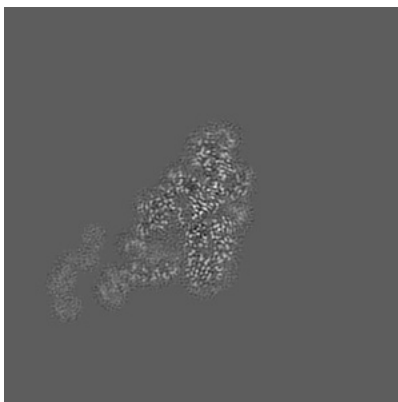
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

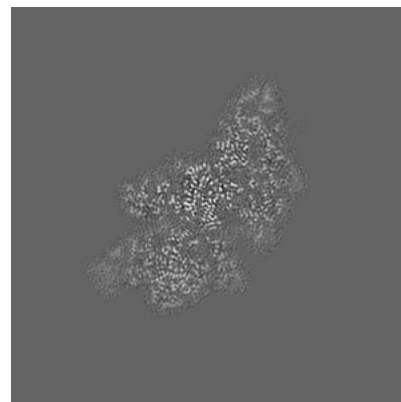
6.2.1 Primary map



X Index: 200

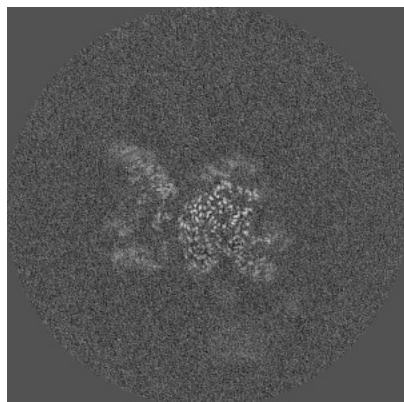


Y Index: 200

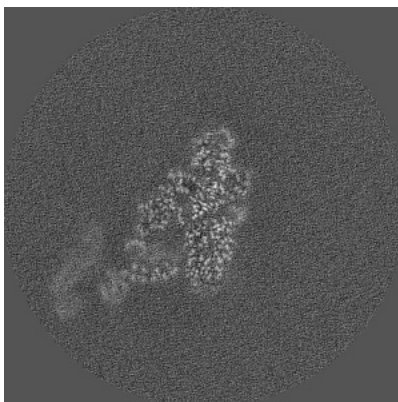


Z Index: 200

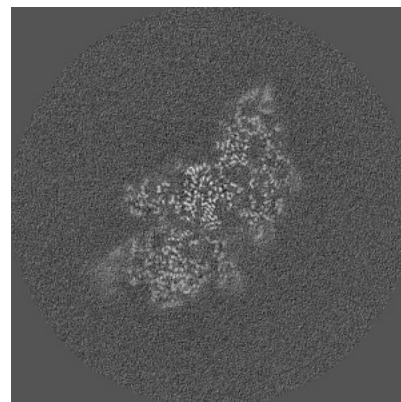
6.2.2 Raw map



X Index: 200



Y Index: 200

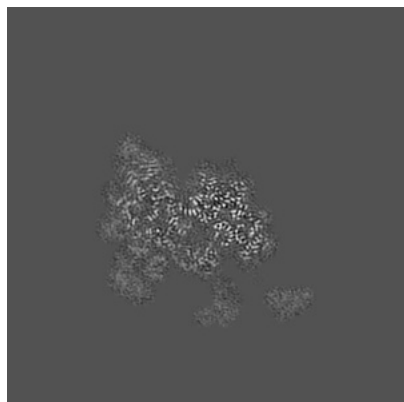


Z Index: 200

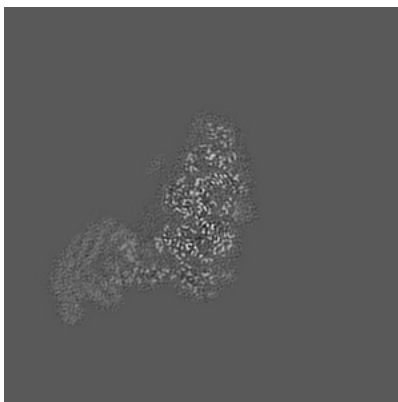
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

