



Full wwPDB EM Validation Report ⓘ

Mar 30, 2026 – 07:05 AM UTC

PDB ID : 6ZVJ / pdb_00006zvj
EMDB ID : EMD-11458
Title : Structure of a human ABCE1-bound 43S pre-initiation complex - State II
Authors : Kratzat, H.; Mackens-Kiani, T.; Ameismeier, A.; Cheng, J.; Berninghausen, O.; Becker, T.; Beckmann, R.
Deposited on : 2020-07-24
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

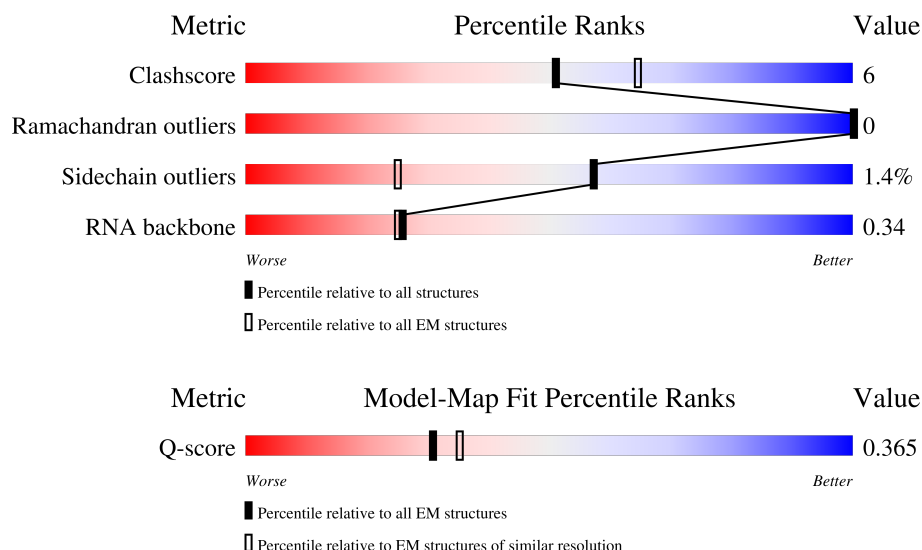
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	10198 (3.30 - 4.30)

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	216	 88% 12%
2	p	211	 81% 19%
3	d	216	 85% 14%

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Mol	Chain	Length	Quality of chain
4	Q	101	
5	q	255	
6	W	24	
7	r	222	
8	s	181	
9	t	205	
10	c	180	
11	n	144	
12	m	149	
13	i	125	
14	y	82	
15	f	129	
16	j	139	
17	z	122	
18	R	82	
19	T	44	
20	2	1720	
21	w	130	
22	g	138	
23	b	224	
24	e	189	
25	u	95	
26	v	116	
27	o	119	
28	k	140	

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Mol	Chain	Length	Quality of chain
29	x	141	
30	h	98	
31	P	70	
32	S	61	
33	l	54	
34	U	62	
35	V	309	
36	I	316	
37	B	566	
38	A	722	
39	C	743	
40	E	429	
41	F	269	
42	H	318	
43	K	217	
44	L	372	
45	M	362	
46	l	595	
47	N	91	
48	D	527	
49	Y	78	
50	G	258	
50	J	258	

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 115020 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	216	Total	C	N	O	S	0	0
			1706	1083	299	316	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	p	211	Total	C	N	O	S	0	0
			1716	1088	307	307	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	d	216	Total	C	N	O	S	0	0
			1675	1085	287	293	10		

- Molecule 4 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Q	101	Total	C	N	O	S	0	0
			815	507	170	133	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	q	255	Total	C	N	O	S	0	0
			2032	1299	377	348	8		

- Molecule 6 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	W	24	Total	C	N	O	S	0	0
			231	139	62	27	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	r	222	Total	C	N	O	S	0	0
			1795	1123	357	309	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	s	173	Total	C	N	O	S	0	0
			1400	898	256	245	1		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
s	8	ILE	GLY	conflict	UNP P62081
s	9	VAL	GLU	conflict	UNP P62081
s	12	ASN	ASP	conflict	UNP P62081

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	t	199	Total	C	N	O	S	0	0
			1639	1027	322	285	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	c	180	Total	C	N	O	S	0	0
			1500	955	300	243	2		

- Molecule 11 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	n	135	Total	C	N	O	S	0	0
			1120	715	211	188	6		

- Molecule 12 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	m	149	Total	C	N	O	S	0	0
			1203	770	228	204	1		

- Molecule 13 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	i	125	Total	C	N	O	S	0	0
			940	574	187	173	6		

- Molecule 14 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	y	82	Total	C	N	O	S	0	0
			626	384	116	121	5		

- Molecule 15 is a protein called 40S ribosomal protein S15a.

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

- Molecule 16 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	j	139	Total	C	N	O	S	0	0
			1081	682	214	182	3		

- Molecule 17 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	z	122	Total	C	N	O	S	0	0
			1000	633	196	166	5		

- Molecule 18 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	82	Total	C	N	O	S	0	0
			641	402	118	114	7		

- Molecule 19 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	44	Total	C	N	O	S	0	0
			355	216	81	57	1		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	54	GLY	VAL	conflict	UNP P62861
T	56	ASN	THR	conflict	UNP P62861
T	57	ALA	PHE	conflict	UNP P62861
T	58	ASN	GLY	conflict	UNP P62861

- Molecule 20 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	2	1720	Total	C	N	O	P	0	0
			36700	16391	6600	11998	1711		

- Molecule 21 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	w	128	Total	C	N	O	S	0	0
			1011	641	182	184	4		

- Molecule 22 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	g	138	Total	C	N	O	S	0	0
			1100	699	208	190	3		

- Molecule 23 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	b	224	Total	C	N	O	S	0	0
			1746	1112	314	313	7		

- Molecule 24 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	e	189	Total	C	N	O	S	0	0
			1495	934	284	270	7		

- Molecule 25 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	u	95	Total	C	N	O	S	0	0
			800	524	139	131	6		

- Molecule 26 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	v	111	Total	C	N	O	S	0	0
			862	544	151	160	7		

- Molecule 27 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	o	119	Total	C	N	O	S	0	0
			980	623	183	167	7		

- Molecule 28 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	k	140	Total	C	N	O	S	0	0
			1163	731	234	197	1		

- Molecule 29 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	x	141	Total	C	N	O	S	0	0
			1095	685	210	197	3		

- Molecule 30 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	h	98	Total	C	N	O	S	0	0
			781	489	148	140	4		

- Molecule 31 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	P	70	Total	C	N	O	S	0	0
			558	358	101	98	1		

- Molecule 32 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	S	61	Total	C	N	O	S	0	0
			480	292	95	91	2		

- Molecule 33 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	1	54	Total	C	N	O	S	0	0
			451	282	93	71	5		

- Molecule 34 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	U	57	Total	C	N	O	S	0	0
			466	295	89	75	7		

- Molecule 35 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	V	296	Total	C	N	O	S	0	0
			2315	1464	404	435	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	I	305	Total	C	N	O	S	0	0
			1497	887	305	305			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	B	536	Total	C	N	O	S	0	0
			2966	1801	580	580	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	A	692	Total	C	N	O	S	0	0
			5384	3378	980	1004	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	C	625	Total	C	N	O	S	0	0
			5073	3205	899	934	35		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	130	MET	-	insertion	UNP B4DVU3
C	131	ASN	HIS	conflict	UNP B4DVU3
C	132	LYS	ASP	conflict	UNP B4DVU3
C	133	ASN	ARG	conflict	UNP B4DVU3
C	134	ASN	LYS	conflict	UNP B4DVU3
C	135	ALA	SER	conflict	UNP B4DVU3
C	137	ALA	ARG	conflict	UNP B4DVU3
C	?	-	ASP	deletion	UNP B4DVU3
C	?	-	GLU	deletion	UNP B4DVU3
C	?	-	GLU	deletion	UNP B4DVU3
C	?	-	GLU	deletion	UNP B4DVU3
C	?	-	GLU	deletion	UNP B4DVU3
C	?	-	ASP	deletion	UNP B4DVU3
C	?	-	ASN	deletion	UNP B4DVU3
C	?	-	GLU	deletion	UNP B4DVU3
C	?	-	GLY	deletion	UNP B4DVU3
C	?	-	GLY	deletion	UNP B4DVU3
C	?	-	GLU	deletion	UNP B4DVU3
C	?	-	TRP	deletion	UNP B4DVU3
C	?	-	GLU	deletion	UNP B4DVU3
C	?	-	ARG	deletion	UNP B4DVU3
C	?	-	VAL	deletion	UNP B4DVU3
C	?	-	ARG	deletion	UNP B4DVU3
C	?	-	GLY	deletion	UNP B4DVU3
C	?	-	GLY	deletion	UNP B4DVU3
C	?	-	VAL	deletion	UNP B4DVU3
C	139	SER	PRO	conflict	UNP B4DVU3
C	140	THR	LEU	conflict	UNP B4DVU3
C	141	LEU	VAL	conflict	UNP B4DVU3
C	142	ARG	LYS	conflict	UNP B4DVU3
C	143	GLN	GLU	conflict	UNP B4DVU3
C	145	ILE	PRO	conflict	UNP B4DVU3
C	146	ARG	LYS	conflict	UNP B4DVU3
C	147	LYS	MET	conflict	UNP B4DVU3
C	148	TYR	PHE	conflict	UNP B4DVU3
C	149	ASN	ALA	conflict	UNP B4DVU3

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	E	416	Total	C	N	O	S	0	0
			3437	2202	585	630	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	F	269	Total	C	N	O	S	0	0
			2090	1317	356	405	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	H	295	Total	C	N	O	S	0	0
			2413	1532	417	449	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	K	217	Total	C	N	O	S	0	0
			1750	1116	288	334	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
44	L	372	Total	C	N	O	S	0	0
			3112	2011	520	564	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
45	M	340	Total	C	N	O	S	0	0
			2718	1734	459	508	17		

- Molecule 46 is a protein called ATP-binding cassette sub-family E member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	1	576	Total	C	N	O	S	0	0
			4542	2899	779	836	28		

- Molecule 47 is a protein called Eukaryotic translation initiation factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	N	91	Total	C	N	O	S	0	0
			728	460	131	135	2		

- Molecule 48 is a protein called Eukaryotic translation initiation factor 3 subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	D	447	Total	C	N	O	S	0	0
			3618	2279	625	692	22		

- Molecule 49 is a protein called RNA recognition motif (unknown).

Mol	Chain	Residues	Atoms				AltConf	Trace
49	Y	78	Total	C	N	O	0	0
			390	234	78	78		

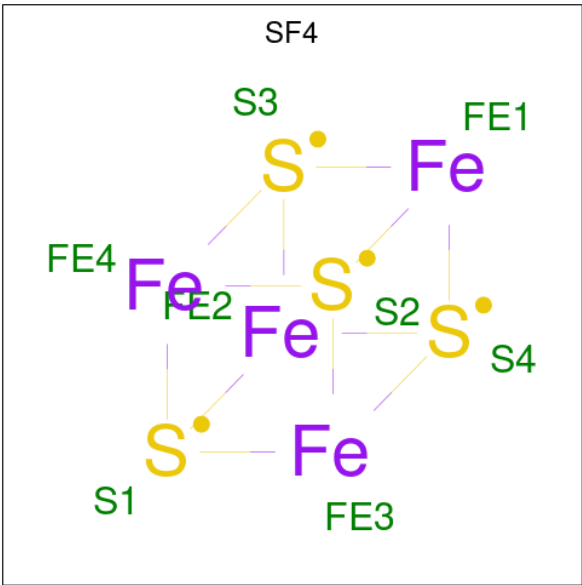
- Molecule 50 is a protein called Eukaryotic translation initiation factor 3 subunit J.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	G	70	Total	C	N	O	0	0
			348	208	70	70		
50	J	73	Total	C	N	O	0	0
			363	217	73	73		

- Molecule 51 is ZINC ION (CCD ID: ZN) (formula: Zn).

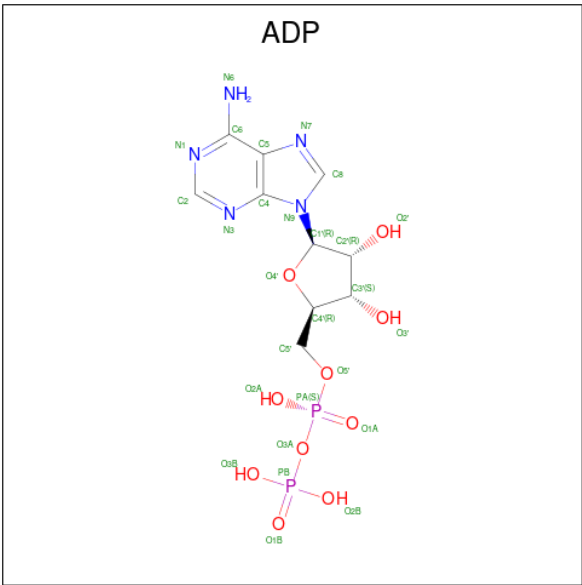
Mol	Chain	Residues	Atoms		AltConf
51	Q	1	Total	Zn	0
			1	1	
51	l	1	Total	Zn	0
			1	1	
51	U	1	Total	Zn	0
			1	1	

- Molecule 52 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			AltConf
52	1	1	Total	Fe	S	0
			8	4	4	
52	1	1	Total	Fe	S	0
			8	4	4	

- Molecule 53 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

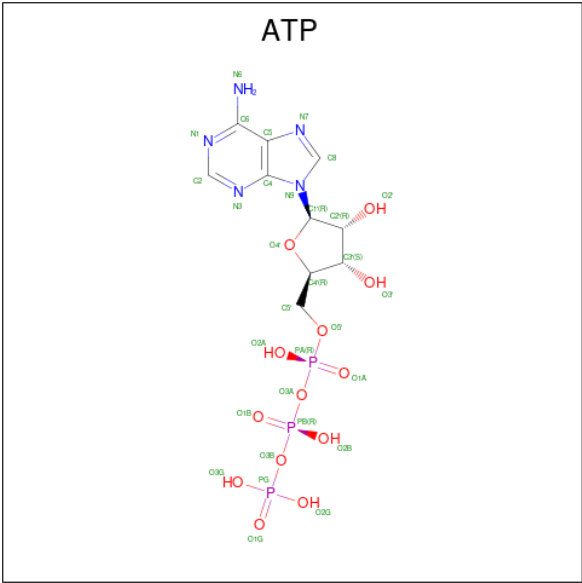


Mol	Chain	Residues	Atoms					AltConf
53	1	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
54	1	2	Total	Mg	0
			2	2	

- Molecule 55 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

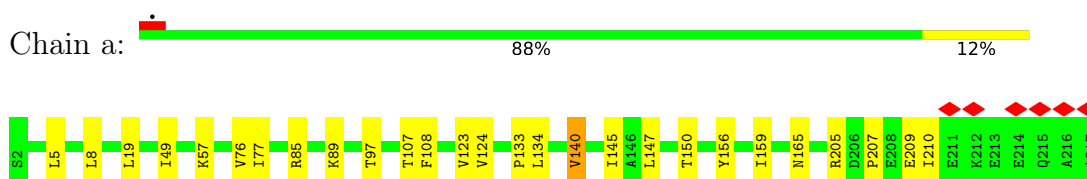


Mol	Chain	Residues	Atoms					AltConf
55	1	1	Total	C	N	O	P	0
			31	10	5	13	3	

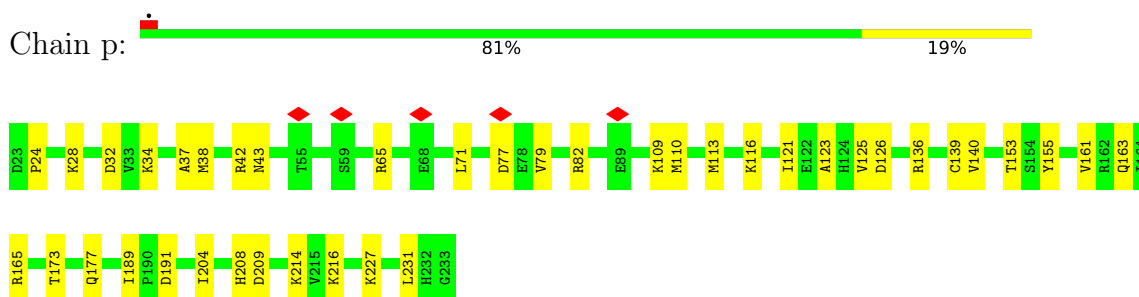
3 Residue-property plots

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.

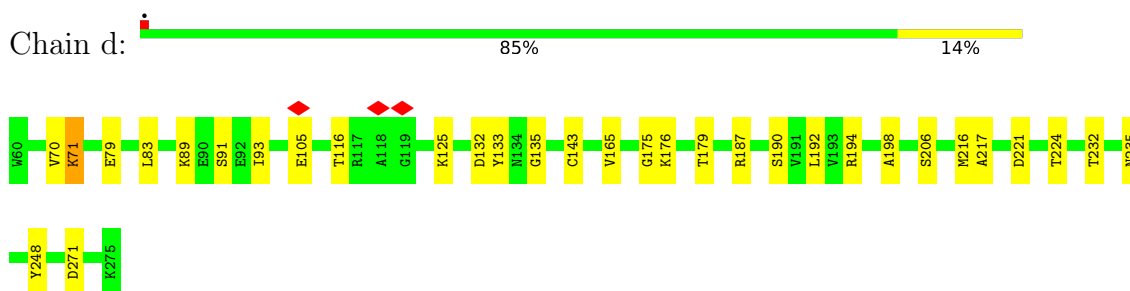
- Molecule 1: 40S ribosomal protein SA



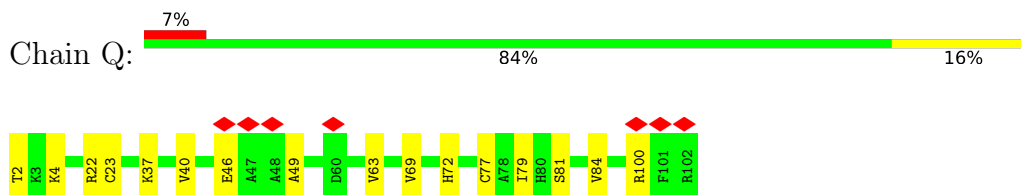
- Molecule 2: 40S ribosomal protein S3a



- Molecule 3: 40S ribosomal protein S2

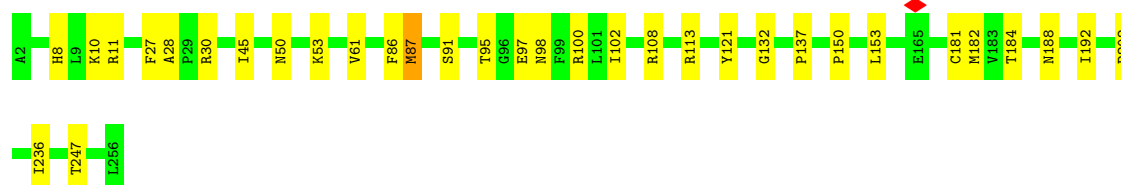


- Molecule 4: 40S ribosomal protein S26



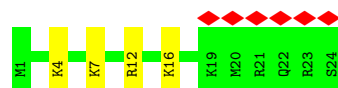
- Molecule 5: 40S ribosomal protein S4, X isoform