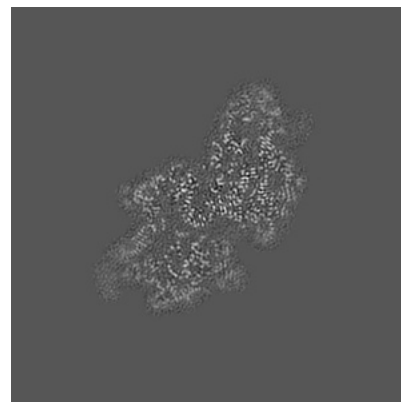
6.3.1 Primary map



X Index: 179

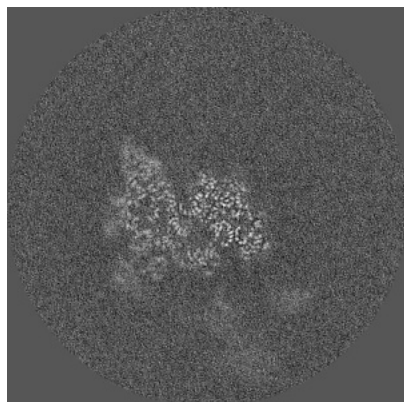


Y Index: 214

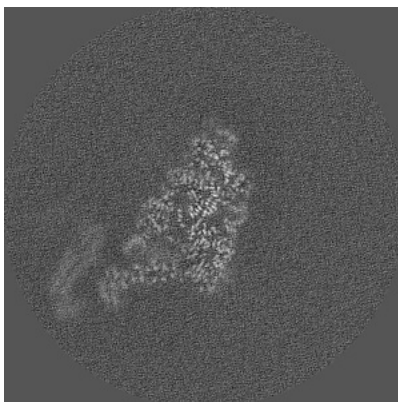


Z Index: 207

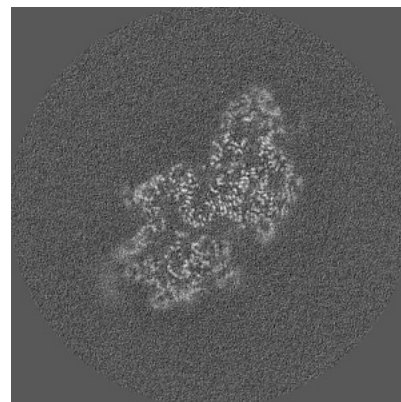
6.3.2 Raw map



X Index: 180



Y Index: 203

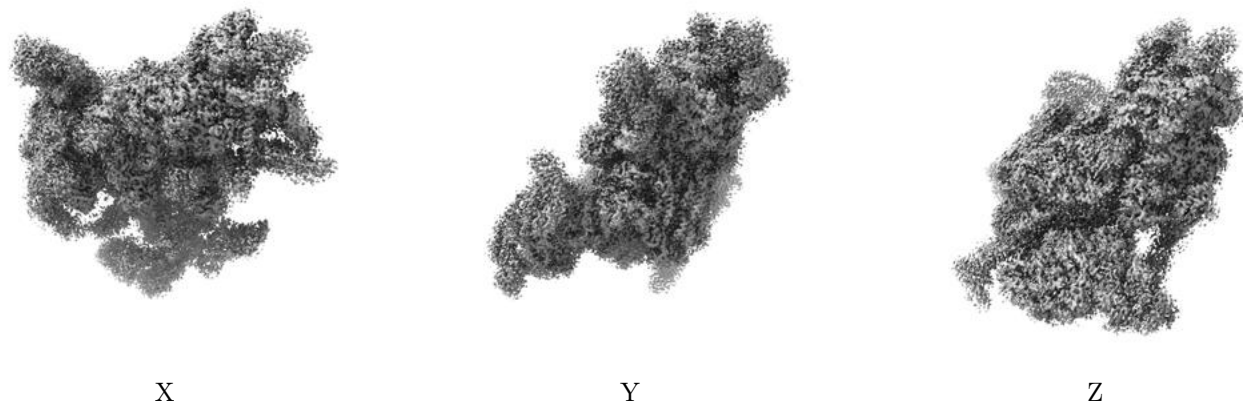


Z Index: 207

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

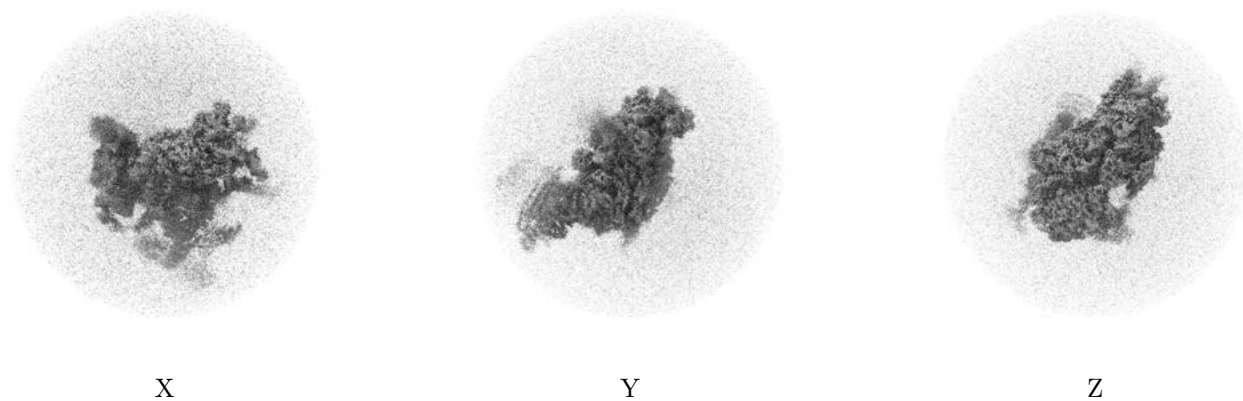
6.4 Orthogonal surface views [i](#)

6.4.1 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.

6.4.2 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.

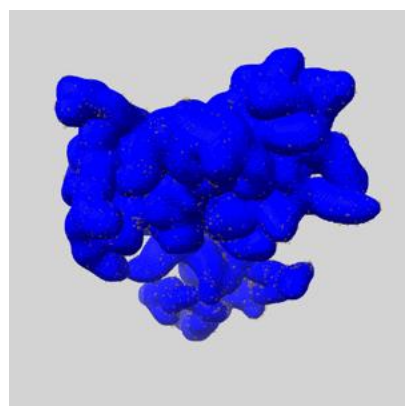
6.5 Mask visualisation [i](#)

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

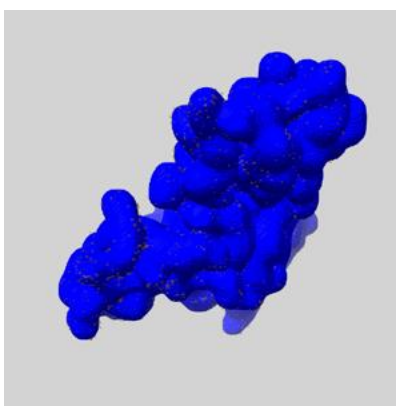
A mask typically either:

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

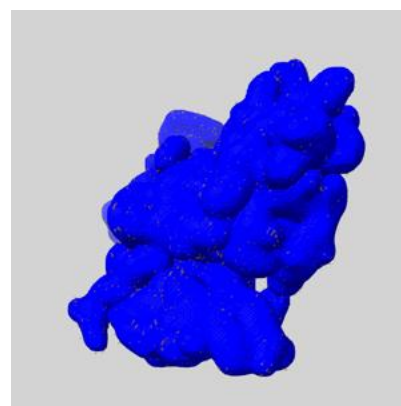
6.5.1 emd_21530_msk_1.map [i](#)