Chain q:  87% 13%



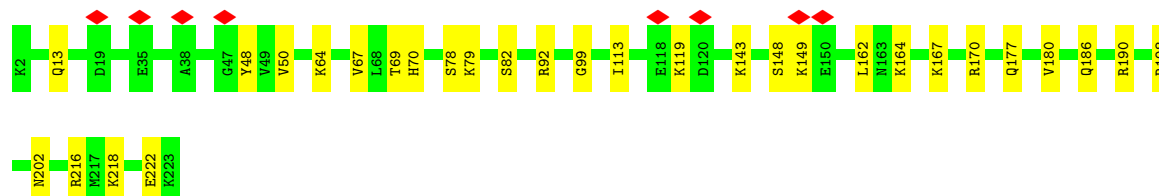
- Molecule 6: 60S ribosomal protein L41

Chain W:  25% 83% 17%



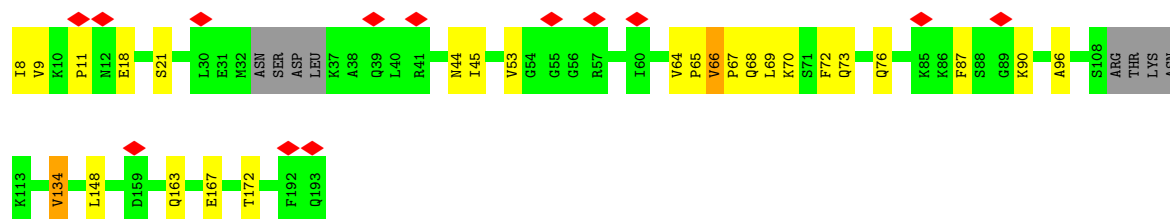
- Molecule 7: 40S ribosomal protein S6

Chain r:  86% 14%



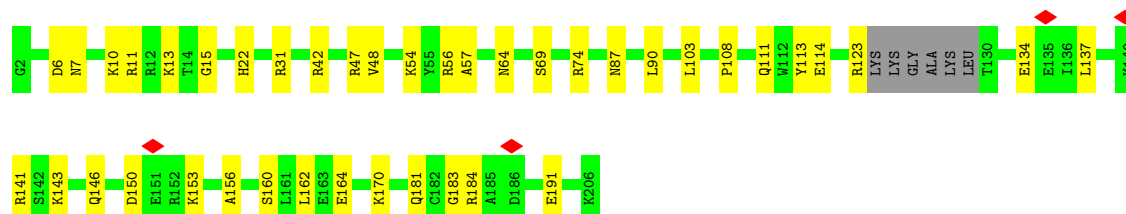
- Molecule 8: 40S ribosomal protein S7

Chain s:  7% 81% 13%



- Molecule 9: 40S ribosomal protein S8

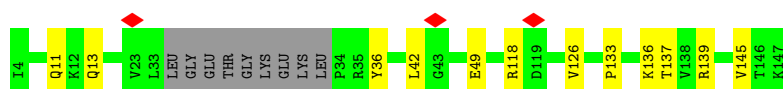
Chain t:  77% 20%



• Molecule 10: 40S ribosomal protein S9

Chain c:  86% 14%

• Molecule 11: 40S ribosomal protein S11

Chain n:  85% 8% 6%

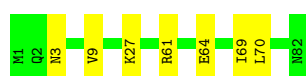
• Molecule 12: 40S ribosomal protein S13

Chain m:  90% 10%

• Molecule 13: 40S ribosomal protein S14

Chain i:  82% 18%

• Molecule 14: 40S ribosomal protein S21

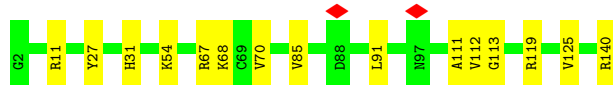
Chain y:  91% 9%

• Molecule 15: 40S ribosomal protein S15a

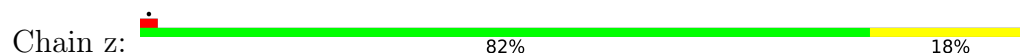
Chain f:  88% 12%

• Molecule 16: 40S ribosomal protein S23

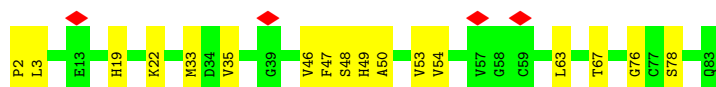
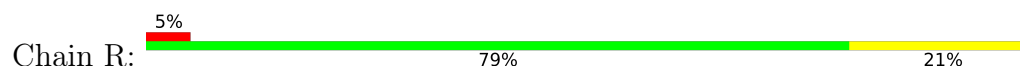
Chain j:  89% 11%



- Molecule 17: 40S ribosomal protein S24



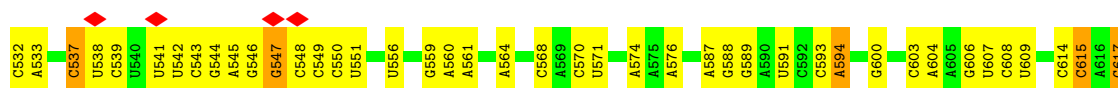
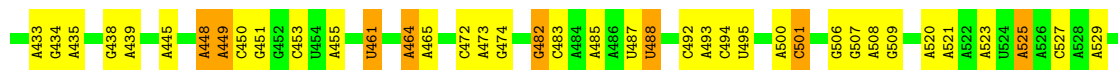
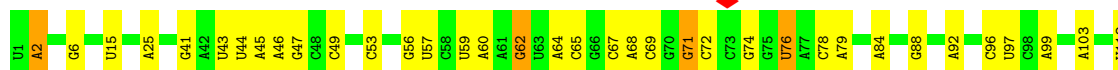
- Molecule 18: 40S ribosomal protein S27

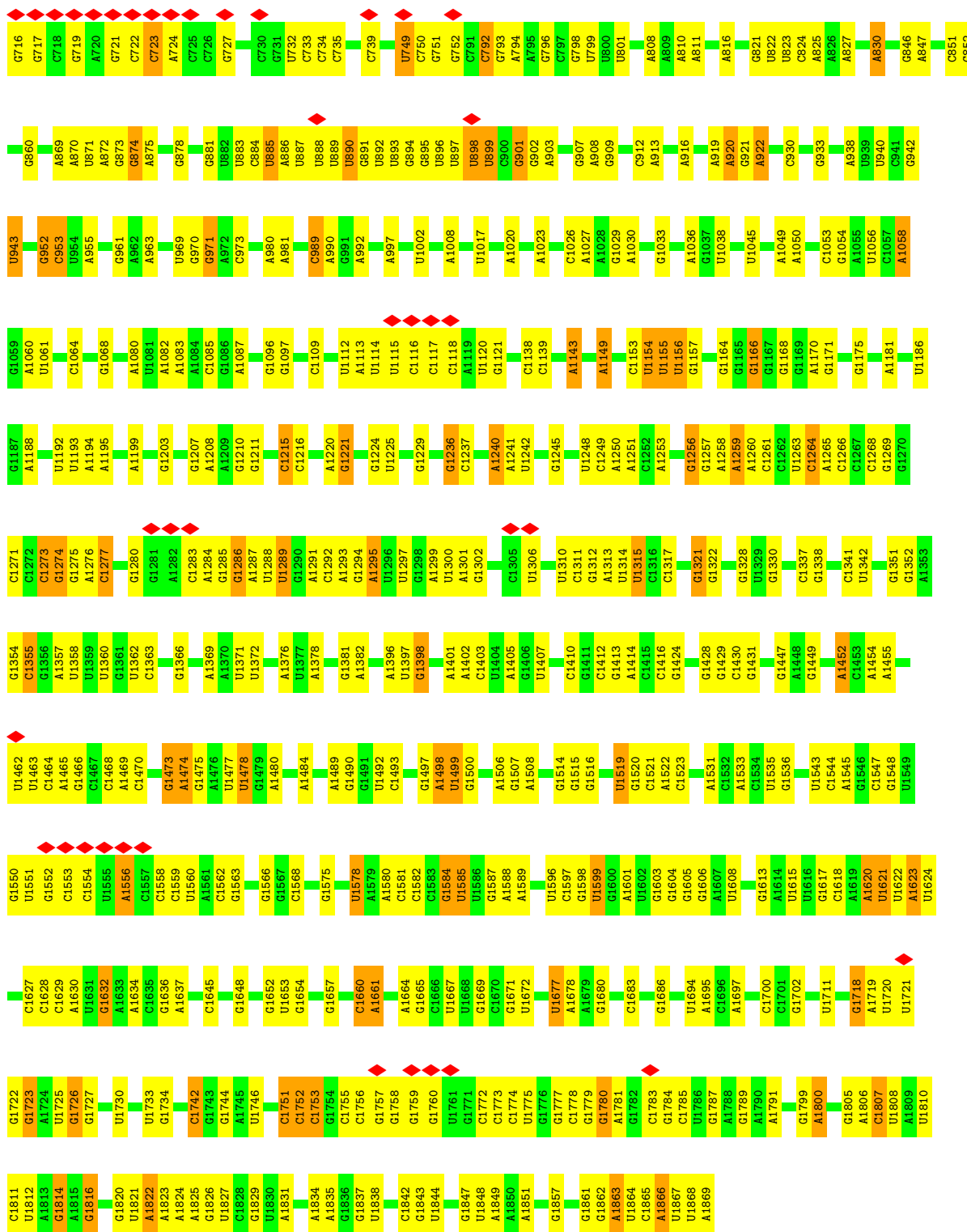


- Molecule 19: 40S ribosomal protein S30

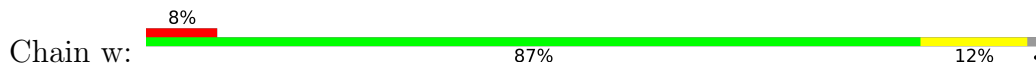


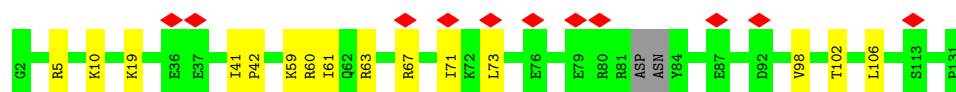
- Molecule 20: 18S ribosomal RNA



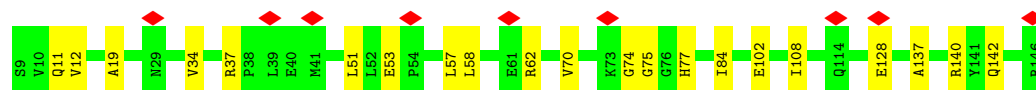
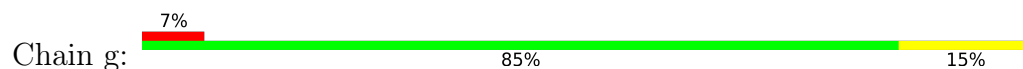


• Molecule 21: 40S ribosomal protein S17

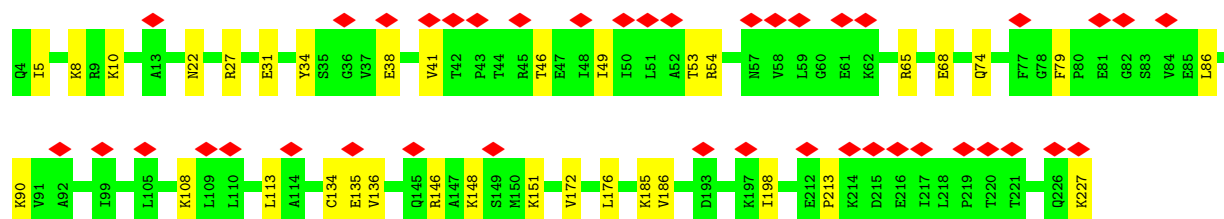
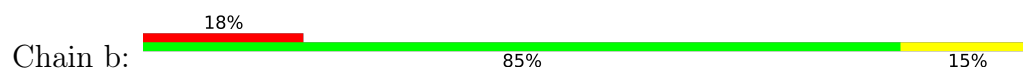




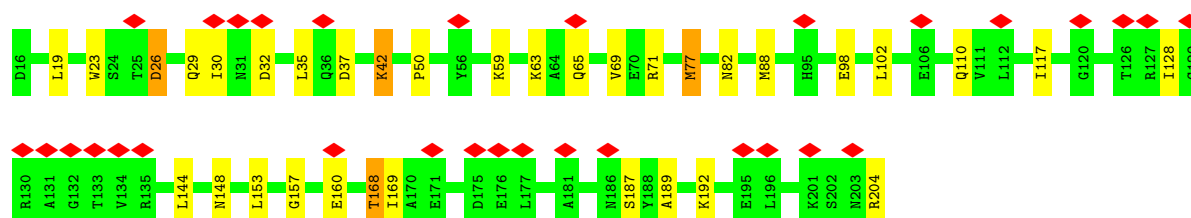
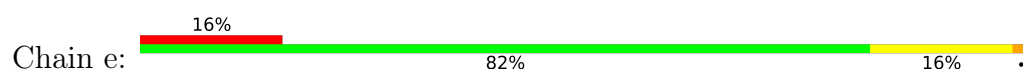
- Molecule 22: 40S ribosomal protein S16



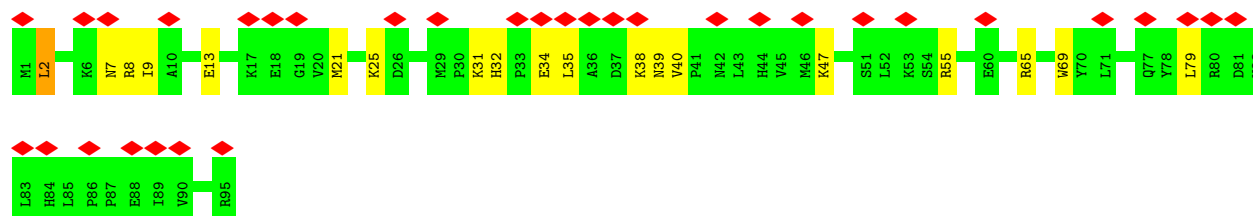
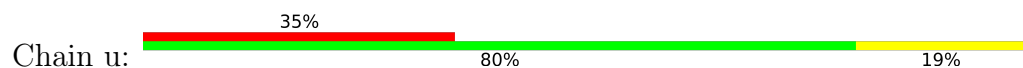
- Molecule 23: 40S ribosomal protein S3



- Molecule 24: 40S ribosomal protein S5

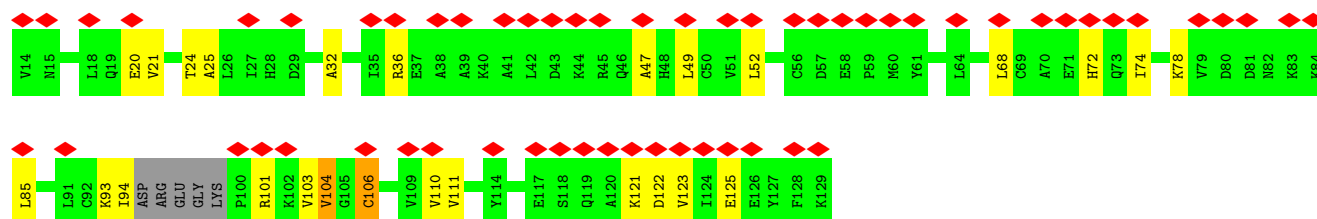


- Molecule 25: 40S ribosomal protein S10

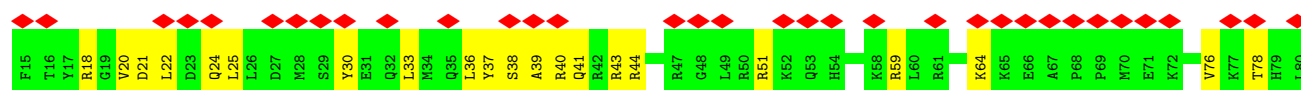


- Molecule 26: 40S ribosomal protein S12

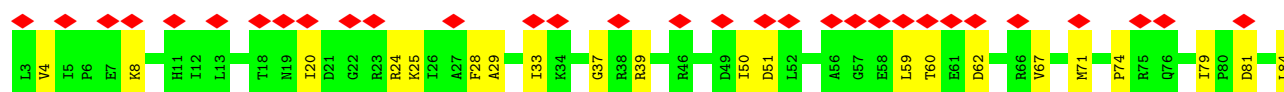




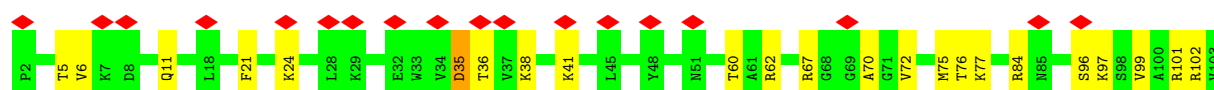
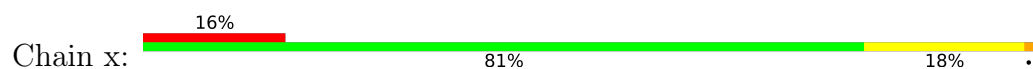
- Molecule 27: 40S ribosomal protein S15



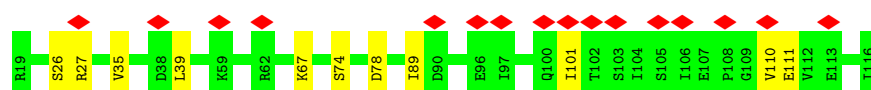
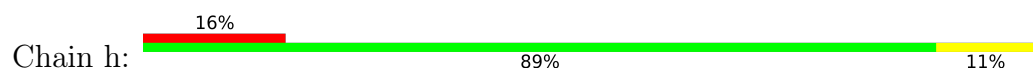
- Molecule 28: 40S ribosomal protein S18



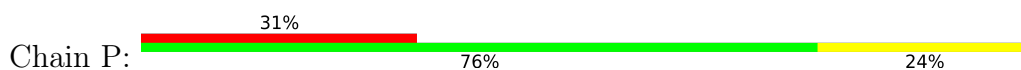
- Molecule 29: 40S ribosomal protein S19



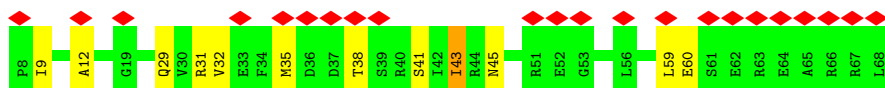
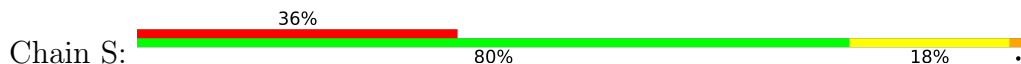
- Molecule 30: 40S ribosomal protein S20



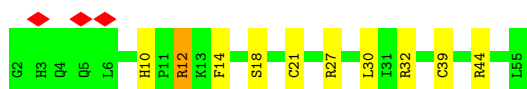
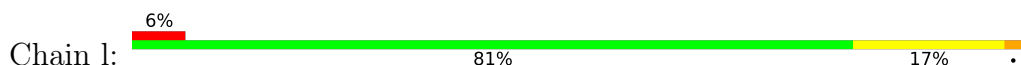
- Molecule 31: 40S ribosomal protein S25



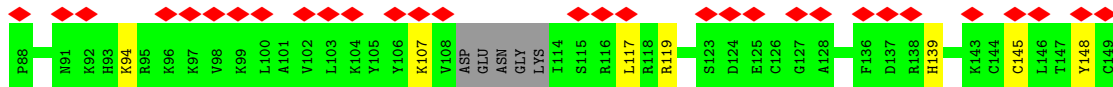
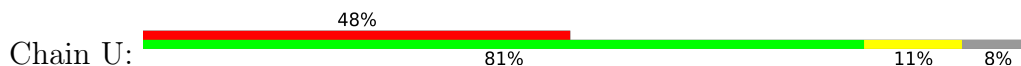
- Molecule 32: 40S ribosomal protein S28



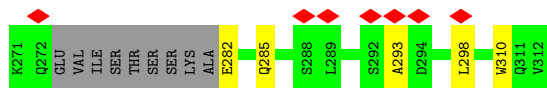
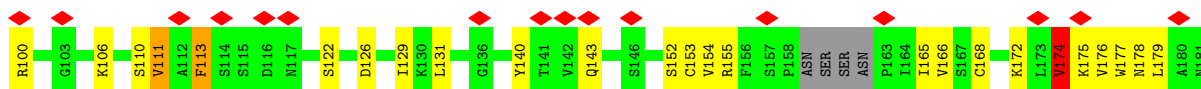
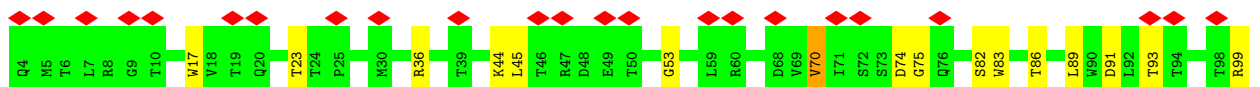
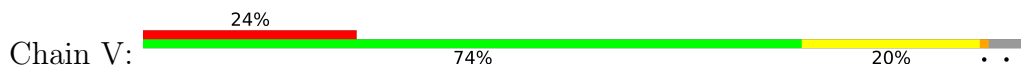
- Molecule 33: 40S ribosomal protein S29