X



Y

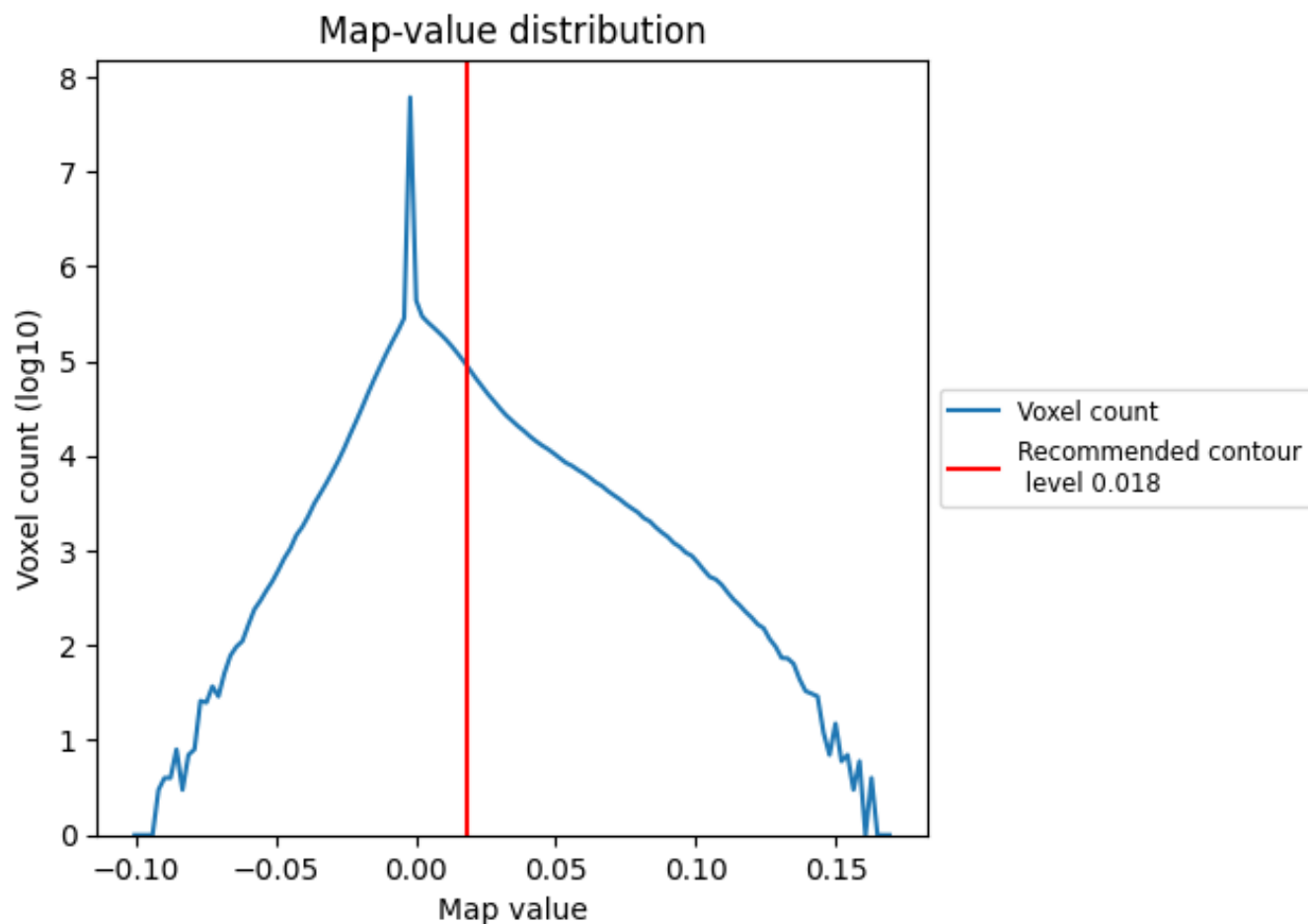


Z

7 Map analysis [i](#)

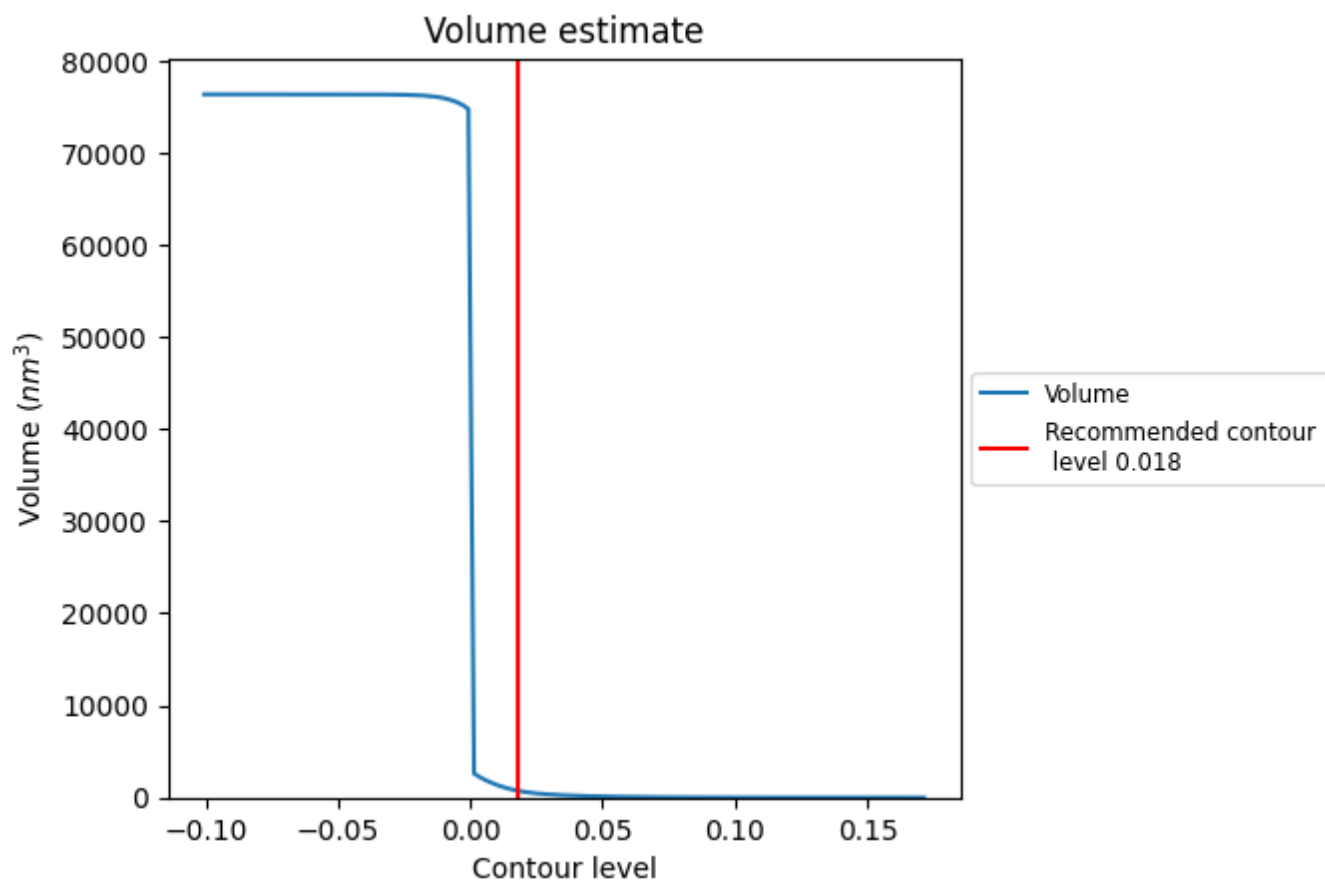
This section contains the results of statistical analysis of the map.