- Molecule 34: Ubiquitin-40S ribosomal protein S27a

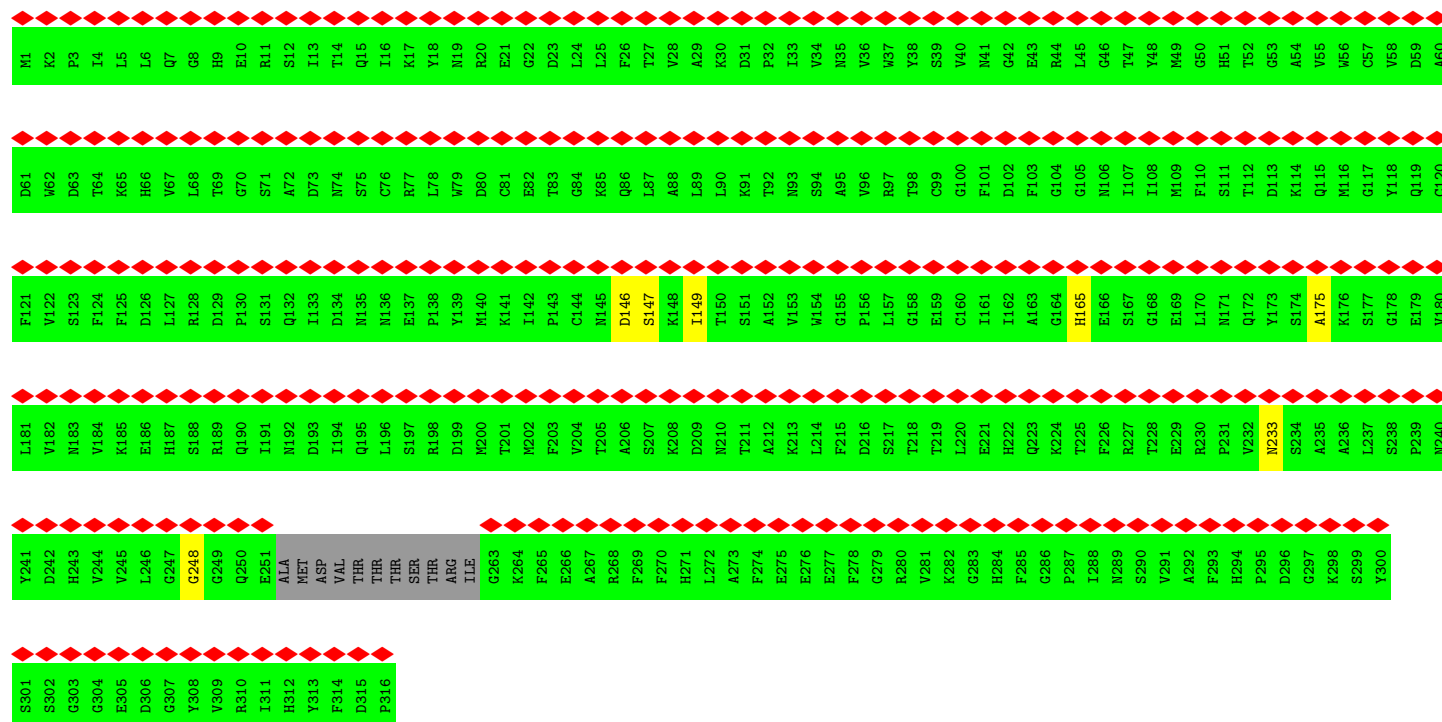


- Molecule 35: Receptor of activated protein C kinase 1

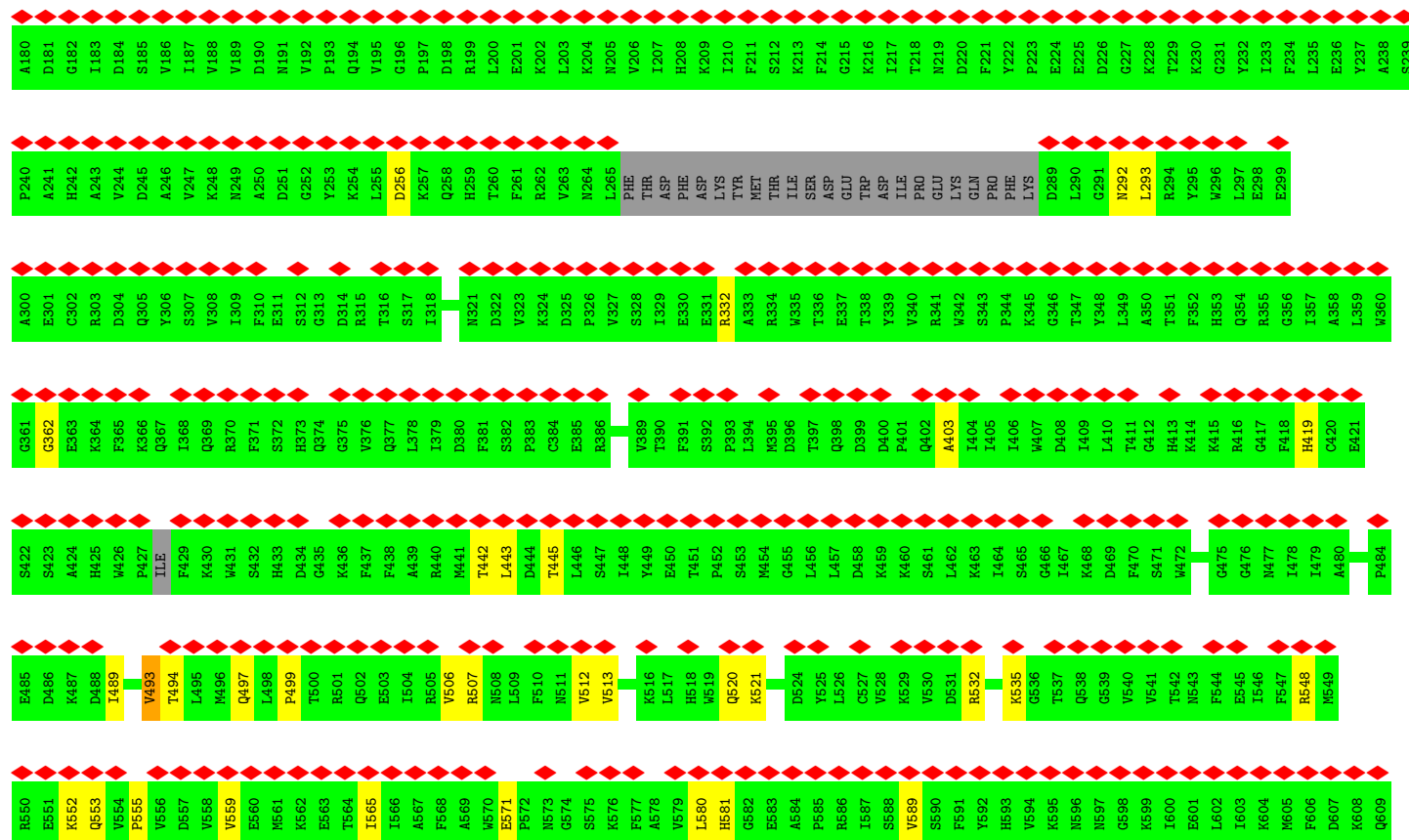
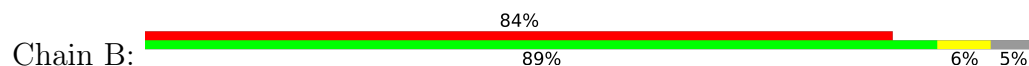


- Molecule 36: Eukaryotic translation initiation factor 3 subunit I





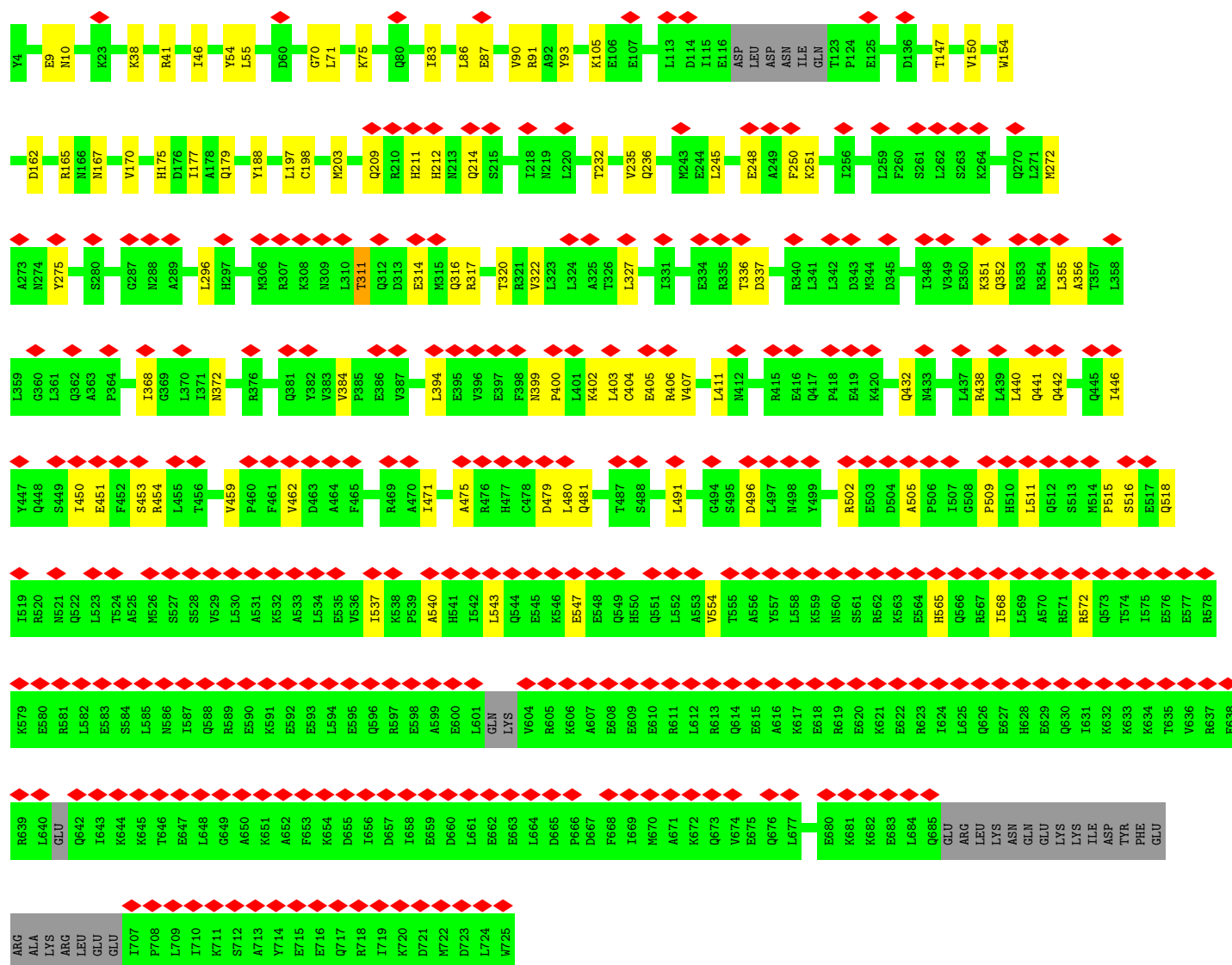
• Molecule 37: Eukaryotic translation initiation factor 3 subunit B



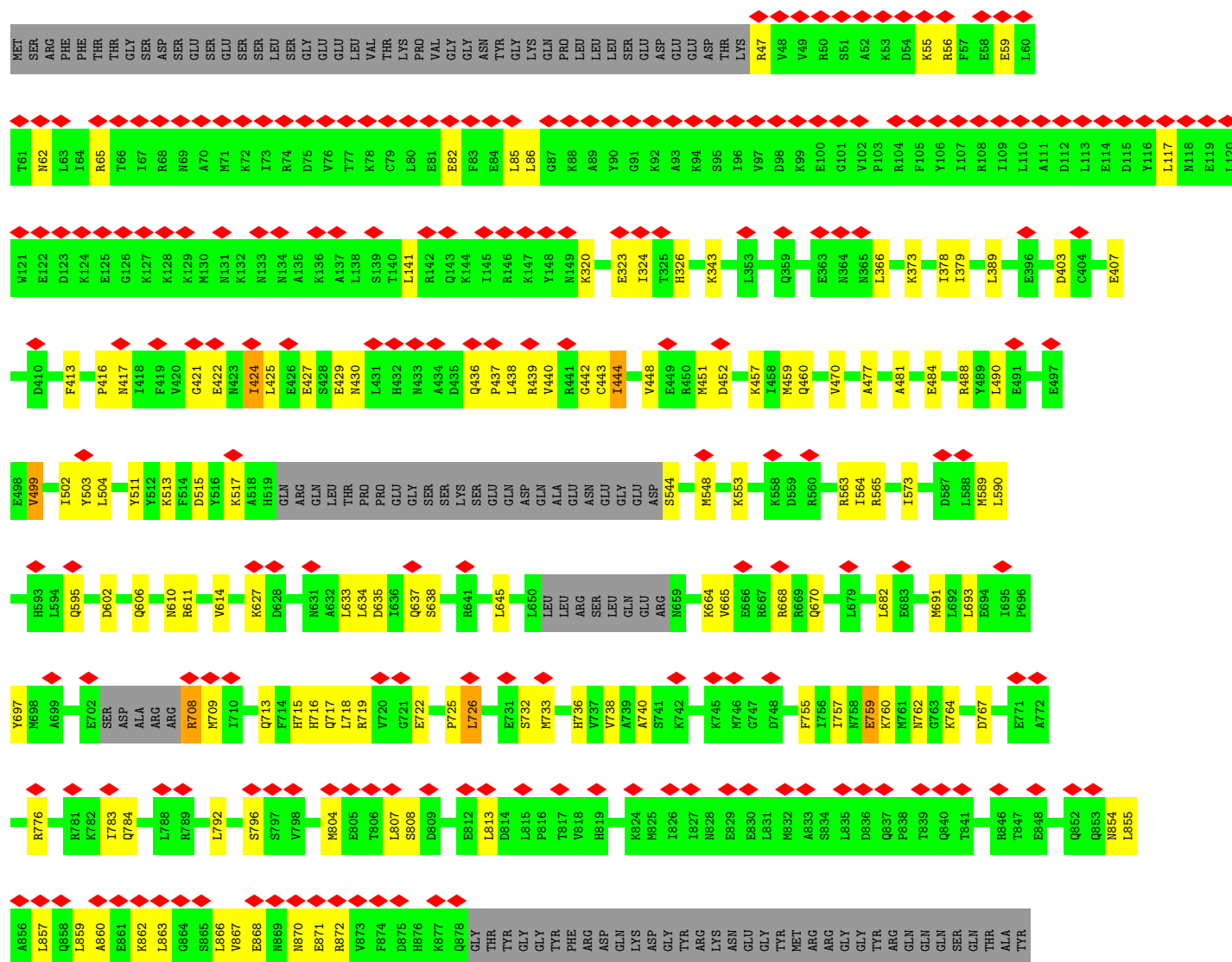


• Molecule 38: Eukaryotic translation initiation factor 3 subunit A

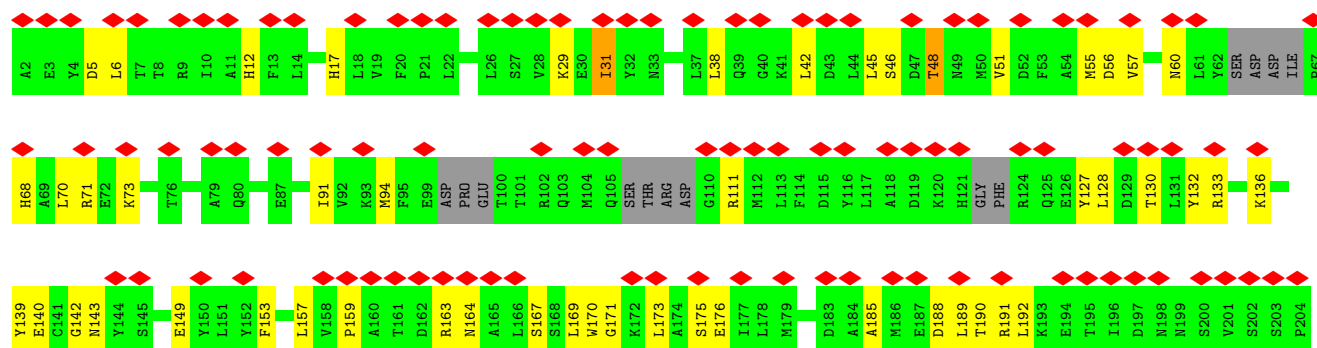
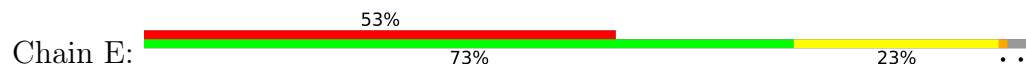
Chain A: 43% 81% 14%

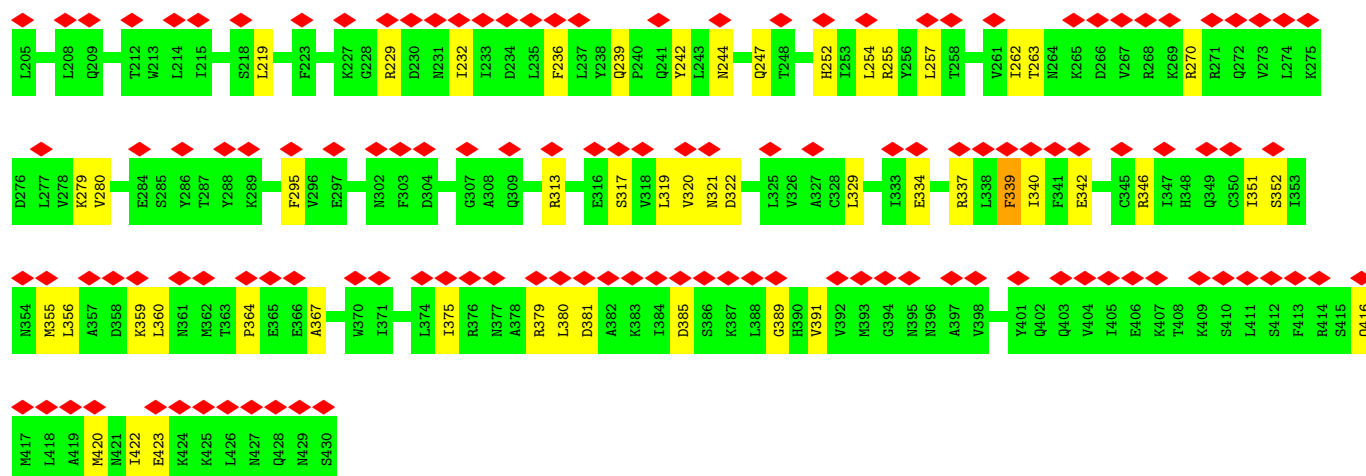


• Molecule 39: Eukaryotic translation initiation factor 3 subunit C

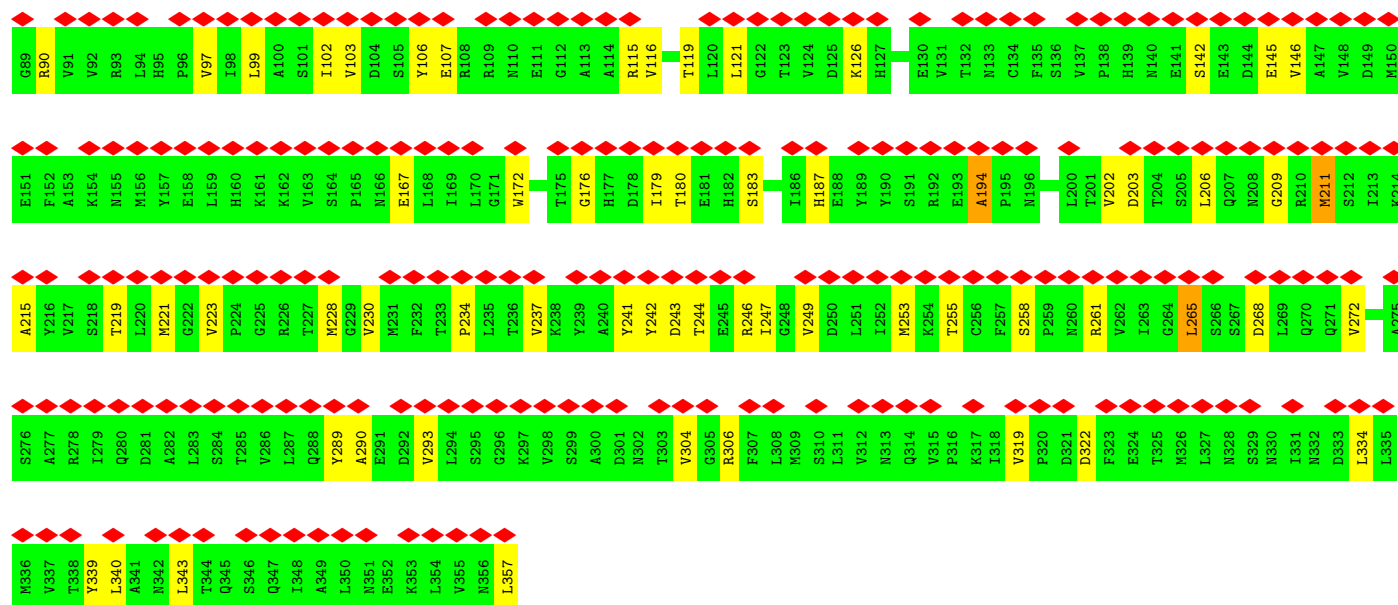
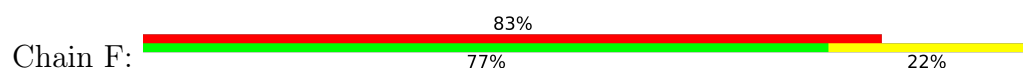


• Molecule 40: Eukaryotic translation initiation factor 3 subunit E

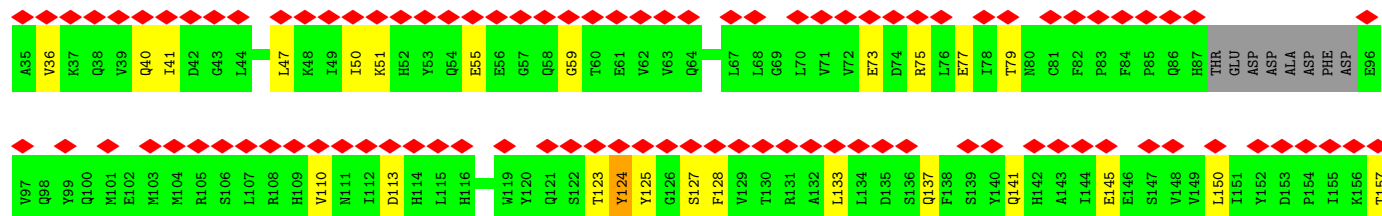
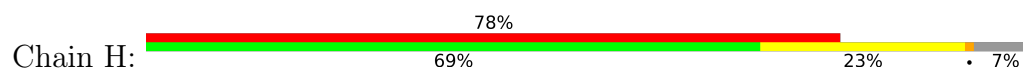


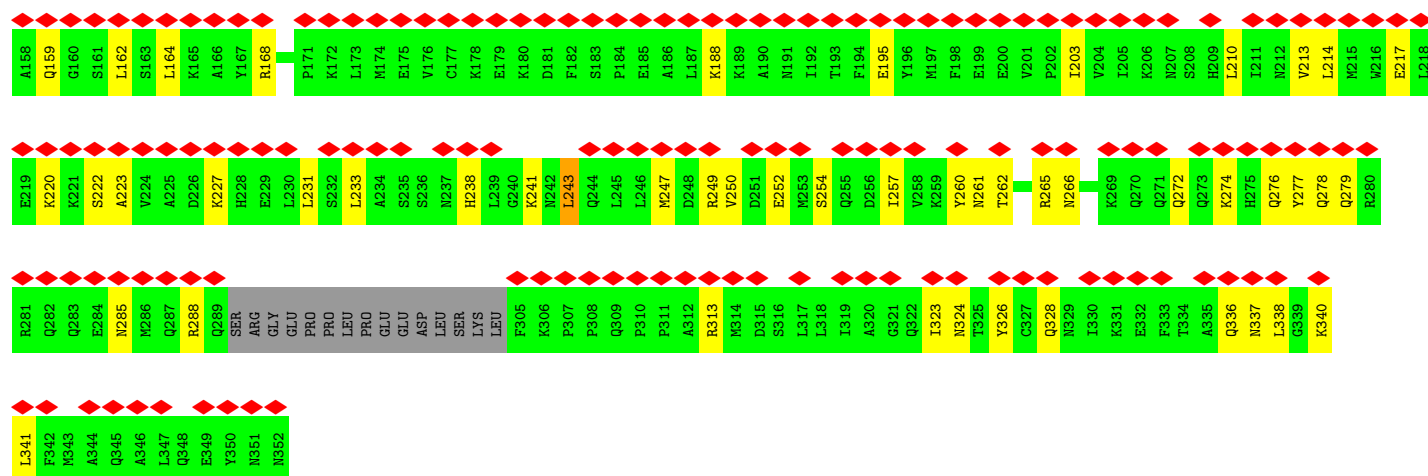


• Molecule 41: Eukaryotic translation initiation factor 3 subunit F

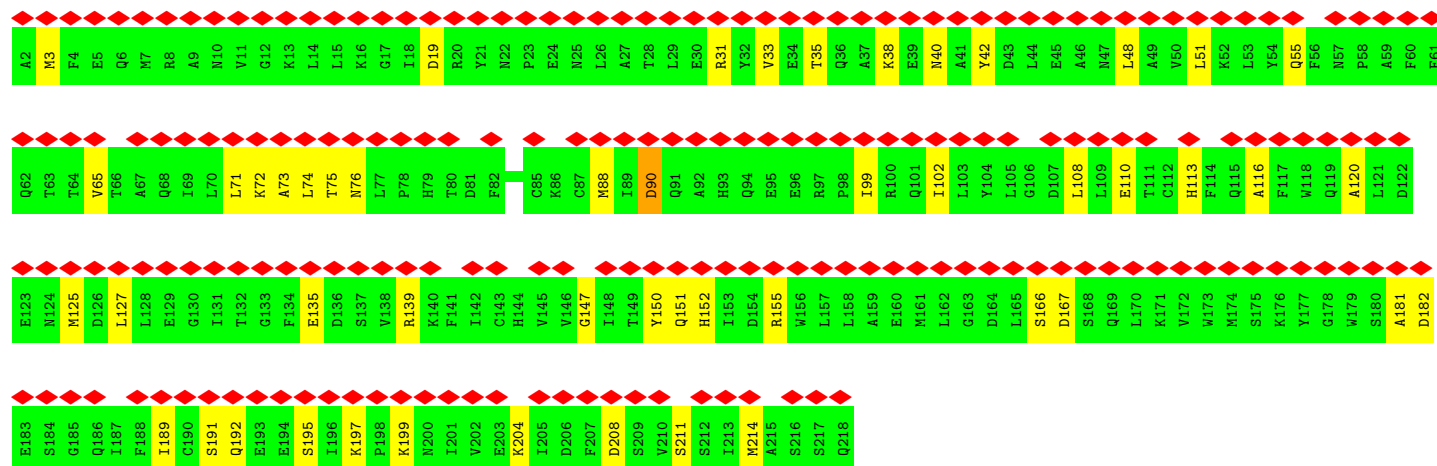
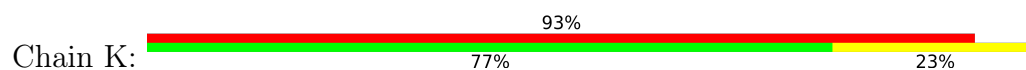


• Molecule 42: Eukaryotic translation initiation factor 3 subunit H

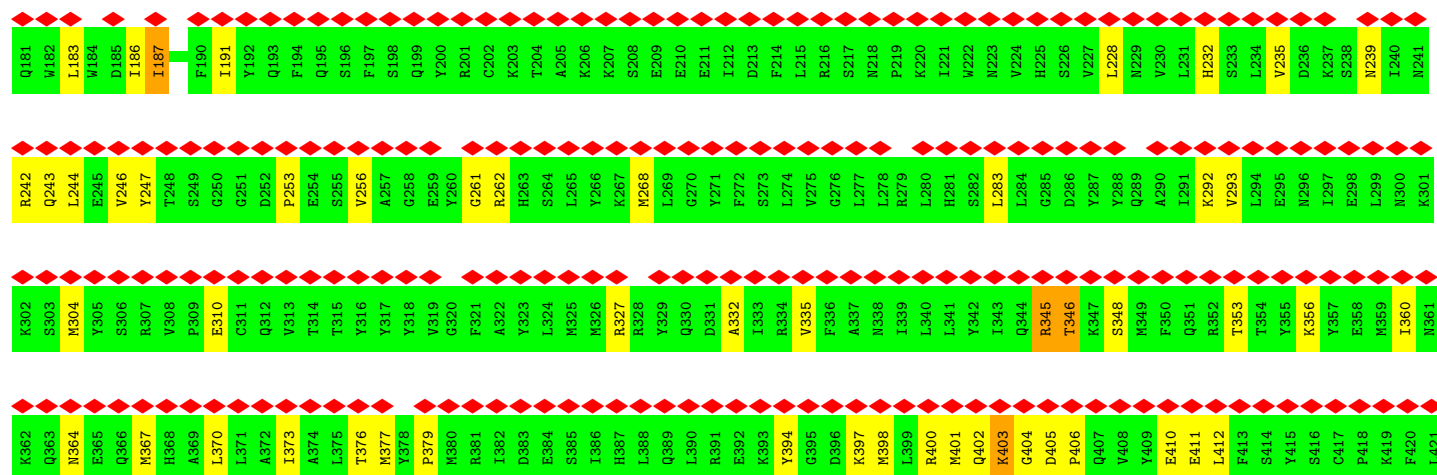
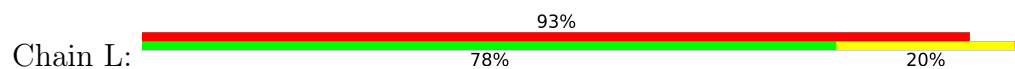


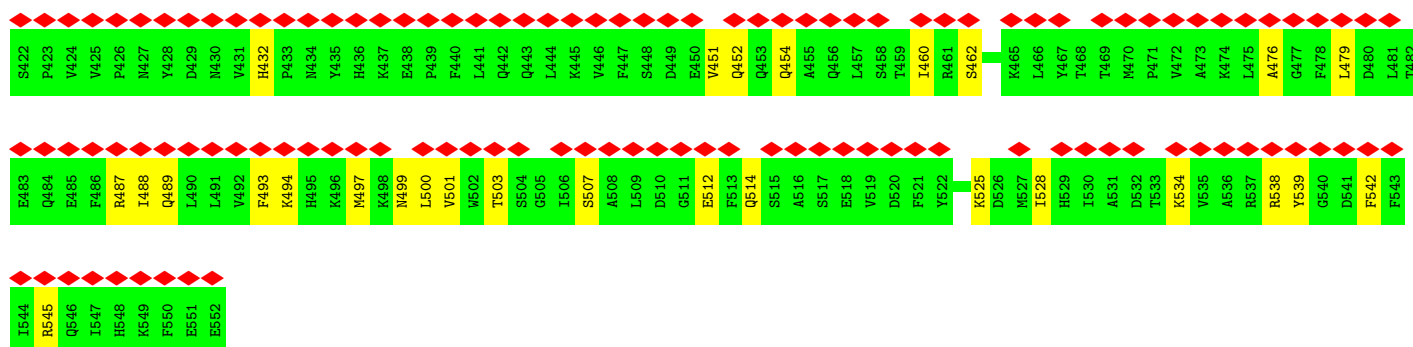


• Molecule 43: Eukaryotic translation initiation factor 3 subunit K

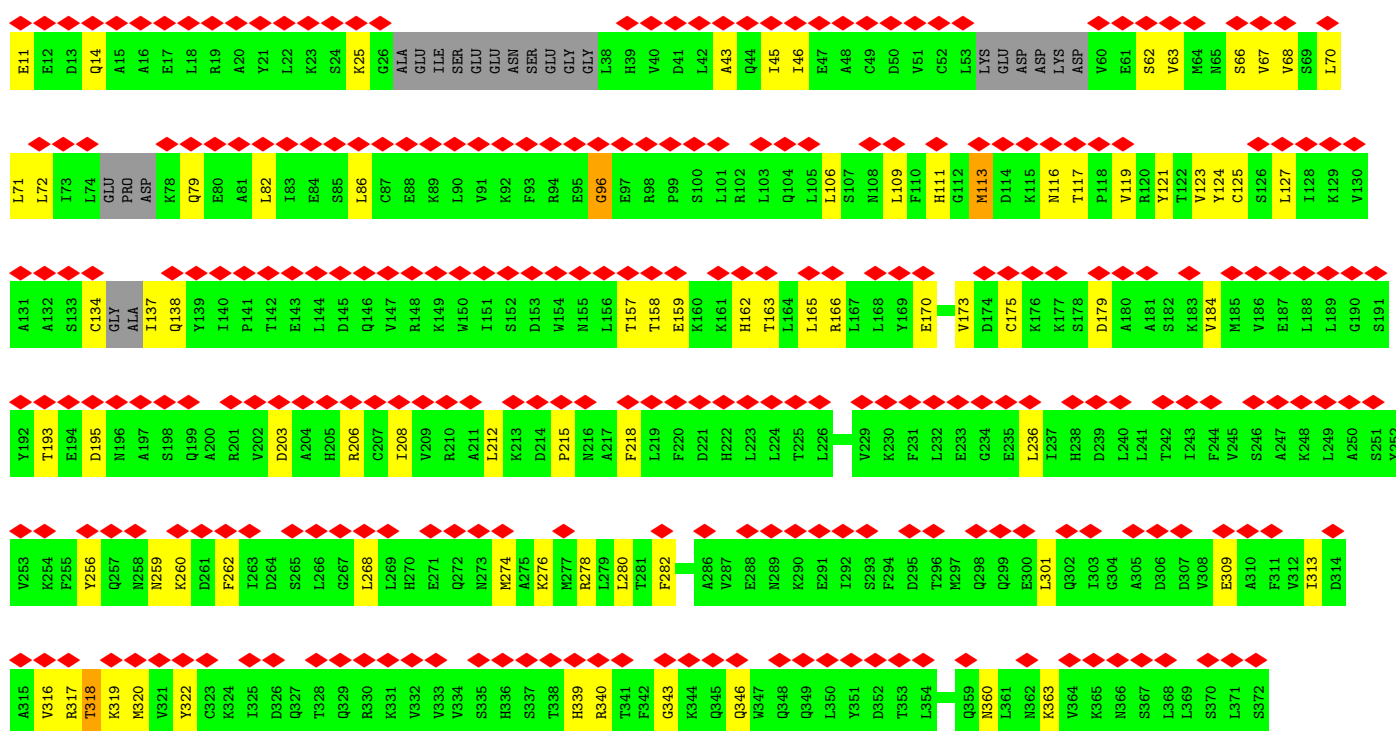
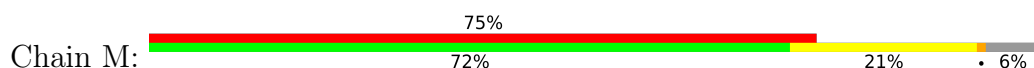


• Molecule 44: Eukaryotic translation initiation factor 3 subunit L

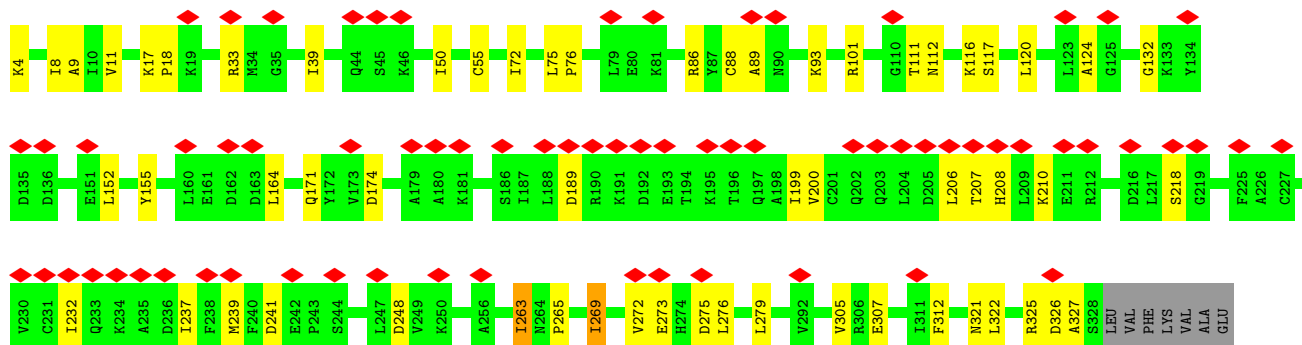
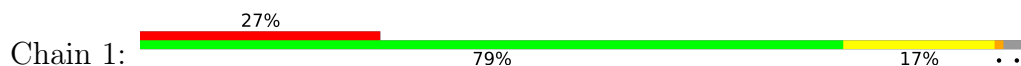


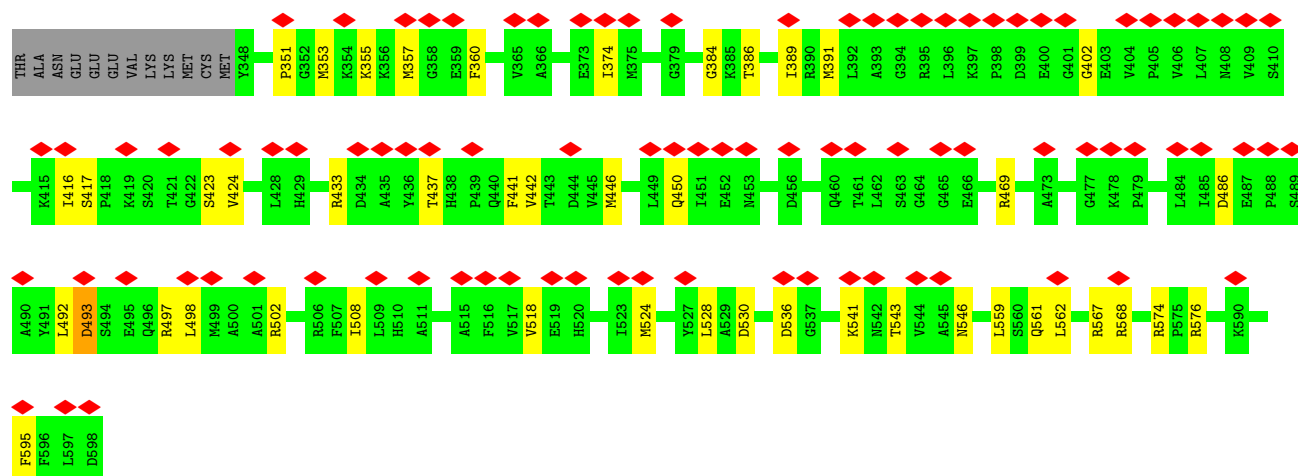


• Molecule 45: Eukaryotic translation initiation factor 3 subunit M

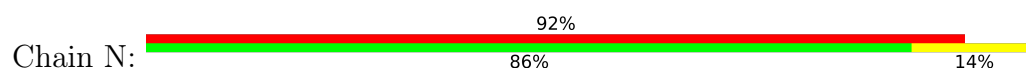


• Molecule 46: ATP-binding cassette sub-family E member 1

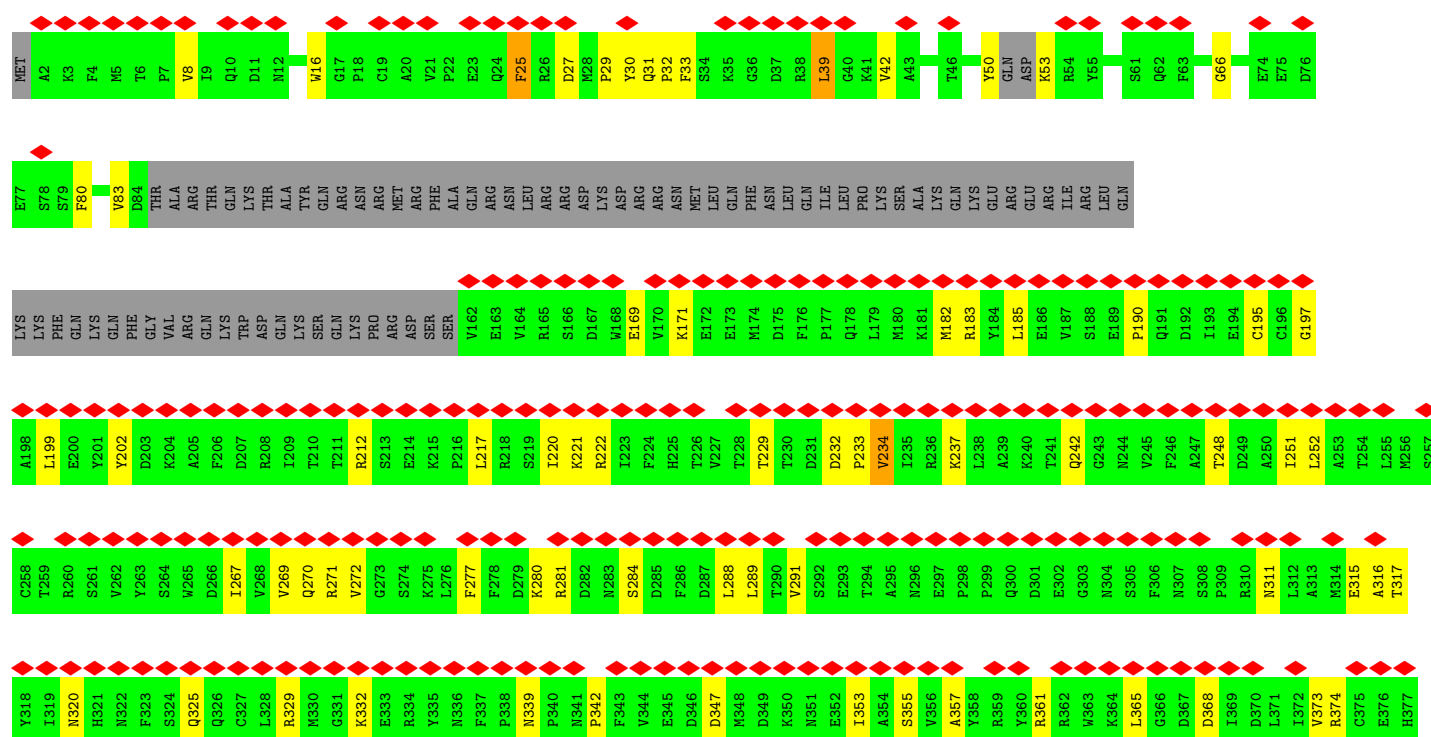




• Molecule 47: Eukaryotic translation initiation factor 1

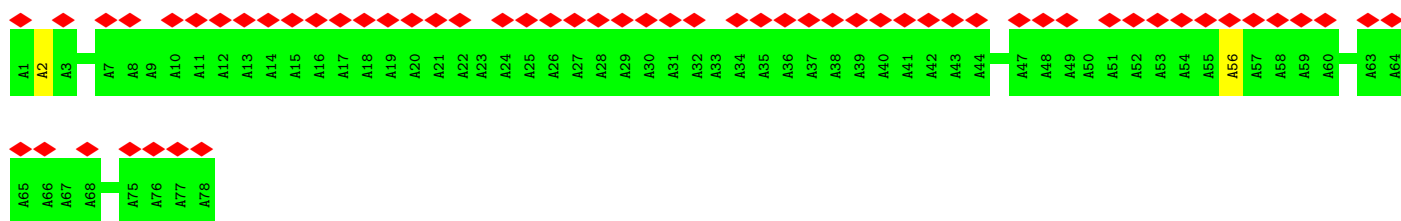
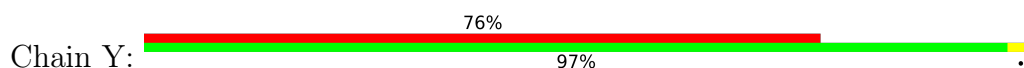