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.

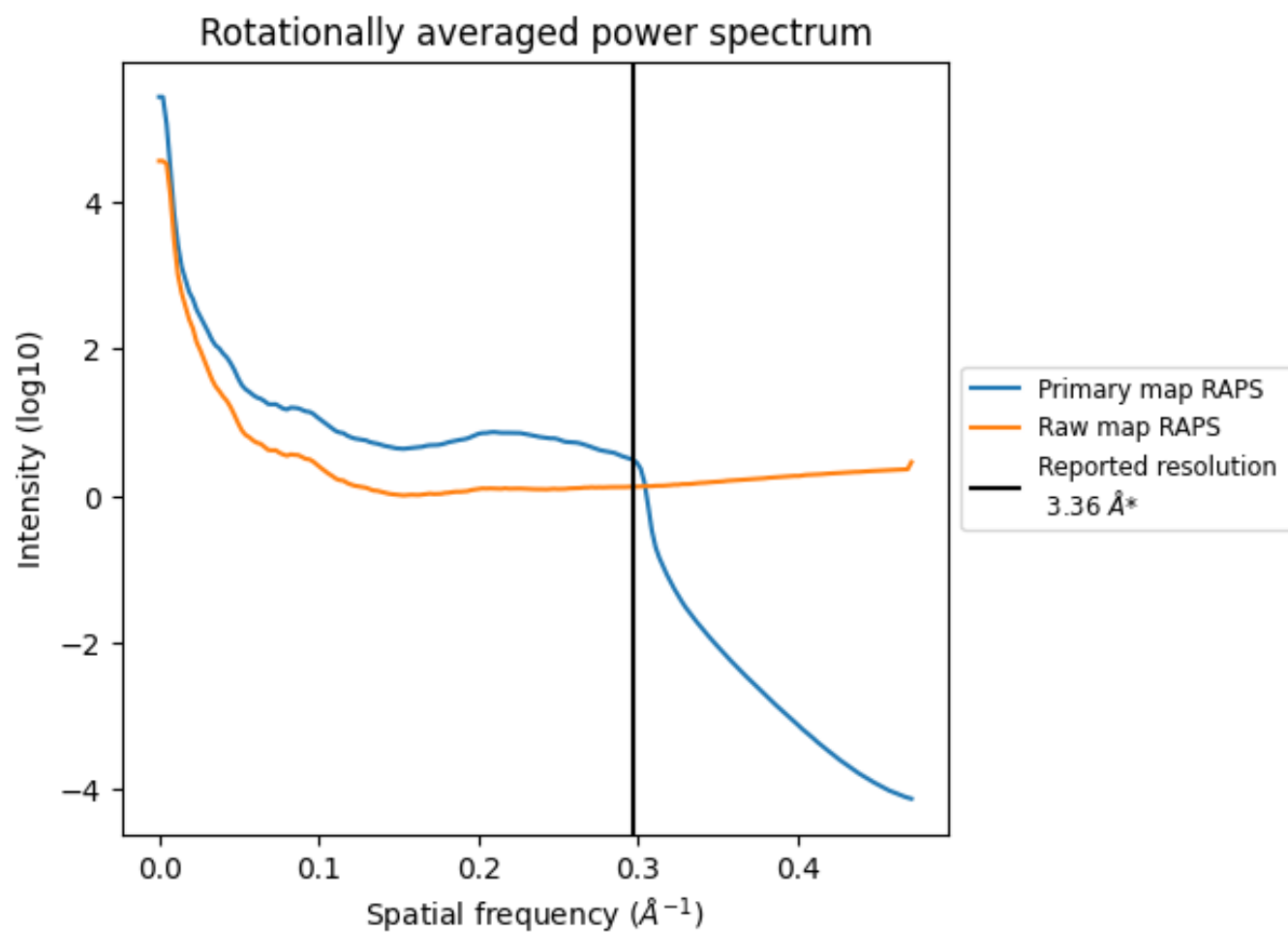
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 744 nm³; this corresponds to an approximate mass of 672 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 ⓘ