• Molecule 48: Eukaryotic translation initiation factor 3 subunit D

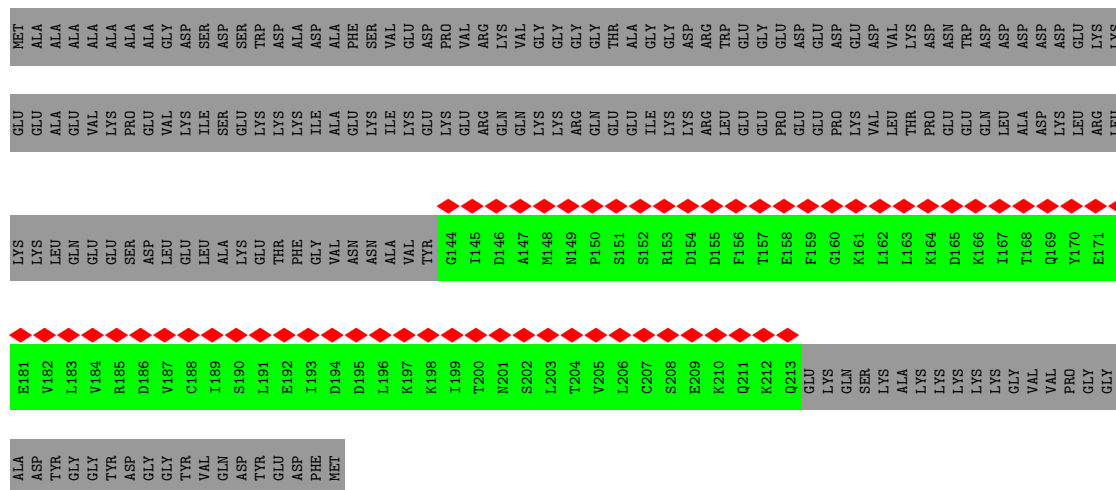




- Molecule 49: RNA recognition motif (unknown)



- Molecule 50: Eukaryotic translation initiation factor 3 subunit J



ALA	ASP	TYR	GLY	GLY	TVR	ASP	GLY	GLY	TVR	VAL	GLN	ASP	TYR	GLU	ASP	PHE	ASP	GLY	GLY	ASN	ASN	ALA	VAL	TYR	G144	G145	D146	A147	M148	N149	P150	S151	S152	R153	D154	D155	F156	T157	E158	F159	G160	K161	L162	L163	K164	D165	L166	L167	T168	Q169	V170	E171	K172	S173	L174	V175	A176	Y177	A177	S178	F179	L180
LYS	LYS	LEU	GLN	GLU	GLU	SER	ASP	LEU	GLU	LEU	ALA	LYS	GLU	THR	PHE	GLY	VAL	ASN	ASN	ALA	VAL	TYR																																								
E181	V182	L183	V184	R185	D186	V187	C188	I189	S190	L191	E192	I193	D194	D195	L196	K197	K198	I199	T200	N201	S202	L203	T204	V205	L206	C207	S208	E209	K210	Q211	K212	Q213	E214	K215	Q216	SER	LYS	ALA	LYS	LYS	LYS	LYS	LYS	GLY	GLY	VAL	VAL	PRO	GLY	GLY	GLY	LEU	LYS	ALA	THR	MET	LYS	ASP	ASP	LEU		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	5231	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 ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.087	Depositor
Minimum map value	-0.033	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	423.6, 423.6, 423.6	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, MG, ATP, ZN, ADP

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	0.56	0/1743	0.69	0/2367
2	p	0.50	0/1743	0.74	1/2330 (0.0%)
3	d	0.58	0/1711	0.81	2/2310 (0.1%)
4	Q	0.63	0/829	0.76	0/1109
5	q	0.56	0/2074	0.77	2/2791 (0.1%)
6	W	0.48	0/232	0.69	0/294
7	r	0.45	0/1818	0.72	0/2421
8	s	0.50	0/1419	0.73	0/1895
9	t	0.49	0/1667	0.69	0/2223
10	c	0.55	0/1525	0.75	1/2035 (0.0%)
11	n	0.60	0/1140	0.69	0/1524
12	m	0.48	0/1227	0.66	0/1649
13	i	0.50	0/952	0.75	0/1275
14	y	0.55	0/632	0.66	0/844
15	f	0.61	0/1051	0.82	0/1406
16	j	0.56	0/1098	0.76	1/1464 (0.1%)
17	z	0.50	0/1017	0.73	0/1349
18	R	0.57	0/654	0.81	0/876
19	T	0.49	0/357	0.70	0/466
20	2	0.54	0/41041	0.63	7/63969 (0.0%)
21	w	0.47	0/1024	0.82	0/1377
22	g	0.43	0/1117	0.77	0/1494
23	b	0.40	0/1774	0.70	0/2387
24	e	0.40	0/1516	0.81	2/2037 (0.1%)
25	u	0.37	0/824	0.75	1/1111 (0.1%)
26	v	0.37	0/871	0.77	2/1168 (0.2%)
27	o	0.38	0/999	0.74	2/1336 (0.1%)
28	k	0.36	0/1181	0.76	0/1581
29	x	0.36	0/1114	0.67	0/1493
30	h	0.40	0/790	0.78	0/1059
31	P	0.35	0/564	0.67	0/758
32	S	0.37	0/482	0.72	0/643

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	I	0.45	0/462	0.85	0/612
34	U	0.38	0/475	0.78	0/626
35	V	0.40	0/2370	0.90	4/3221 (0.1%)
36	I	0.14	0/1495	0.47	0/2073
37	B	0.29	0/2981	0.71	0/4115
38	A	0.36	0/5468	0.71	2/7401 (0.0%)
39	C	0.39	0/5157	0.78	5/6946 (0.1%)
40	E	0.35	0/3503	0.72	3/4728 (0.1%)
41	F	0.37	0/2126	0.79	3/2890 (0.1%)
42	H	0.38	0/2458	0.79	5/3313 (0.2%)
43	K	0.35	0/1785	0.78	1/2414 (0.0%)
44	L	0.41	0/3188	0.90	7/4299 (0.2%)
45	M	0.35	0/2757	0.73	2/3717 (0.1%)
46	I	0.40	0/4627	0.80	3/6247 (0.0%)
47	N	0.39	0/739	0.87	1/989 (0.1%)
48	D	0.37	0/3700	0.75	1/5001 (0.0%)
49	Y	0.27	0/389	0.69	0/543
50	G	0.14	0/347	0.40	0/483
50	J	0.14	0/362	0.39	0/504
All	All	0.47	0/120575	0.71	58/171163 (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
3	d	0	2
5	q	0	3
8	s	0	1
15	f	0	2
17	z	0	2
21	w	0	3
24	e	0	3
28	k	0	1
32	S	0	1
33	I	0	1
35	V	0	6
36	I	0	3
37	B	0	7
39	C	0	7
40	E	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
41	F	0	6
42	H	0	4
43	K	0	5
44	L	0	5
45	M	0	5
46	1	0	5
48	D	0	3
All	All	0	77

There are no bond length outliers.

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	L	379	PRO	CA-C-N	7.85	135.83	121.70
44	L	379	PRO	C-N-CA	7.85	135.83	121.70
35	V	174	VAL	CA-C-N	7.69	138.48	122.41
35	V	174	VAL	C-N-CA	7.69	138.48	122.41
39	C	499	VAL	N-CA-C	-7.13	104.02	111.58
3	d	71	LYS	CA-C-N	7.07	136.27	121.91
3	d	71	LYS	C-N-CA	7.07	136.27	121.91
44	L	348	SER	CA-C-N	6.92	134.16	121.70
44	L	348	SER	C-N-CA	6.92	134.16	121.70
44	L	353	THR	CA-C-N	6.83	133.98	121.70
44	L	353	THR	C-N-CA	6.83	133.98	121.70
45	M	96	GLY	CA-C-N	6.74	130.93	120.82
45	M	96	GLY	C-N-CA	6.74	130.93	120.82
27	o	107	ILE	CA-C-N	6.71	143.04	122.71
27	o	107	ILE	C-N-CA	6.71	143.04	122.71
2	p	208	HIS	N-CA-C	-6.61	100.18	109.69
48	D	413	LEU	CA-CB-CG	6.54	139.19	116.30
44	L	404	GLY	N-CA-C	6.32	128.16	113.18
5	q	86	PHE	CA-C-N	6.20	131.67	122.74
5	q	86	PHE	C-N-CA	6.20	131.67	122.74
41	F	319	VAL	N-CA-C	-6.05	103.39	109.02
42	H	73	GLU	CA-C-N	5.84	132.21	123.05
42	H	73	GLU	C-N-CA	5.84	132.21	123.05
39	C	417	ASN	N-CA-C	-5.78	106.08	114.12
40	E	132	TYR	N-CA-C	-5.67	105.08	112.23
25	u	25	LYS	CA-CB-CG	5.65	125.39	114.10
46	1	206	LEU	CA-C-N	5.64	132.11	123.47
46	1	206	LEU	C-N-CA	5.64	132.11	123.47
41	F	261	ARG	CA-CB-CG	5.62	125.35	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	1	433	ARG	CA-CB-CG	5.60	125.31	114.10
42	H	231	LEU	CA-CB-CG	5.59	135.86	116.30
16	j	113	GLY	N-CA-C	-5.56	100.00	113.18
10	c	138	ARG	CA-CB-CG	5.54	125.18	114.10
39	C	436	GLN	CA-CB-CG	5.46	125.02	114.10
35	V	184	LEU	CA-C-N	5.38	127.81	120.54
35	V	184	LEU	C-N-CA	5.38	127.81	120.54
47	N	29	ASP	N-CA-C	5.36	117.82	111.33
20	2	1807	C	C2'-C3'-O3'	5.30	121.66	113.70
20	2	367	U	P-O3'-C3'	5.30	128.15	120.20
39	C	425	LEU	CA-C-N	-5.30	112.64	122.60
39	C	425	LEU	C-N-CA	-5.30	112.64	122.60
26	v	104	VAL	CA-C-N	-5.22	118.10	121.65
26	v	104	VAL	C-N-CA	-5.22	118.10	121.65
20	2	501	C	C2-N1-C1'	5.20	134.40	118.80
42	H	124	TYR	CA-C-N	5.17	129.41	121.19
42	H	124	TYR	C-N-CA	5.17	129.41	121.19
41	F	194	ALA	N-CA-C	5.17	121.23	109.81
20	2	1474	A	P-O3'-C3'	5.15	127.92	120.20
20	2	367	U	C4'-C3'-O3'	5.14	117.11	109.40
40	E	48	THR	CA-C-N	5.13	129.41	122.07
40	E	48	THR	C-N-CA	5.13	129.41	122.07
20	2	368	U	P-O3'-C3'	5.13	127.89	120.20
43	K	197	LYS	CA-CB-CG	5.08	124.26	114.10
38	A	537	ILE	CA-C-N	5.03	128.26	122.83
38	A	537	ILE	C-N-CA	5.03	128.26	122.83
20	2	1775	U	C2-N1-C1'	5.01	132.72	117.70
24	e	42	LYS	CA-C-N	5.00	127.69	120.38
24	e	42	LYS	C-N-CA	5.00	127.69	120.38

There are no chirality outliers.

All (77) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
46	1	189	ASP	Peptide
46	1	263	ILE	Peptide
46	1	33	ARG	Peptide
46	1	357	MET	Peptide
46	1	528	LEU	Peptide
37	B	256	ASP	Peptide
37	B	292	ASN	Peptide
37	B	332	ARG	Peptide

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Mol	Chain	Res	Type	Group
37	B	442	THR	Peptide
37	B	443	LEU	Peptide
37	B	445	THR	Peptide
37	B	678	ASP	Peptide
39	C	416	PRO	Peptide
39	C	422	GLU	Peptide
39	C	424	ILE	Peptide
39	C	427	GLU	Peptide
39	C	437	PRO	Peptide
39	C	708	ARG	Peptide
39	C	759	GLU	Peptide
48	D	242	GLN	Peptide
48	D	25	PHE	Peptide
48	D	39	LEU	Peptide
40	E	176	GLU	Peptide
40	E	31	ILE	Peptide
41	F	126	LYS	Peptide
41	F	194	ALA	Peptide
41	F	203	ASP	Peptide
41	F	211	MET	Peptide
41	F	228	MET	Peptide
41	F	265	LEU	Peptide
42	H	313	ARG	Peptide
42	H	41	ILE	Peptide
42	H	55	GLU	Peptide
42	H	59	GLY	Peptide
36	I	146	ASP	Peptide
36	I	147	SER	Peptide
36	I	175	ALA	Peptide
43	K	150	TYR	Peptide
43	K	182	ASP	Peptide
43	K	195	SER	Peptide
43	K	199	LYS	Peptide
43	K	42	TYR	Peptide
44	L	261	GLY	Peptide
44	L	345	ARG	Peptide
44	L	403	LYS	Peptide
44	L	432	HIS	Peptide
44	L	500	LEU	Peptide
45	M	113	MET	Peptide
45	M	116	ASN	Peptide
45	M	236	LEU	Peptide

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Mol	Chain	Res	Type	Group
45	M	318	THR	Peptide
45	M	96	GLY	Peptide
32	S	35	MET	Peptide
35	V	143	GLN	Peptide
35	V	174	VAL	Peptide
35	V	175	LYS	Peptide
35	V	241	PHE	Peptide
35	V	293	ALA	Peptide
35	V	75	GLY	Peptide
3	d	133	TYR	Peptide
3	d	135	GLY	Peptide
24	e	42	LYS	Peptide
24	e	65	GLN	Peptide
24	e	77	MET	Peptide
15	f	54	ASP	Peptide
15	f	65	LEU	Peptide
28	k	99	LEU	Peptide
33	l	12	ARG	Peptide
5	q	132	GLY	Peptide
5	q	184	THR	Peptide
5	q	87	MET	Peptide
8	s	134	VAL	Peptide
21	w	42	PRO	Peptide
21	w	60	ARG	Peptide
21	w	71	ILE	Peptide
17	z	10	ARG	Peptide
17	z	102	THR	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	1706	0	1706	17	0
2	p	1716	0	1785	25	0
3	d	1675	0	1764	24	0
4	Q	815	0	864	12	0
5	q	2032	0	2133	19	0
6	W	231	0	276	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	r	1795	0	1942	19	0
8	s	1400	0	1492	14	0
9	t	1639	0	1710	29	0
10	c	1500	0	1618	16	0
11	n	1120	0	1186	8	0
12	m	1203	0	1289	9	0
13	i	940	0	965	14	0
14	y	626	0	628	7	0
15	f	1034	0	1080	10	0
16	j	1081	0	1147	9	0
17	z	1000	0	1071	13	0
18	R	641	0	665	11	0
19	T	355	0	388	4	0
20	2	36700	0	18556	226	0
21	w	1011	0	1053	8	0
22	g	1100	0	1166	14	0
23	b	1746	0	1839	19	0
24	e	1495	0	1549	20	0
25	u	800	0	823	15	0
26	v	862	0	895	16	0
27	o	980	0	1025	24	0
28	k	1163	0	1221	29	0
29	x	1095	0	1120	20	0
30	h	781	0	850	8	0
31	P	558	0	610	12	0
32	S	480	0	507	6	0
33	l	451	0	448	9	0
34	U	466	0	484	5	0
35	V	2315	0	2273	37	0
36	I	1497	0	676	2	0
37	B	2966	0	1764	15	0
38	A	5384	0	5171	66	0
39	C	5073	0	5114	82	0
40	E	3437	0	3433	63	0
41	F	2090	0	2092	37	0
42	H	2413	0	2411	46	0
43	K	1750	0	1717	30	0
44	L	3112	0	3085	49	0
45	M	2718	0	2769	46	0
46	1	4542	0	4666	64	0
47	N	728	0	736	7	0
48	D	3618	0	3495	66	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	Y	390	0	392	1	0
50	G	348	0	146	0	0
50	J	363	0	152	0	0
51	Q	1	0	0	0	0
51	U	1	0	0	0	0
51	l	1	0	0	0	0
52	1	16	0	0	0	0
53	1	27	0	12	2	0
54	1	2	0	0	0	0
55	1	31	0	12	4	0
All	All	115020	0	95971	1117	0

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

All (1117) 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)
46:1:218:SER:OG	55:1:605:ATP:O2B	1.73	1.05
20:2:1276:A:H62	20:2:1321:G:N2	1.55	1.04
20:2:537:C:N4	20:2:545:A:C6	2.27	1.02
20:2:191:A:H62	20:2:208:G:H21	1.01	0.95
20:2:1276:A:N6	20:2:1321:G:H21	1.65	0.93
39:C:697:TYR:HH	39:C:708:ARG:N	1.71	0.87
8:s:163:GLN:O	8:s:167:GLU:HB2	1.74	0.87
46:1:116:LYS:HB2	53:1:603:ADP:O2B	1.76	0.85
8:s:68:GLN:O	8:s:72:PHE:HB2	1.75	0.84
46:1:112:ASN:OD1	53:1:603:ADP:O1B	1.96	0.84
20:2:1276:A:H62	20:2:1321:G:H21	0.82	0.80
20:2:1050:A:H62	20:2:1068:G:H21	1.30	0.78
20:2:537:C:N4	20:2:545:A:C5	2.52	0.78
20:2:1351:G:H1	20:2:1360:U:H3	1.31	0.76
20:2:537:C:C4	20:2:545:A:N6	2.53	0.76
20:2:191:A:H62	20:2:208:G:N2	1.82	0.74
2:p:173:THR:O	2:p:177:GLN:HB2	1.89	0.72
20:2:1166:G:H1	20:2:1193:U:H3	1.40	0.70
37:B:548:ARG:HB2	37:B:555:PRO:HD2	1.74	0.69
20:2:1221:G:H1	20:2:1645:C:H42	1.43	0.67
39:C:565:ARG:HH12	48:D:29:PRO:HG2	1.61	0.65
7:r:170:ARG:NH2	20:2:71:G:N7	2.44	0.64
46:1:351:PRO:HG2	46:1:402:GLY:H	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:c:160:SER:HB2	10:c:163:SER:HB3	1.81	0.63
29:x:11:GLN:HE21	29:x:62:ARG:HH11	1.47	0.63
38:A:316:GLN:HE21	38:A:384:VAL:HG22	1.64	0.62
32:S:31:ARG:HH11	32:S:43:ILE:HG23	1.64	0.62
45:M:134:CYS:HG	45:M:137:ILE:N	1.98	0.62
20:2:537:C:N4	20:2:545:A:N6	2.46	0.62
20:2:1711:U:H3	20:2:1822:A:H61	1.47	0.62
44:L:253:PRO:HA	44:L:256:VAL:HG12	1.80	0.62
43:K:71:LEU:HA	43:K:74:LEU:HD12	1.81	0.62
20:2:1366:G:H21	20:2:1465:A:H8	1.46	0.62
41:F:115:ARG:HH22	41:F:180:THR:H	1.46	0.61
38:A:402:LYS:HB3	38:A:406:ARG:HD2	1.83	0.61
41:F:99:LEU:HB3	42:H:214:LEU:HD11	1.83	0.61
37:B:403:ALA:H	37:B:419:HIS:HA	1.64	0.61
45:M:68:VAL:HG22	45:M:109:LEU:HD13	1.82	0.61
43:K:147:GLY:HA2	43:K:189:ILE:HD13	1.83	0.61
3:d:79:GLU:O	3:d:83:LEU:HB2	2.01	0.60
44:L:534:LYS:HB3	44:L:538:ARG:HH21	1.66	0.60
48:D:365:LEU:HD23	48:D:492:ARG:HD3	1.84	0.60
20:2:1677:U:H2'	20:2:1678:A:H8	1.66	0.60
20:2:851:C:H5''	20:2:852:G:H5'	1.82	0.60
38:A:165:ARG:NH1	38:A:203:MET:SD	2.75	0.60
28:k:33:ILE:HG23	28:k:100:ALA:HB2	1.83	0.60
48:D:281:ARG:HE	48:D:284:SER:HB3	1.67	0.60
11:n:133:PRO:HG2	20:2:383:G:H21	1.67	0.60
43:K:108:LEU:HB2	43:K:113:HIS:HB2	1.84	0.60
20:2:1050:A:H62	20:2:1068:G:N2	1.98	0.59
40:E:29:LYS:NZ	40:E:320:VAL:O	2.35	0.59
2:p:227:LYS:O	2:p:231:LEU:HB2	2.03	0.59
8:s:69:LEU:HD22	8:s:96:ALA:HB2	1.85	0.59
17:z:20:ARG:HE	17:z:22:GLN:HE21	1.51	0.59
38:A:400:PRO:HB3	38:A:442:GLN:HB3	1.85	0.59
2:p:37:ALA:HA	2:p:42:ARG:HH12	1.67	0.59
44:L:239:ASN:HD22	44:L:253:PRO:HG3	1.67	0.59
1:a:76:VAL:HG12	1:a:123:VAL:HB	1.84	0.59
44:L:460:ILE:HG13	44:L:499:ASN:HB2	1.85	0.59
18:R:33:MET:HE2	18:R:48:SER:HA	1.85	0.59
28:k:71:MET:HE2	28:k:99:LEU:HD13	1.84	0.59
44:L:310:GLU:HG2	44:L:356:LYS:HE2	1.85	0.59
45:M:134:CYS:SG	45:M:137:ILE:N	2.76	0.59
46:1:374:ILE:HG12	46:1:508:ILE:HD11	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:2:1266:C:O2	20:2:1516:G:N2	2.36	0.58
40:E:55:MET:HA	40:E:70:LEU:HD13	1.84	0.58
1:a:108:PHE:HB3	1:a:140:VAL:HG21	1.85	0.58
4:Q:4:LYS:NZ	20:2:1863:A:OP2	2.35	0.58
20:2:1608:U:O4	20:2:1632:G:N2	2.36	0.58
48:D:451:TYR:OH	48:D:469:GLN:NE2	2.37	0.58
39:C:715:HIS:HB3	39:C:719:ARG:HH11	1.68	0.58
40:E:319:LEU:HB3	40:E:329:LEU:HG	1.84	0.58
46:1:273:GLU:HG3	46:1:275:ASP:H	1.68	0.58
35:V:196:ASN:H	35:V:211:GLY:HA2	1.68	0.58
35:V:298:LEU:HB3	35:V:310:TRP:HB2	1.84	0.58
37:B:493:VAL:HG22	37:B:507:ARG:HB3	1.85	0.58
20:2:667:U:O4	20:2:1143:A:N6	2.36	0.58
46:1:355:LYS:NZ	46:1:391:MET:SD	2.76	0.58
3:d:187:ARG:HD2	3:d:192:LEU:HD12	1.84	0.58
45:M:72:LEU:HA	45:M:79:GLN:HE22	1.69	0.58
13:i:34:PHE:HB3	13:i:41:PHE:HB2	1.84	0.58
35:V:218:LEU:HB2	35:V:228:TYR:HB2	1.84	0.58
41:F:142:SER:HB2	41:F:145:GLU:HB3	1.86	0.58
43:K:71:LEU:HD13	43:K:102:ILE:HD11	1.84	0.58
47:N:46:THR:HG22	47:N:84:GLN:HG2	1.86	0.58
11:n:13:GLN:HE22	11:n:36:TYR:H	1.53	0.57
20:2:940:U:H3	20:2:1002:U:H3	1.51	0.57
20:2:1622:U:O4	27:o:81:ARG:NH2	2.37	0.57
29:x:35:ASP:OD1	29:x:35:ASP:N	2.37	0.57
4:Q:2:THR:N	20:2:1199:A:OP1	2.37	0.57
40:E:17:HIS:NE2	40:E:139:TYR:O	2.38	0.57
20:2:1264:C:OP2	33:l:27:ARG:NH2	2.36	0.57
47:N:71:GLY:HA3	47:N:85:LEU:HD23	1.84	0.57
2:p:82:ARG:NH1	2:p:191:ASP:OD2	2.38	0.57
46:1:384:GLY:N	55:1:605:ATP:O2A	2.37	0.57
2:p:121:ILE:HG12	2:p:161:VAL:HG13	1.86	0.57
9:t:11:ARG:NH1	9:t:15:GLY:O	2.37	0.57
44:L:373:ILE:HD11	44:L:394:TYR:HB3	1.85	0.57
3:d:70:VAL:HG11	3:d:93:ILE:HG23	1.87	0.57
20:2:547:G:N7	37:B:535:LYS:NZ	2.50	0.57
24:e:102:LEU:HD21	31:P:100:VAL:HG21	1.86	0.57
28:k:89:ASP:HB3	28:k:93:GLY:H	1.69	0.57
43:K:116:ALA:HA	43:K:120:ALA:HB3	1.87	0.57
13:i:32:HIS:HB2	13:i:43:HIS:HB3	1.87	0.57
15:f:26:LEU:HD21	15:f:60:LYS:HD3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:C:606:GLN:O	39:C:610:ASN:ND2	2.38	0.57
45:M:203:ASP:HA	45:M:206:ARG:HB2	1.85	0.57
20:2:722:C:H5''	20:2:723:C:H5'	1.87	0.56
20:2:1657:G:H1	20:2:1667:U:H3	1.51	0.56
20:2:1723:G:N2	20:2:1812:U:O2	2.39	0.56
23:b:134:CYS:SG	23:b:135:GLU:N	2.78	0.56
12:m:87:ASP:OD1	12:m:87:ASP:N	2.39	0.56
18:R:19:HIS:HB3	18:R:22:LYS:HG3	1.86	0.56
40:E:379:ARG:NH2	44:L:377:MET:SD	2.76	0.56
45:M:212:LEU:HB3	45:M:268:LEU:HD21	1.87	0.56
22:g:58:LEU:HB3	22:g:62:ARG:HD2	1.86	0.56
7:r:198:ARG:NH1	20:2:126:G:OP1	2.37	0.56
20:2:1139:C:H41	20:2:1149:A:H62	1.53	0.56
40:E:170:TRP:HB3	48:D:16:TRP:HB2	1.86	0.56
20:2:1535:U:O2'	24:e:82:ASN:ND2	2.39	0.56
21:w:5:ARG:O	21:w:10:LYS:NZ	2.38	0.56
30:h:26:SER:OG	30:h:27:ARG:N	2.39	0.56
20:2:698:G:H1	20:2:732:U:H3	1.53	0.56
28:k:24:ARG:NH2	28:k:28:PHE:O	2.37	0.56
46:1:72:ILE:O	46:1:321:ASN:ND2	2.39	0.56
46:1:312:PHE:O	46:1:325:ARG:NH2	2.39	0.56
20:2:830:A:OP2	20:2:846:G:N2	2.39	0.56
38:A:404:CYS:SG	38:A:405:GLU:N	2.78	0.56
44:L:228:LEU:O	44:L:232:HIS:ND1	2.39	0.56
5:q:181:CYS:SG	5:q:182:MET:N	2.79	0.55
7:r:13:GLN:HE22	20:2:153:G:H21	1.53	0.55
27:o:123:TYR:OH	28:k:124:ARG:NH1	2.39	0.55
38:A:179:GLN:HG2	38:A:235:VAL:HG21	1.86	0.55
28:k:114:LEU:HD22	28:k:122:GLY:H	1.72	0.55
40:E:167:SER:HA	40:E:170:TRP:HB2	1.88	0.55
40:E:247:GLN:NE2	40:E:280:VAL:O	2.39	0.55
20:2:1314:U:O2'	25:u:8:ARG:NH2	2.39	0.55
27:o:30:TYR:HA	27:o:33:LEU:HD12	1.87	0.55
46:1:39:ILE:HG12	46:1:50:ILE:HG12	1.87	0.55
35:V:86:THR:HG21	35:V:100:ARG:HH11	1.72	0.55
40:E:313:ARG:HH22	40:E:359:LYS:HA	1.71	0.55
44:L:304:MET:SD	44:L:304:MET:N	2.80	0.55
4:Q:22:ARG:NH2	13:i:145:GLY:O	2.40	0.55
20:2:488:U:O4	46:1:101:ARG:NH2	2.39	0.55
27:o:44:ARG:NH1	27:o:82:ASP:O	2.40	0.55
39:C:718:LEU:HD23	39:C:738:VAL:HG13	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:K:155:ARG:HH21	43:K:181:ALA:HB1	1.71	0.55
10:c:108:ARG:NH2	10:c:149:VAL:O	2.39	0.55
24:e:63:LYS:O	24:e:71:ARG:NH1	2.38	0.55
35:V:214:GLY:HA2	35:V:236:ILE:HG12	1.87	0.55
40:E:68:HIS:HA	40:E:71:ARG:HG3	1.87	0.55
44:L:398:MET:O	44:L:402:GLN:NE2	2.40	0.55
46:1:207:THR:HA	46:1:210:LYS:HG3	1.88	0.55
20:2:1286:G:O2'	20:2:1312:G:N2	2.39	0.55
38:A:565:HIS:ND1	41:F:107:GLU:O	2.39	0.55
39:C:515:ASP:OD2	39:C:544:SER:N	2.40	0.55
20:2:1036:A:N3	20:2:1844:U:O2'	2.39	0.55
20:2:1498:A:OP2	23:b:27:ARG:NH2	2.40	0.55
20:2:1753:C:H2'	20:2:1779:G:H22	1.71	0.55
35:V:282:GLU:OE2	35:V:285:GLN:NE2	2.40	0.55
38:A:147:THR:HA	38:A:150:VAL:HG22	1.89	0.55
42:H:145:GLU:O	42:H:168:ARG:NH2	2.39	0.55
45:M:256:TYR:OH	45:M:260:LYS:NZ	2.40	0.55
27:o:37:TYR:O	28:k:88:LYS:NZ	2.40	0.55
43:K:40:ASN:OD1	43:K:72:LYS:NZ	2.40	0.55
43:K:55:GLN:NE2	43:K:88:MET:O	2.40	0.55
43:K:152:HIS:HD2	44:L:507:SER:HA	1.72	0.55
20:2:1585:U:OP1	29:x:67:ARG:NH2	2.40	0.55
38:A:209:GLN:O	38:A:212:HIS:NE2	2.40	0.54
4:Q:23:CYS:O	13:i:142:ARG:NH1	2.41	0.54
20:2:1719:A:N6	20:2:1814:G:O2'	2.40	0.54
39:C:484:GLU:OE2	39:C:488:ARG:NH1	2.40	0.54
39:C:590:LEU:HG	48:D:33:PHE:HB2	1.88	0.54
20:2:191:A:N6	20:2:208:G:H21	1.86	0.54
12:m:96:VAL:HG22	12:m:146:ALA:HB1	1.90	0.54
42:H:40:GLN:OE1	42:H:75:ARG:NH1	2.40	0.54
17:z:126:GLY:HA3	46:1:265:PRO:HG3	1.88	0.54
45:M:280:LEU:O	45:M:340:ARG:NH2	2.40	0.54
21:w:59:LYS:O	21:w:63:ARG:NH1	2.41	0.54
36:I:149:ILE:HA	36:I:165:HIS:HA	1.88	0.54
41:F:121:LEU:HB3	41:F:167:GLU:HB3	1.90	0.54
41:F:241:TYR:O	41:F:246:ARG:NH2	2.40	0.54
2:p:65:ARG:NH2	13:i:51:GLU:OE1	2.41	0.54
24:e:204:ARG:NH1	32:S:60:GLU:OE1	2.40	0.54
28:k:124:ARG:HD2	28:k:129:LEU:HD12	1.89	0.54
42:H:137:GLN:NE2	42:H:141:GLN:OE1	2.40	0.54
17:z:108:LYS:NZ	20:2:506:G:OP1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:2:1256:G:N2	33:l:30:LEU:O	2.39	0.54
22:g:51:LEU:HD23	22:g:84:ILE:HG21	1.90	0.54
9:t:134:GLU:HA	9:t:137:LEU:HB2	1.89	0.54
16:j:119:ARG:NH2	20:2:1192:U:OP1	2.41	0.54
24:e:144:LEU:O	24:e:148:ASN:ND2	2.40	0.54
31:P:98:LYS:NZ	31:P:99:LEU:O	2.39	0.54
40:E:317:SER:O	40:E:321:ASN:ND2	2.40	0.54
20:2:885:U:H2'	20:2:901:G:H22	1.72	0.54
28:k:67:VAL:O	28:k:71:MET:HB2	2.08	0.54
44:L:489:GLN:O	44:L:493:PHE:N	2.37	0.54
45:M:113:MET:HE1	45:M:123:VAL:HG21	1.90	0.54
45:M:158:THR:O	45:M:162:HIS:N	2.40	0.54
46:1:9:ALA:HB3	46:1:50:ILE:HG21	1.90	0.54
46:1:276:LEU:O	46:1:574:ARG:NH1	2.40	0.54
20:2:1315:U:H4'	25:u:2:LEU:HB3	1.89	0.53
37:B:520:GLN:NE2	37:B:571:GLU:O	2.41	0.53
38:A:438:ARG:NH1	38:A:441:GLN:OE1	2.41	0.53
39:C:757:ILE:O	39:C:762:ASN:ND2	2.41	0.53
43:K:35:THR:HA	43:K:38:LYS:HE2	1.90	0.53
44:L:451:VAL:HA	44:L:454:GLN:HG2	1.90	0.53
9:t:184:ARG:NH1	20:2:303:C:O2	2.38	0.53
35:V:70:VAL:HG11	35:V:113:PHE:H	1.73	0.53
9:t:181:GLN:NE2	20:2:379:C:OP2	2.42	0.53
37:B:497:GLN:HG3	37:B:499:PRO:HD2	1.89	0.53
2:p:214:LYS:NZ	20:2:943:U:OP1	2.42	0.53
5:q:10:LYS:NZ	20:2:429:C:OP1	2.42	0.53
5:q:45:ILE:HA	5:q:61:VAL:HG11	1.90	0.53
34:U:139:HIS:HB2	34:U:148:TYR:HB2	1.90	0.53
39:C:504:LEU:HD22	39:C:564:ILE:HG23	1.90	0.53
38:A:296:LEU:HB3	38:A:322:VAL:HG12	1.89	0.53
46:1:536:ASP:OD2	46:1:546:ASN:ND2	2.41	0.53
9:t:114:GLU:OE2	9:t:123:ARG:NH2	2.41	0.53
20:2:1556:A:N6	33:l:18:SER:OG	2.42	0.53
20:2:1597:C:OP2	31:P:85:ARG:NH2	2.38	0.53
21:w:19:LYS:HD3	23:b:213:PRO:HD3	1.90	0.53
44:L:332:ALA:HA	44:L:335:VAL:HG22	1.90	0.53
9:t:47:ARG:NH1	9:t:48:VAL:O	2.42	0.53
16:j:111:ALA:HB2	16:j:119:ARG:HE	1.74	0.53
27:o:64:LYS:NZ	27:o:88:GLU:O	2.42	0.53
40:E:244:ASN:ND2	48:D:33:PHE:O	2.38	0.53
1:a:145:ILE:HG12	1:a:159:ILE:HB	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:w:98:VAL:HG13	21:w:102:THR:HB	1.91	0.53
46:1:111:THR:O	46:1:116:LYS:NZ	2.42	0.53
46:1:536:ASP:OD1	46:1:561:GLN:NE2	2.42	0.53
3:d:125:LYS:NZ	20:2:1357:A:OP1	2.41	0.53
9:t:103:LEU:HD22	9:t:170:LYS:HB3	1.91	0.53
18:R:67:THR:HG22	39:C:343:LYS:HD2	1.91	0.53
40:E:128:LEU:HD21	40:E:157:LEU:HD13	1.91	0.53
48:D:289:LEU:HD12	48:D:316:ALA:HB1	1.91	0.53
26:v:52:LEU:HD12	26:v:78:LYS:HG3	1.91	0.52
30:h:67:LYS:O	33:l:44:ARG:NH1	2.42	0.52
40:E:111:ARG:HH11	40:E:159:PRO:HG2	1.72	0.52
40:E:334:GLU:HA	40:E:337:ARG:HB2	1.91	0.52
41:F:176:GLY:N	41:F:202:VAL:O	2.41	0.52
41:F:211:MET:HB3	42:H:217:GLU:HG3	1.91	0.52
20:2:1827:U:OP1	47:N:41:ARG:NH2	2.41	0.52
20:2:1300:U:O2	27:o:51:ARG:NH1	2.42	0.52
28:k:137:LYS:O	28:k:141:ARG:NH2	2.43	0.52
41:F:272:VAL:HG22	42:H:340:LYS:HE3	1.92	0.52
9:t:64:ASN:ND2	20:2:302:A:O2'	2.40	0.52
9:t:87:ASN:HB3	9:t:90:LEU:HG	1.92	0.52
41:F:265:LEU:HD13	42:H:203:ILE:HD13	1.92	0.52
45:M:121:TYR:O	45:M:125:CYS:N	2.41	0.52
48:D:229:THR:HG22	48:D:248:THR:HG23	1.89	0.52
3:d:125:LYS:HG3	3:d:143:CYS:HB2	1.92	0.52
7:r:78:SER:OG	7:r:79:LYS:N	2.42	0.52
20:2:1617:G:N1	20:2:1620:A:OP2	2.43	0.52
26:v:49:LEU:HB3	26:v:111:VAL:HB	1.91	0.52
31:P:56:ASP:O	31:P:60:LYS:HB2	2.09	0.52
7:r:218:LYS:NZ	7:r:222:GLU:OE2	2.43	0.52
11:n:126:VAL:HG12	11:n:145:VAL:HG22	1.91	0.52