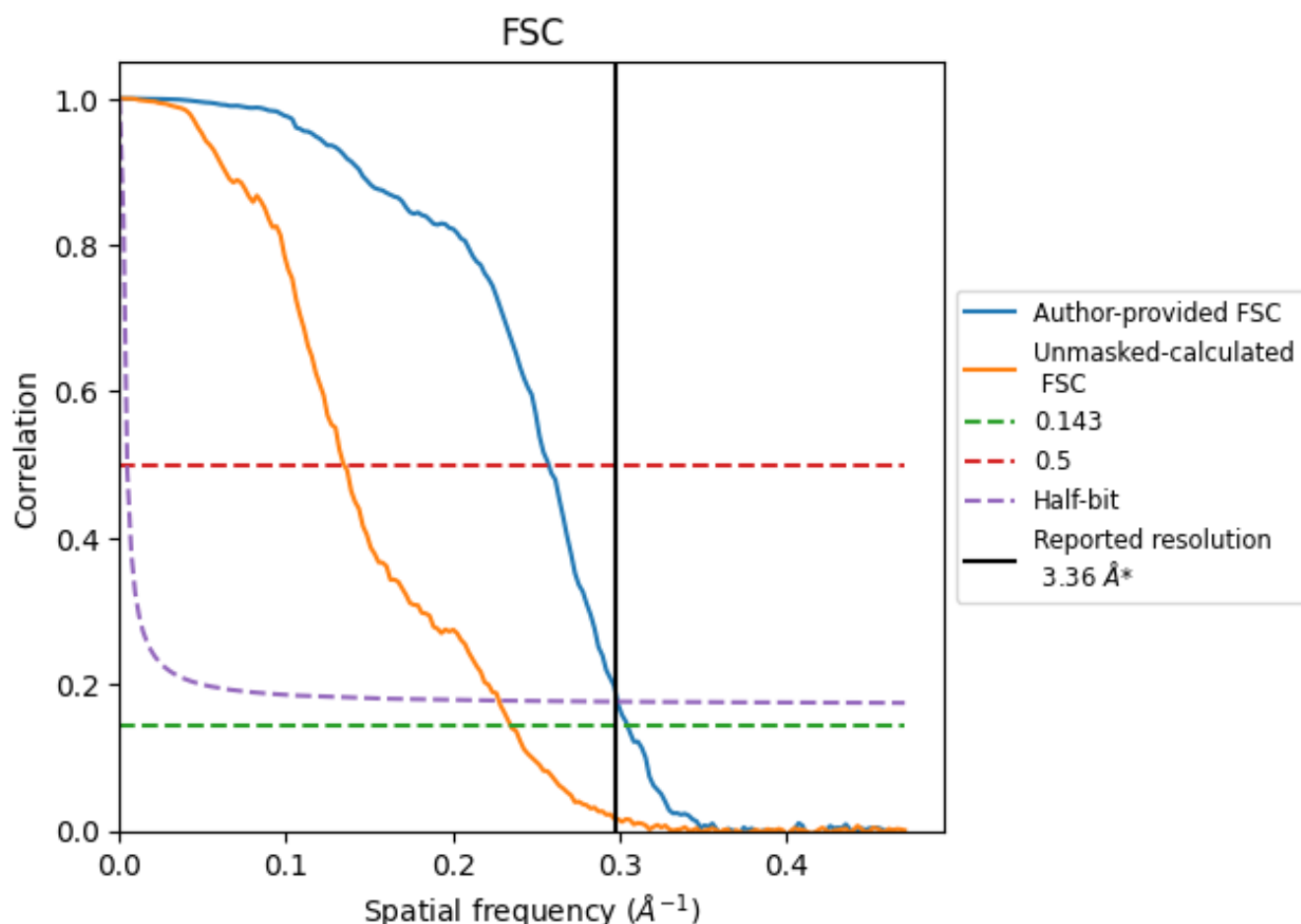


*Reported resolution corresponds to spatial frequency of 0.298 Å⁻¹

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 0.298 Å⁻¹

8.2 Resolution estimates [i](#)

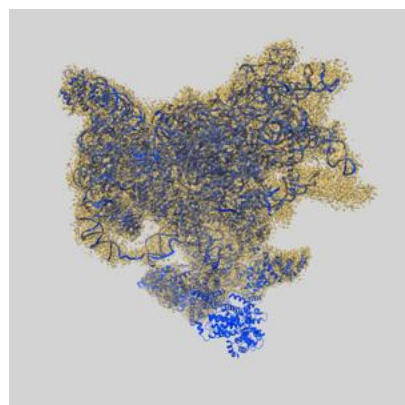
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.36	-	-
Author-provided FSC curve	3.28	3.88	3.34
Unmasked-calculated*	4.26	7.42	4.39

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.26 differs from the reported value 3.36 by more than 10 %

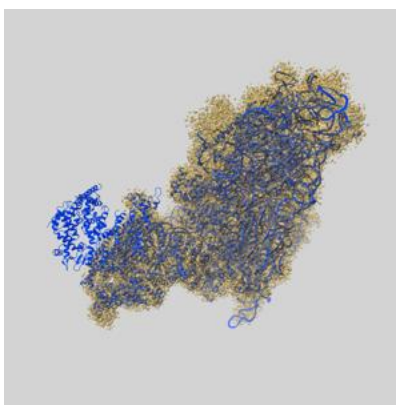
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21530 and PDB model 6W2T. Per-residue inclusion information can be found in section [3](#) on page [13](#).