20:2:1284:A:N3	20:2:1286:G:N2	2.57	0.52
27:o:20:VAL:HG13	27:o:24:GLN:HG3	1.92	0.52
44:L:370:LEU:HD12	44:L:412:LEU:HG	1.91	0.52
48:D:522:LEU:HD21	48:D:526:THR:HB	1.91	0.52
13:i:102:GLY:O	13:i:106:LYS:NZ	2.37	0.52
20:2:1605:G:OP1	29:x:84:ARG:NH2	2.43	0.52
26:v:21:VAL:O	26:v:25:ALA:HB2	2.09	0.52
39:C:665:VAL:HA	39:C:668:ARG:HG2	1.91	0.52
48:D:183:ARG:HE	48:D:185:LEU:HD13	1.74	0.52
20:2:1236:G:O6	28:k:137:LYS:NZ	2.43	0.52
22:g:137:ALA:O	22:g:140:ARG:NH2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A:368:ILE:O	38:A:372:ASN:ND2	2.42	0.52
2:p:71:LEU:HD21	2:p:189:ILE:HG23	1.92	0.52
39:C:713:GLN:NE2	39:C:717:GLN:OE1	2.43	0.52
40:E:319:LEU:HD13	40:E:329:LEU:HA	1.91	0.52
4:Q:84:VAL:HG13	20:2:1866:A:H62	1.75	0.52
10:c:134:HIS:HE1	10:c:164:PRO:HD2	1.75	0.52
38:A:38:LYS:O	38:A:41:ARG:NH2	2.42	0.52
15:f:31:SER:H	15:f:34:ILE:HD12	1.74	0.51
20:2:1628:C:OP1	29:x:38:LYS:NZ	2.37	0.51
37:B:512:VAL:HG12	37:B:532:ARG:HD3	1.92	0.51
44:L:403:LYS:NZ	44:L:462:SER:O	2.40	0.51
45:M:124:TYR:HA	45:M:127:LEU:HB2	1.92	0.51
20:2:952:G:O2'	20:2:953:C:O2	2.28	0.51
23:b:65:ARG:HA	23:b:68:GLU:HB2	1.92	0.51
38:A:442:GLN:NE2	38:A:509:PRO:O	2.43	0.51
47:N:69:CYS:SG	47:N:89:GLN:NE2	2.77	0.51
3:d:175:GLY:O	14:y:3:ASN:ND2	2.41	0.51
15:f:58:ALA:HB2	20:2:685:A:H1'	1.92	0.51
17:z:103:SER:O	17:z:107:ARG:NE	2.43	0.51
38:A:451:GLU:HG2	38:A:453:SER:H	1.74	0.51
20:2:1058:A:N7	47:N:38:ARG:NH1	2.58	0.51
20:2:1543:U:OP1	22:g:37:ARG:NH2	2.43	0.51
27:o:21:ASP:N	27:o:21:ASP:OD1	2.44	0.51
40:E:163:ARG:HD3	40:E:164:ASN:HB2	1.91	0.51
41:F:234:PRO:HG2	45:M:111:HIS:HB3	1.92	0.51
3:d:194:ARG:NH1	20:2:1156:U:O4	2.44	0.51
28:k:60:THR:OG1	28:k:62:ASP:OD1	2.28	0.51
41:F:268:ASP:OD2	42:H:336:GLN:NE2	2.43	0.51
2:p:139:CYS:SG	2:p:140:VAL:N	2.83	0.51
20:2:706:U:O4	20:2:721:G:N2	2.44	0.51
23:b:108:LYS:HB3	23:b:113:LEU:HD12	1.92	0.51
23:b:146:ARG:O	23:b:148:LYS:NZ	2.39	0.51
29:x:60:THR:HG23	29:x:75:MET:HE3	1.93	0.51
38:A:352:GLN:O	38:A:356:ALA:N	2.38	0.51
39:C:563:ARG:NH2	39:C:602:ASP:OD2	2.43	0.51
39:C:664:LYS:O	39:C:668:ARG:NH1	2.44	0.51
42:H:150:LEU:HB3	42:H:164:LEU:HD12	1.91	0.51
48:D:510:LYS:NZ	48:D:511:ASP:O	2.42	0.51
24:e:50:PRO:HB3	24:e:69:VAL:HG12	1.93	0.51
38:A:154:TRP:HH2	38:A:197:LEU:HB2	1.75	0.51
38:A:515:PRO:HA	38:A:518:GLN:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:K:110:GLU:OE2	44:L:327:ARG:NH1	2.44	0.51
46:1:120:LEU:HD13	46:1:239:MET:HB3	1.92	0.51
46:1:498:LEU:O	46:1:502:ARG:NH1	2.43	0.51
48:D:202:TYR:HB3	48:D:381:MET:HB3	1.93	0.51
18:R:35:VAL:HG11	18:R:63:LEU:HB3	1.93	0.51
20:2:1225:U:O2'	22:g:142:GLN:NE2	2.44	0.51
21:w:61:ILE:HG12	21:w:73:LEU:HD21	1.92	0.51
23:b:31:GLU:O	23:b:54:ARG:NH1	2.38	0.51
39:C:511:TYR:OH	39:C:611:ARG:NH2	2.41	0.51
39:C:862:LYS:O	39:C:866:LEU:N	2.43	0.51
5:q:27:PHE:O	20:2:495:U:O2'	2.29	0.51
45:M:259:ASN:HD22	45:M:262:PHE:HB3	1.74	0.51
20:2:1215:C:H42	20:2:1220:A:H61	1.59	0.51
46:1:567:ARG:HH11	46:1:576:ARG:HD2	1.75	0.51
5:q:91:SER:OG	5:q:98:ASN:ND2	2.44	0.50
9:t:162:LEU:HD11	9:t:191:GLU:HG2	1.93	0.50
32:S:31:ARG:NH2	32:S:41:SER:O	2.43	0.50
39:C:62:ASN:HA	39:C:65:ARG:HE	1.76	0.50
42:H:47:LEU:HD12	42:H:50:ILE:HD12	1.93	0.50
42:H:257:ILE:HA	42:H:260:TYR:HB3	1.92	0.50
1:a:57:LYS:HD3	14:y:70:LEU:HD13	1.93	0.50
2:p:116:LYS:HE3	20:2:989:C:H5''	1.93	0.50
8:s:18:GLU:HG3	8:s:21:SER:H	1.76	0.50
15:f:112:ASP:OD1	15:f:112:ASP:N	2.44	0.50
24:e:35:LEU:HD12	24:e:117:ILE:HG12	1.93	0.50
40:E:45:LEU:HA	40:E:48:THR:HG22	1.93	0.50
41:F:339:TYR:O	41:F:343:LEU:N	2.42	0.50
45:M:11:GLU:N	45:M:14:GLN:OE1	2.44	0.50
45:M:343:GLY:H	45:M:346:GLN:HB2	1.76	0.50
48:D:42:VAL:O	48:D:50:TYR:OH	2.29	0.50
38:A:87:GLU:OE2	38:A:91:ARG:NH1	2.44	0.50
43:K:211:SER:HA	43:K:214:MET:HB2	1.93	0.50
45:M:162:HIS:HB3	45:M:166:ARG:HH11	1.74	0.50
48:D:251:ILE:HD11	48:D:280:LYS:HB3	1.93	0.50
18:R:46:VAL:HG23	18:R:54:VAL:HG21	1.92	0.50
20:2:1033:G:N1	20:2:1080:A:O2'	2.39	0.50
40:E:352:SER:OG	40:E:355:MET:SD	2.68	0.50
48:D:217:LEU:HB2	48:D:465:ILE:HG13	1.91	0.50
20:2:146:G:N2	20:2:174:C:O2	2.45	0.50
20:2:1396:A:O2'	20:2:1398:G:N7	2.42	0.50
35:V:89:LEU:HD12	35:V:99:ARG:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:C:56:ARG:NH1	39:C:59:GLU:OE1	2.45	0.50
13:i:53:ILE:HG23	13:i:88:LEU:HD22	1.93	0.50
27:o:38:SER:OG	27:o:41:GLN:OE1	2.29	0.50
27:o:59:ARG:HH21	27:o:76:VAL:HG22	1.76	0.50
35:V:106:LYS:HB2	35:V:126:ASP:HB3	1.92	0.50
44:L:345:ARG:HH21	44:L:539:TYR:HD2	1.60	0.50
45:M:208:ILE:O	45:M:212:LEU:N	2.39	0.50
48:D:232:ASP:OD2	48:D:374:ARG:NH1	2.45	0.50
48:D:251:ILE:HG23	48:D:267:ILE:HD13	1.94	0.50
7:r:186:GLN:NE2	20:2:318:A:N1	2.55	0.50
9:t:150:ASP:OD1	9:t:153:LYS:NZ	2.42	0.50
26:v:94:ILE:HG13	26:v:101:ARG:HH21	1.77	0.50
35:V:154:VAL:O	35:V:155:ARG:NH1	2.45	0.50
38:A:440:LEU:HD11	38:A:471:ILE:HG12	1.93	0.50
40:E:423:GLU:OE2	44:L:346:THR:OG1	2.25	0.50
41:F:290:ALA:HA	41:F:293:VAL:HG12	1.94	0.50
27:o:22:LEU:HD13	27:o:109:PRO:HB3	1.94	0.50
33:l:30:LEU:HA	33:l:39:CYS:HA	1.92	0.50
38:A:399:ASN:HB3	38:A:402:LYS:HB2	1.94	0.50
38:A:547:GLU:OE2	42:H:220:LYS:NZ	2.45	0.50
44:L:370:LEU:HD22	44:L:373:ILE:HD12	1.92	0.50
7:r:148:SER:OG	7:r:149:LYS:N	2.42	0.50
20:2:955:A:H62	20:2:971:G:N2	2.10	0.50
38:A:320:THR:HG21	38:A:384:VAL:HG23	1.94	0.50
16:j:68:LYS:NZ	20:2:617:G:OP2	2.43	0.49
25:u:21:MET:HB3	25:u:69:TRP:HB2	1.93	0.49
41:F:97:VAL:HG11	42:H:51:LYS:HE3	1.93	0.49
41:F:357:LEU:O	42:H:188:LYS:NZ	2.45	0.49
48:D:252:LEU:HD12	48:D:373:VAL:HG22	1.93	0.49
20:2:1241:A:HO2'	20:2:1266:C:HO2'	1.59	0.49
38:A:272:MET:HA	38:A:275:TYR:HB3	1.93	0.49
40:E:262:ILE:O	40:E:270:ARG:NH2	2.45	0.49
46:1:493:ASP:OD1	46:1:493:ASP:N	2.33	0.49
1:a:205:ARG:HE	1:a:210:ILE:HD13	1.78	0.49
2:p:24:PRO:O	2:p:28:LYS:NZ	2.43	0.49
12:m:70:LYS:NZ	20:2:1020:A:N7	2.61	0.49
38:A:411:LEU:HD13	38:A:432:GLN:HE22	1.77	0.49
40:E:381:ASP:OD1	40:E:381:ASP:N	2.43	0.49
44:L:243:GLN:O	44:L:247:TYR:N	2.39	0.49
7:r:164:LYS:HD3	7:r:167:LYS:HG3	1.94	0.49
9:t:160:SER:OG	9:t:164:GLU:OE1	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:x:108:GLU:OE1	29:x:115:LYS:NZ	2.44	0.49
37:B:580:LEU:HA	37:B:589:VAL:HA	1.94	0.49
38:A:475:ALA:HA	38:A:480:LEU:HB2	1.94	0.49
1:a:49:ILE:HD11	1:a:150:THR:HG22	1.94	0.49
6:W:7:LYS:NZ	20:2:1843:G:OP1	2.41	0.49
20:2:1268:C:N4	20:2:1269:G:O6	2.45	0.49
20:2:1468:C:H2'	20:2:1469:A:H8	1.77	0.49
43:K:90:ASP:OD1	43:K:90:ASP:N	2.45	0.49
44:L:367:MET:HA	44:L:370:LEU:HB2	1.95	0.49
20:2:1584:G:OP1	29:x:77:LYS:NZ	2.42	0.49
20:2:1734:G:O2'	20:2:1800:A:N6	2.45	0.49
38:A:511:LEU:HD11	45:M:316:VAL:HG13	1.94	0.49
12:m:73:ARG:HH21	20:2:916:A:H1'	1.77	0.49
46:1:152:LEU:HA	46:1:155:TYR:HB3	1.93	0.49
48:D:498:CYS:HA	48:D:501:LEU:HG	1.95	0.49
7:r:67:VAL:HB	7:r:99:GLY:HA2	1.95	0.49
20:2:1661:A:C8	33:l:14:PHE:HB2	2.48	0.49
25:u:31:LYS:NZ	25:u:39:ASN:OD1	2.46	0.49
42:H:123:THR:OG1	42:H:127:SER:O	2.29	0.49
7:r:143:LYS:NZ	20:2:146:G:OP1	2.45	0.49
20:2:1038:U:O3'	39:C:47:ARG:NH2	2.45	0.49
20:2:1277:C:H5'	25:u:55:ARG:HH11	1.77	0.49
23:b:22:ASN:OD1	23:b:34:TYR:OH	2.30	0.49
38:A:355:LEU:HD11	39:C:725:PRO:HB2	1.95	0.49
39:C:804:MET:O	39:C:808:SER:N	2.44	0.49
39:C:855:LEU:HB3	42:H:243:LEU:HD22	1.93	0.49
45:M:193:THR:HG23	45:M:195:ASP:H	1.78	0.49
10:c:45:ARG:NH1	20:2:521:A:OP1	2.46	0.49
12:m:99:ARG:NH2	12:m:119:GLU:OE2	2.46	0.49
35:V:152:SER:OG	35:V:168:CYS:SG	2.69	0.49
38:A:71:LEU:HD21	38:A:90:VAL:HG22	1.95	0.49
38:A:75:LYS:HG2	38:A:86:LEU:HD21	1.94	0.49
1:a:77:ILE:HG21	1:a:133:PRO:HG3	1.94	0.48
8:s:53:VAL:HG11	8:s:172:THR:HA	1.95	0.48
20:2:890:U:O2'	20:2:896:U:O4	2.30	0.48
20:2:1414:A:O2'	29:x:128:GLN:NE2	2.46	0.48
20:2:1416:C:N4	20:2:1424:G:O6	2.39	0.48
41:F:102:ILE:HG21	41:F:202:VAL:HG11	1.94	0.48
43:K:3:MET:HE1	43:K:38:LYS:HE3	1.95	0.48
45:M:313:ILE:HA	45:M:316:VAL:HG12	1.94	0.48
3:d:179:THR:HG21	3:d:198:ALA:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:s:87:PHE:HB3	8:s:90:LYS:HE2	1.94	0.48
20:2:1273:C:H4'	20:2:1274:G:H21	1.76	0.48
20:2:1566:G:OP1	29:x:102:ARG:NH2	2.46	0.48
35:V:176:VAL:HB	35:V:186:THR:HB	1.93	0.48
39:C:719:ARG:HA	39:C:722:GLU:HB3	1.95	0.48
41:F:253:MET:HE1	42:H:227:LYS:HE2	1.96	0.48
42:H:262:THR:O	42:H:266:ASN:N	2.46	0.48
4:Q:100:ARG:NH1	20:2:1868:U:O2'	2.46	0.48
8:s:66:VAL:HG23	8:s:67:PRO:HD3	1.95	0.48
9:t:7:ASN:ND2	20:2:351:G:OP1	2.46	0.48
20:2:448:A:H4'	20:2:449:A:H5''	1.93	0.48
24:e:32:ASP:O	48:D:479:GLN:NE2	2.46	0.48
38:A:352:GLN:HA	38:A:355:LEU:HB2	1.93	0.48
41:F:306:ARG:NH1	45:M:339:HIS:O	2.46	0.48
45:M:274:MET:SD	45:M:278:ARG:NH1	2.86	0.48
45:M:360:ASN:OD1	45:M:363:LYS:NZ	2.45	0.48
7:r:64:LYS:NZ	7:r:82:SER:OG	2.45	0.48
17:z:37:LYS:HD2	17:z:57:VAL:HG23	1.94	0.48
25:u:65:ARG:NH1	33:l:21:CYS:O	2.46	0.48
38:A:175:HIS:O	38:A:179:GLN:NE2	2.46	0.48
43:K:72:LYS:O	43:K:76:ASN:ND2	2.46	0.48
43:K:151:GLN:NE2	43:K:191:SER:O	2.46	0.48
44:L:183:LEU:O	44:L:242:ARG:NH1	2.46	0.48
46:1:450:GLN:O	46:1:469:ARG:NH2	2.47	0.48
48:D:222:ARG:NH1	48:D:353:ILE:O	2.46	0.48
4:Q:37:LYS:HG2	4:Q:72:HIS:HD2	1.78	0.48
14:y:64:GLU:HG3	18:R:3:LEU:HD13	1.96	0.48
16:j:27:TYR:O	16:j:31:HIS:HB2	2.12	0.48
20:2:1470:C:O2'	48:D:212:ARG:NH1	2.46	0.48
30:h:67:LYS:HG3	30:h:78:ASP:HB2	1.95	0.48
40:E:6:LEU:HD23	40:E:252:HIS:HD2	1.78	0.48
40:E:356:LEU:O	40:E:360:LEU:N	2.45	0.48
45:M:43:ALA:HA	45:M:46:ILE:HD12	1.96	0.48
46:1:86:ARG:HB3	46:1:132:GLY:HA2	1.95	0.48
9:t:57:ALA:HB2	9:t:183:GLY:HA2	1.94	0.48
20:2:1337:C:H2'	20:2:1338:G:H8	1.78	0.48
20:2:1615:U:H3'	27:o:43:ARG:HH22	1.79	0.48
40:E:185:ALA:HA	40:E:188:ASP:HB2	1.95	0.48
48:D:31:GLN:NE2	48:D:66:GLY:O	2.46	0.48
48:D:289:LEU:HD13	48:D:431:LYS:HD2	1.96	0.48
48:D:311:ASN:O	48:D:315:GLU:N	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:2:350:C:O2'	20:2:383:G:N1	2.46	0.48
28:k:4:VAL:HA	31:P:50:PHE:HB2	1.95	0.48
38:A:54:TYR:HE2	38:A:70:GLY:HA3	1.79	0.48
38:A:248:GLU:HA	38:A:251:LYS:HB2	1.95	0.48
2:p:216:LYS:NZ	20:2:942:G:OP1	2.46	0.48
17:z:78:SER:OG	17:z:79:LEU:N	2.47	0.48
19:T:13:ARG:NH1	20:2:634:A:OP1	2.47	0.48
20:2:920:A:O2'	20:2:922:A:OP1	2.32	0.48
23:b:74:GLN:HA	23:b:79:PHE:HB2	1.96	0.48
39:C:424:ILE:HG21	39:C:439:ARG:HB3	1.95	0.48
44:L:525:LYS:HD3	44:L:528:ILE:HD12	1.96	0.48
4:Q:46:GLU:HG3	4:Q:49:ALA:H	1.79	0.48
26:v:93:LYS:O	26:v:101:ARG:NE	2.39	0.48
27:o:98:ASN:HD22	27:o:122:THR:HA	1.79	0.48
35:V:17:TRP:HB2	35:V:36:ARG:HD2	1.95	0.48
39:C:697:TYR:OH	39:C:708:ARG:N	2.42	0.48
40:E:128:LEU:HD11	40:E:157:LEU:HD22	1.96	0.48
42:H:123:THR:HG21	42:H:128:PHE:HB3	1.96	0.48
43:K:166:SER:OG	43:K:167:ASP:N	2.47	0.48
2:p:155:TYR:OH	20:2:989:C:OP2	2.28	0.48
2:p:216:LYS:NZ	20:2:943:U:OP2	2.41	0.47
5:q:182:MET:HG3	5:q:192:ILE:HG12	1.95	0.47
39:C:859:LEU:HD12	39:C:862:LYS:HB3	1.95	0.47
40:E:337:ARG:HA	40:E:340:ILE:HG22	1.95	0.47
42:H:157:THR:HG22	42:H:162:LEU:HA	1.95	0.47
48:D:271:ARG:HG2	48:D:503:GLU:HG2	1.96	0.47
2:p:123:ALA:HB2	2:p:165:ARG:HG3	1.96	0.47
3:d:271:ASP:OD1	3:d:271:ASP:N	2.44	0.47
5:q:87:MET:HE2	5:q:236:ILE:HD13	1.96	0.47
18:R:48:SER:OG	18:R:49:HIS:ND1	2.46	0.47
20:2:1259:A:H61	20:2:1519:U:H5'	1.79	0.47
38:A:311:THR:HB	38:A:314:GLU:H	1.79	0.47
41:F:249:VAL:O	41:F:253:MET:N	2.47	0.47
42:H:241:LYS:HD2	42:H:241:LYS:HA	1.69	0.47
5:q:97:GLU:OE1	5:q:113:ARG:NH1	2.40	0.47
7:r:48:TYR:OH	7:r:119:LYS:O	2.30	0.47
11:n:136:LYS:O	11:n:139:ARG:NH1	2.48	0.47
30:h:35:VAL:HG11	30:h:110:VAL:HG21	1.96	0.47
35:V:91:ASP:OD1	35:V:93:THR:OG1	2.31	0.47
37:B:512:VAL:HA	37:B:532:ARG:HG3	1.97	0.47
39:C:403:ASP:O	39:C:407:GLU:N	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:N:60:VAL:HA	47:N:63:PHE:HB2	1.95	0.47
48:D:269:VAL:HB	48:D:506:TYR:HB2	1.96	0.47