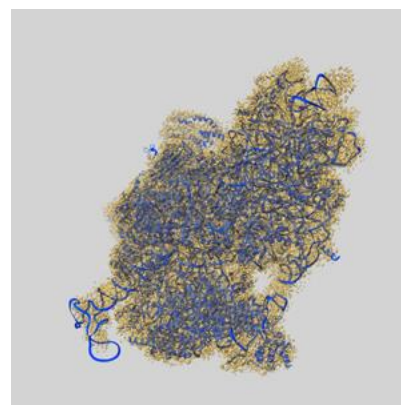
9.1 Map-model overlay [i](#)



X



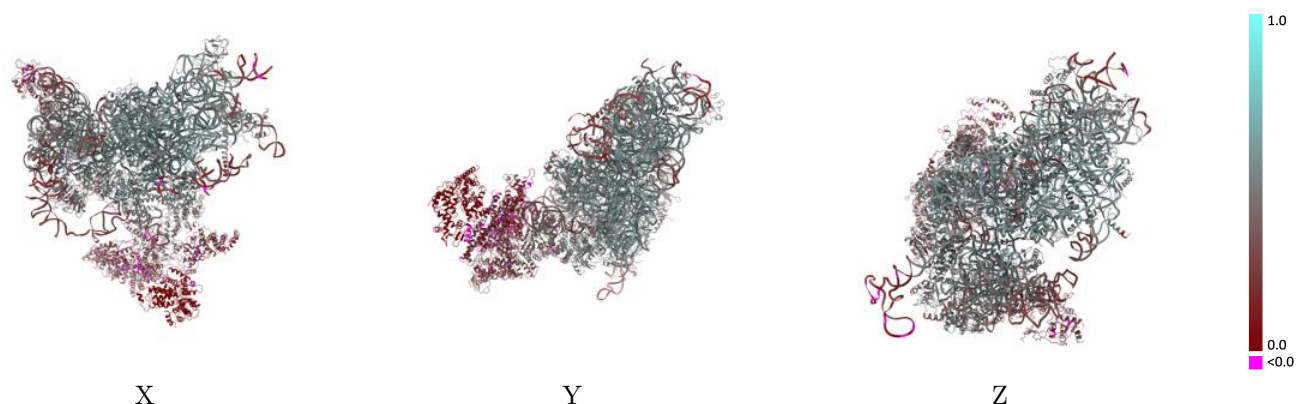
Y



Z

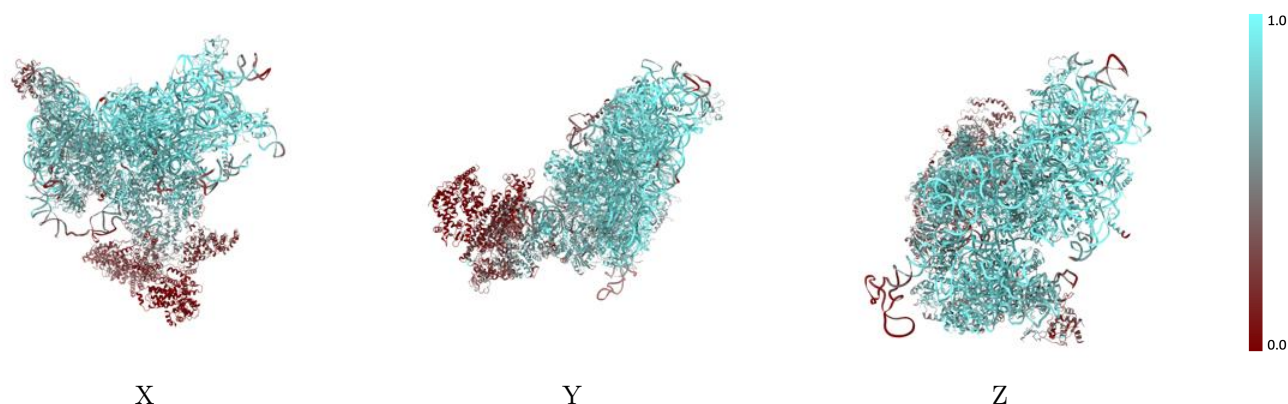
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



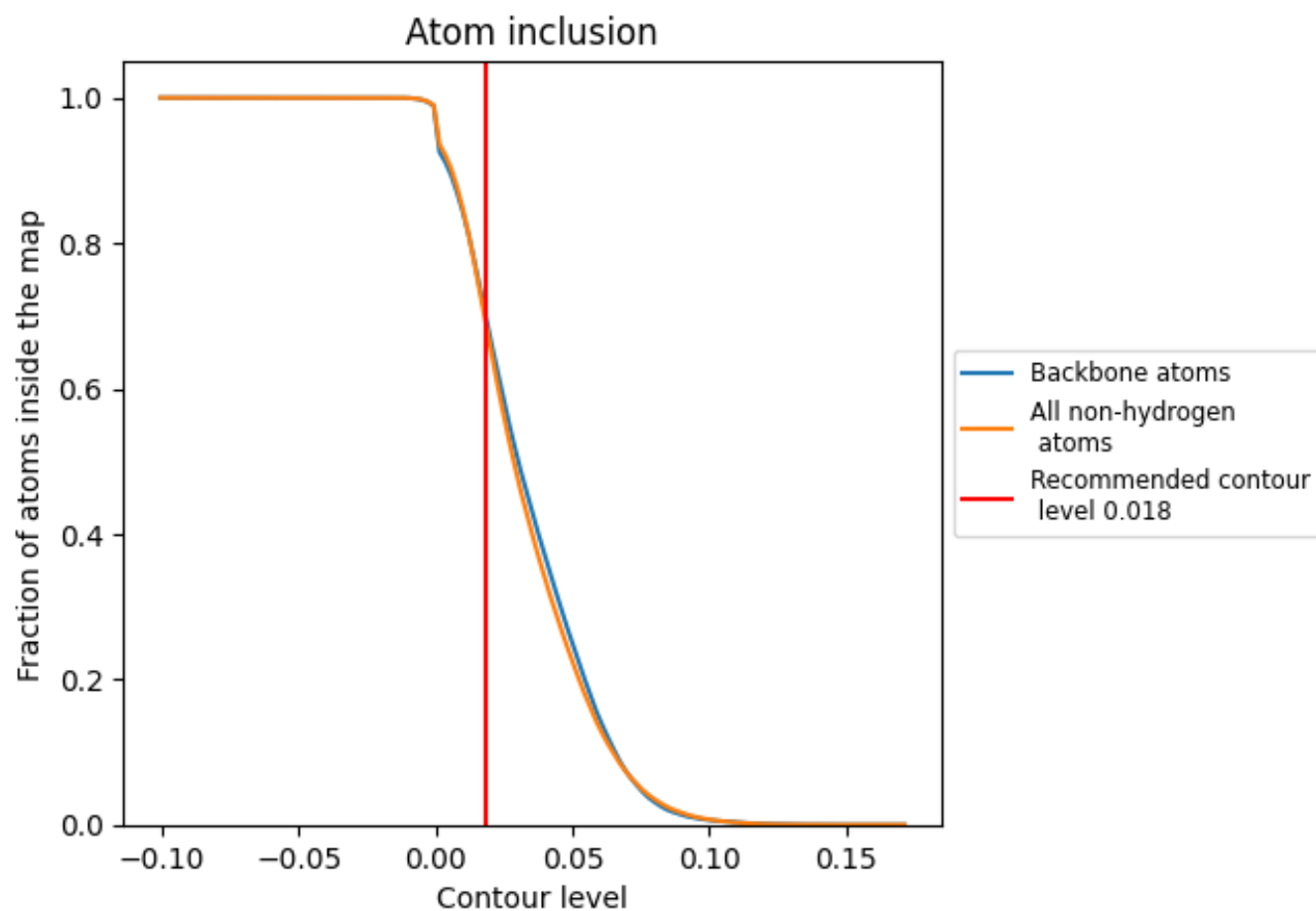
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 70% 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	 0.6971	 0.4200
1	 0.5875	 0.3650
2	 0.6053	 0.3800
3	 0.2038	 0.2040
4	 0.1624	 0.2030
5	 0.1474	 0.1910
6	 0.0088	 0.0160
7	 0.0072	 0.0140
8	 0.1808	 0.2210
9	 0.6433	 0.4360
A	 0.5407	 0.2720
B	 0.8364	 0.5310
C	 0.8458	 0.5390
D	 0.8629	 0.5460
E	 0.7467	 0.4640
F	 0.8710	 0.5530
G	 0.8014	 0.5090
H	 0.7811	 0.4670
I	 0.7988	 0.4940
J	 0.8525	 0.5120
K	 0.8567	 0.5260
L	 0.6772	 0.3900
M	 0.8965	 0.5610
N	 0.2919	 0.2630
O	 0.8688	 0.5460
P	 0.8318	 0.5390
Q	 0.6080	 0.3530
R	 0.8288	 0.5210
S	 0.7736	 0.4880
T	 0.6952	 0.4180
U	 0.8285	 0.5070
V	 0.7455	 0.4630
W	 0.8742	 0.5430
X	 0.9069	 0.5650
Y	 0.8824	 0.5520



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Chain	Atom inclusion	Q-score
Z	 0.8583	 0.5240
a	 0.9084	 0.5020
b	 0.8533	 0.5480
c	 0.8294	 0.5350
d	 0.7170	 0.4940
e	 0.8390	 0.4950
f	 0.6909	 0.4590
g	 0.3759	 0.3030
h	 0.7060	 0.4240
i	 0.7050	 0.4470