9:t:74:ARG:NH1	20:2:301:A:O2'	2.47	0.47
20:2:461:U:O2'	46:1:307:GLU:OE1	2.25	0.47
26:v:122:ASP:OD1	26:v:122:ASP:N	2.48	0.47
28:k:84:LEU:HD13	28:k:95:TYR:HB3	1.95	0.47
31:P:110:THR:OG1	31:P:111:ARG:N	2.46	0.47
32:S:12:ALA:HB1	32:S:32:VAL:HB	1.97	0.47
35:V:111:VAL:HG13	35:V:122:SER:HB3	1.95	0.47
38:A:162:ASP:OD1	38:A:165:ARG:NH1	2.47	0.47
39:C:460:GLN:NE2	39:C:670:GLN:O	2.47	0.47
39:C:490:LEU:HB3	39:C:499:VAL:HG22	1.97	0.47
44:L:183:LEU:HG	44:L:186:ILE:HD12	1.97	0.47
46:1:374:ILE:H	46:1:530:ASP:HB2	1.77	0.47
48:D:50:TYR:O	48:D:53:LYS:NZ	2.42	0.47
20:2:1751:C:N3	20:2:1752:C:N4	2.62	0.47
28:k:74:PRO:HB2	28:k:79:ILE:HB	1.96	0.47
41:F:244:THR:HA	41:F:247:ILE:HG22	1.97	0.47
46:1:248:ASP:OD1	46:1:248:ASP:N	2.44	0.47
48:D:195:CYS:O	48:D:339:ASN:ND2	2.42	0.47
11:n:49:GLU:HG2	11:n:118:ARG:HH11	1.79	0.47
28:k:114:LEU:HB3	28:k:122:GLY:HA3	1.97	0.47
40:E:229:ARG:NH1	40:E:263:THR:O	2.48	0.47
45:M:316:VAL:HG23	45:M:322:TYR:HA	1.95	0.47
48:D:183:ARG:HH11	48:D:185:LEU:H	1.61	0.47
6:W:12:ARG:NH2	20:2:1847:G:N7	2.63	0.47
10:c:164:PRO:HG2	20:2:561:A:H5''	1.96	0.47
13:i:93:LEU:O	13:i:127:GLY:N	2.44	0.47
20:2:520:A:O2'	20:2:825:A:N3	2.44	0.47
20:2:1240:A:OP1	27:o:100:LYS:NZ	2.46	0.47
20:2:1452:A:N6	20:2:1473:G:H21	2.11	0.47
38:A:337:ASP:OD1	38:A:337:ASP:N	2.47	0.47
38:A:351:LYS:HE2	38:A:351:LYS:HB3	1.83	0.47
40:E:190:THR:OG1	40:E:191:ARG:NH1	2.48	0.47
40:E:254:LEU:HA	40:E:257:LEU:HB2	1.95	0.47
41:F:215:ALA:HB2	41:F:237:VAL:HB	1.96	0.47
43:K:19:ASP:OD1	43:K:19:ASP:N	2.47	0.47
44:L:538:ARG:O	44:L:542:PHE:N	2.48	0.47
46:1:208:HIS:HB2	46:1:541:LYS:HE3	1.94	0.47
20:2:1288:U:H3	20:2:1311:C:H42	1.60	0.47
20:2:1615:U:OP2	27:o:43:ARG:NH1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:g:53:GLU:O	22:g:57:LEU:HB2	2.15	0.47
40:E:416:GLN:O	40:E:420:MET:N	2.48	0.47
42:H:285:ASN:HA	42:H:288:ARG:HD2	1.97	0.47
10:c:170:PRO:O	10:c:175:ARG:NH1	2.41	0.47
13:i:139:SER:OG	13:i:140:THR:N	2.45	0.47
20:2:1617:G:O6	27:o:40:ARG:NH2	2.48	0.47
26:v:47:ALA:HB3	26:v:74:ILE:HD12	1.97	0.47
35:V:110:SER:HB2	35:V:153:CYS:HA	1.96	0.47
20:2:1599:U:H5''	31:P:44:LEU:HB2	1.97	0.47
23:b:38:GLU:HB3	23:b:49:ILE:HB	1.96	0.47
23:b:151:LYS:HB2	23:b:151:LYS:HE3	1.74	0.47
37:B:552:LYS:HG3	37:B:553:GLN:HG3	1.97	0.47
38:A:55:LEU:HD13	38:A:93:TYR:HB2	1.96	0.47
39:C:430:ASN:HB2	39:C:438:LEU:HA	1.96	0.47
40:E:351:ILE:HB	40:E:391:VAL:HB	1.97	0.47
46:1:437:THR:HG23	46:1:441:PHE:HB2	1.96	0.47
12:m:22:VAL:HG13	12:m:26:LEU:HD23	1.97	0.46
24:e:37:ASP:HB3	48:D:418:GLY:H	1.80	0.46
35:V:129:ILE:HD13	35:V:154:VAL:HG11	1.97	0.46
41:F:206:LEU:HD23	41:F:209:GLY:HA3	1.98	0.46
44:L:394:TYR:HA	44:L:397:LYS:HD2	1.97	0.46
45:M:360:ASN:HA	45:M:363:LYS:HD2	1.96	0.46
1:a:5:LEU:HD12	1:a:8:LEU:HD12	1.96	0.46
1:a:207:PRO:HA	1:a:210:ILE:HG22	1.97	0.46
3:d:206:SER:HG	3:d:224:THR:HG1	1.63	0.46
3:d:235:ASN:ND2	20:2:1355:C:O2	2.47	0.46
5:q:100:ARG:NH2	5:q:121:TYR:O	2.41	0.46
20:2:59:U:N3	20:2:62:G:OP2	2.42	0.46
20:2:898:U:OP2	20:2:899:U:N3	2.44	0.46
36:I:233:ASN:H	36:I:248:GLY:HA2	1.80	0.46
48:D:171:LYS:HE2	48:D:521:SER:HB2	1.97	0.46
20:2:1283:C:H2'	26:v:104:VAL:HG23	1.96	0.46
35:V:44:LYS:HA	35:V:44:LYS:HD3	1.75	0.46
35:V:131:LEU:H	35:V:140:TYR:HE1	1.61	0.46
48:D:25:PHE:HE2	48:D:30:TYR:HA	1.79	0.46
4:Q:40:VAL:HG23	4:Q:69:VAL:HB	1.97	0.46
19:T:26:LYS:NZ	20:2:525:A:OP2	2.48	0.46
38:A:481:GLN:HE22	38:A:516:SER:HB3	1.81	0.46
38:A:568:ILE:O	38:A:572:ARG:N	2.48	0.46
42:H:195:GLU:HG2	44:L:545:ARG:HH21	1.81	0.46
48:D:347:ASP:N	48:D:347:ASP:OD1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:r:190:ARG:NH1	20:2:333:G:OP2	2.48	0.46
13:i:98:ARG:NH1	13:i:99:ALA:O	2.48	0.46
17:z:60:PHE:O	20:2:571:U:O2'	2.33	0.46
40:E:91:ILE:HG12	40:E:127:TYR:HD1	1.79	0.46
40:E:364:PRO:HA	40:E:367:ALA:HB3	1.98	0.46
44:L:376:THR:HA	44:L:377:MET:HA	1.62	0.46
48:D:317:THR:HA	48:D:320:ASN:HB2	1.97	0.46
5:q:11:ARG:HA	5:q:28:ALA:HB2	1.97	0.46
16:j:125:VAL:HG22	16:j:140:ARG:HH12	1.80	0.46
42:H:250:VAL:O	42:H:254:SER:N	2.44	0.46
27:o:22:LEU:HA	27:o:25:LEU:HB3	1.98	0.46
39:C:373:LYS:HE2	39:C:429:GLU:HG2	1.98	0.46
40:E:346:ARG:HE	40:E:346:ARG:HB2	1.65	0.46
44:L:360:ILE:O	44:L:364:ASN:ND2	2.49	0.46
46:l:86:ARG:HB2	46:l:93:LYS:HG3	1.97	0.46
2:p:32:ASP:OD2	2:p:34:LYS:NZ	2.46	0.46
5:q:137:PRO:HG2	5:q:150:PRO:HD2	1.97	0.46
23:b:41:VAL:HG13	23:b:46:THR:HG22	1.98	0.46
43:K:73:ALA:HA	43:K:76:ASN:HD22	1.81	0.46
46:l:360:PHE:CE1	55:l:605:ATP:H4'	2.51	0.46
3:d:105:GLU:HB2	3:d:216:MET:HE1	1.98	0.46
4:Q:81:SER:O	4:Q:81:SER:OG	2.34	0.46
20:2:1291:A:HO2'	34:U:145:CYS:HG	1.58	0.46
27:o:18:ARG:HG3	27:o:36:LEU:HB3	1.98	0.46
37:B:494:THR:HG22	37:B:506:VAL:HG12	1.98	0.46
48:D:289:LEU:HD22	48:D:431:LYS:HG3	1.98	0.46
4:Q:79:ILE:HD12	20:2:1863:A:H1'	1.97	0.46
5:q:108:ARG:NH2	20:2:846:G:OP2	2.44	0.46
38:A:250:PHE:HB2	39:C:726:LEU:HD22	1.98	0.46
20:2:96:C:O2	20:2:473:A:O2'	2.34	0.45
28:k:39:ARG:NH2	29:x:36:THR:O	2.48	0.45
38:A:479:ASP:HB3	38:A:505:ALA:HB2	1.97	0.45
40:E:420:MET:HE3	44:L:346:THR:HG21	1.98	0.45
44:L:232:HIS:HA	44:L:235:VAL:HG12	1.97	0.45
44:L:507:SER:HB3	44:L:512:GLU:H	1.81	0.45
24:e:168:THR:OG1	24:e:169:ILE:N	2.48	0.45
25:u:32:HIS:HD2	25:u:34:GLU:H	1.62	0.45
38:A:540:ALA:HA	38:A:543:LEU:HD12	1.97	0.45
45:M:66:SER:O	45:M:70:LEU:N	2.48	0.45
45:M:282:PHE:HB2	45:M:301:LEU:HD11	1.98	0.45
15:f:96:SER:OG	15:f:97:ARG:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:T:11:LYS:NZ	20:2:615:C:O2	2.40	0.45
28:k:20:ILE:HG23	28:k:29:ALA:HB1	1.97	0.45
40:E:295:PHE:HE1	40:E:340:ILE:HD12	1.80	0.45
41:F:255:THR:O	41:F:258:SER:OG	2.34	0.45
42:H:262:THR:HA	42:H:265:ARG:HB2	1.98	0.45
45:M:179:ASP:OD1	45:M:179:ASP:N	2.47	0.45
7:r:50:VAL:HG12	7:r:113:ILE:HA	1.98	0.45
20:2:1050:A:N6	20:2:1068:G:H21	2.05	0.45
35:V:172:LYS:HD3	35:V:193:GLY:H	1.81	0.45
39:C:448:VAL:HG23	39:C:451:MET:HE3	1.97	0.45
39:C:627:LYS:HA	39:C:693:LEU:HD21	1.98	0.45
39:C:767:ASP:OD1	39:C:776:ARG:NH2	2.50	0.45
46:1:263:ILE:HD13	46:1:269:ILE:HD13	1.97	0.45
9:t:10:LYS:NZ	20:2:385:G:O2'	2.45	0.45
20:2:482:G:N1	20:2:485:A:OP2	2.48	0.45
20:2:1220:A:N3	20:2:1677:U:O2'	2.42	0.45
23:b:53:THR:O	23:b:90:LYS:NZ	2.43	0.45
38:A:211:HIS:HB3	38:A:214:GLN:HE22	1.81	0.45
38:A:496:ASP:OD1	38:A:496:ASP:N	2.45	0.45
39:C:389:LEU:O	39:C:457:LYS:NZ	2.47	0.45
40:E:51:VAL:O	40:E:55:MET:N	2.50	0.45
41:F:221:MET:HG3	45:M:62:SER:HB2	1.98	0.45
45:M:318:THR:HA	45:M:319:LYS:HD2	1.99	0.45
13:i:124:MET:HE3	13:i:124:MET:HB3	1.86	0.45
26:v:85:LEU:HD22	26:v:106:CYS:HB2	1.98	0.45
35:V:178:ASN:ND2	35:V:179:LEU:O	2.49	0.45
38:A:198:CYS:SG	38:A:236:GLN:NE2	2.89	0.45
41:F:306:ARG:HA	41:F:306:ARG:HD3	1.81	0.45
45:M:46:ILE:HG12	45:M:86:LEU:HD13	1.98	0.45
46:1:237:ILE:HG22	46:1:239:MET:HE1	1.98	0.45
46:1:492:LEU:O	46:1:497:ARG:NH2	2.50	0.45
7:r:92:ARG:O	20:2:453:C:O2'	2.31	0.45
39:C:859:LEU:O	39:C:863:LEU:N	2.42	0.45
42:H:123:THR:OG1	42:H:124:TYR:N	2.49	0.45
42:H:125:TYR:HE2	42:H:238:HIS:HA	1.81	0.45
44:L:494:LYS:HA	44:L:497:MET:HG2	1.98	0.45
45:M:163:THR:HA	45:M:166:ARG:HG2	1.99	0.45
46:1:524:MET:HE3	46:1:524:MET:HB3	1.83	0.45
47:N:110:VAL:HG12	47:N:112:GLY:H	1.81	0.45
48:D:329:ARG:HD2	48:D:332:LYS:HG2	1.99	0.45
7:r:177:GLN:NE2	20:2:315:C:OP1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:2:669:A:N3	20:2:1164:G:O2'	2.48	0.45
39:C:611:ARG:HA	39:C:614:VAL:HG12	1.99	0.45
39:C:868:GLU:HA	39:C:871:GLU:HG2	1.99	0.45
46:1:276:LEU:HA	46:1:279:LEU:HB2	1.99	0.45
22:g:58:LEU:HD13	22:g:108:ILE:HD11	1.99	0.45
30:h:39:LEU:HD23	30:h:89:ILE:HD12	1.99	0.45
35:V:129:ILE:O	35:V:140:TYR:OH	2.35	0.45
38:A:399:ASN:OD1	45:M:317:ARG:NH2	2.41	0.45
38:A:554:VAL:HG12	42:H:213:VAL:HG13	1.99	0.45
42:H:323:ILE:HA	42:H:326:TYR:HD2	1.81	0.45
44:L:268:MET:SD	44:L:268:MET:N	2.86	0.45
46:1:200:VAL:HG11	46:1:232:ILE:HG12	1.98	0.45
20:2:43:U:OP2	20:2:485:A:N6	2.50	0.44
20:2:1543:U:O2'	22:g:77:HIS:NE2	2.43	0.44
29:x:72:VAL:HG23	29:x:121:ARG:HH12	1.82	0.44
32:S:29:GLN:HA	32:S:45:ASN:HA	2.00	0.44
35:V:212:LYS:HA	35:V:235:ILE:HG23	1.98	0.44
39:C:634:LEU:O	39:C:638:SER:OG	2.32	0.44
40:E:185:ALA:O	40:E:189:LEU:N	2.48	0.44
46:1:353:MET:HE3	46:1:353:MET:HB2	1.74	0.44
5:q:8:HIS:O	5:q:30:ARG:NH1	2.50	0.44
6:W:16:LYS:HB3	6:W:16:LYS:HE2	1.75	0.44
8:s:148:LEU:HD12	15:f:49:GLU:HG3	1.98	0.44
17:z:120:THR:OG1	20:2:151:C:OP1	2.34	0.44
20:2:53:C:O2'	20:2:507:G:N7	2.50	0.44
31:P:79:ILE:HB	31:P:83:LEU:HD12	1.99	0.44
35:V:126:ASP:OD1	35:V:126:ASP:N	2.37	0.44
40:E:149:GLU:O	40:E:153:PHE:N	2.47	0.44
46:1:423:SER:OG	46:1:424:VAL:N	2.50	0.44
48:D:182:MET:HE2	48:D:493:CYS:HB3	1.99	0.44
3:d:79:GLU:O	3:d:83:LEU:CB	2.65	0.44
5:q:95:THR:HG22	17:z:16:ARG:HB2	1.99	0.44
7:r:202:ASN:ND2	20:2:125:C:OP1	2.41	0.44
20:2:955:A:H62	20:2:971:G:H21	1.65	0.44
20:2:1410:C:N4	20:2:1431:G:O6	2.50	0.44
20:2:1746:U:O4	20:2:1789:G:N2	2.51	0.44
23:b:136:VAL:HG22	23:b:186:VAL:HG22	1.99	0.44
38:A:327:LEU:HD22	38:A:394:LEU:HD23	1.98	0.44
39:C:553:LYS:NZ	48:D:27:ASP:O	2.40	0.44
39:C:716:HIS:HA	39:C:719:ARG:HG2	1.99	0.44
48:D:190:PRO:HB2	48:D:361:ARG:HB3	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:p:126:ASP:OD1	2:p:136:ARG:NE	2.48	0.44
9:t:6:ASP:OD1	9:t:6:ASP:N	2.48	0.44
10:c:155:LYS:HD3	37:B:555:PRO:HB3	1.99	0.44
27:o:104:GLN:H	27:o:104:GLN:HG2	1.55	0.44
30:h:39:LEU:HD11	30:h:101:ILE:HB	1.99	0.44
39:C:82:GLU:O	39:C:86:LEU:N	2.45	0.44
39:C:736:HIS:ND1	39:C:755:PHE:O	2.50	0.44
45:M:45:ILE:HD12	45:M:45:ILE:HA	1.81	0.44
48:D:171:LYS:HB2	48:D:519:VAL:HG13	1.99	0.44
9:t:69:SER:OG	9:t:191:GLU:OE2	2.28	0.44
12:m:5:HIS:HB3	12:m:117:LEU:HD13	1.98	0.44
12:m:69:ASN:OD1	12:m:69:ASN:N	2.50	0.44
20:2:76:U:O2'	20:2:78:C:OP2	2.33	0.44
20:2:594:A:H61	20:2:643:A:H5''	1.83	0.44
20:2:1376:A:OP2	21:w:67:ARG:NH1	2.50	0.44
20:2:1478:U:O2'	22:g:128:GLU:OE2	2.36	0.44
20:2:1562:C:H2'	20:2:1563:G:H8	1.83	0.44
28:k:84:LEU:HB2	28:k:87:GLN:HG2	2.00	0.44
41:F:179:ILE:HG23	41:F:183:SER:HB3	1.99	0.44
2:p:110:MET:HA	2:p:113:MET:HE2	1.99	0.44
7:r:69:THR:OG1	7:r:70:HIS:N	2.48	0.44
9:t:141:ARG:HH11	9:t:146:GLN:HE22	1.66	0.44
17:z:8:ARG:HB2	17:z:26:ASP:HB2	1.99	0.44
20:2:380:G:N1	20:2:383:G:OP2	2.51	0.44
20:2:1550:G:OP2	23:b:8:LYS:NZ	2.48	0.44
25:u:32:HIS:HB3	25:u:35:LEU:HB2	2.00	0.44
35:V:165:ILE:HB	35:V:177:TRP:HB2	2.00	0.44
39:C:421:GLY:N	39:C:442:GLY:O	2.47	0.44
3:d:116:THR:HA	20:2:1203:G:H4'	1.99	0.44
8:s:9:VAL:HG12	8:s:11:PRO:HD3	1.99	0.44
35:V:226:HIS:NE2	35:V:228:TYR:O	2.51	0.44
43:K:151:GLN:HE22	43:K:192:GLN:HA	1.83	0.44
45:M:67:VAL:O	45:M:71:LEU:N	2.46	0.44
46:1:164:LEU:HB3	46:1:237:ILE:HD11	2.00	0.44
20:2:190:G:O2'	20:2:209:A:N6	2.51	0.44
28:k:50:ILE:HG21	28:k:59:LEU:HD21	1.99	0.44
29:x:5:THR:OG1	29:x:6:VAL:N	2.51	0.44
38:A:245:LEU:HB3	38:A:248:GLU:HB2	2.00	0.44
39:C:866:LEU:O	39:C:870:ASN:N	2.51	0.44
40:E:255:ARG:NH2	40:E:322:ASP:OD2	2.48	0.44
46:1:111:THR:OG1	46:1:112:ASN:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:D:197:GLY:HA3	48:D:357:ALA:HA	1.99	0.44
1:a:205:ARG:NH1	1:a:209:GLU:OE1	2.51	0.44
3:d:224:THR:O	20:2:2:A:O2'	2.36	0.44
5:q:50:ASN:O	5:q:53:LYS:NZ	2.38	0.44
9:t:22:HIS:HB3	20:2:433:A:H5''	2.00	0.44
16:j:68:LYS:HB3	16:j:91:LEU:HD22	2.00	0.44
24:e:29:GLN:N	24:e:110:GLN:OE1	2.41	0.44
45:M:165:LEU:HD12	45:M:184:VAL:HG13	2.00	0.44
48:D:491:LEU:HD23	48:D:492:ARG:HG2	2.00	0.44
48:D:524:ASP:OD1	48:D:524:ASP:N	2.49	0.44
4:Q:77:CYS:O	4:Q:81:SER:HB3	2.18	0.43
10:c:50:LEU:HD12	10:c:105:PHE:HE2	1.81	0.43
18:R:78:SER:HB2	48:D:80:PHE:HB3	2.00	0.43
26:v:68:LEU:O	26:v:72:HIS:HB2	2.18	0.43
38:A:83:ILE:HG21	38:A:170:VAL:HG12	1.99	0.43
39:C:82:GLU:HA	39:C:85:LEU:HB2	2.00	0.43
39:C:867:VAL:HA	39:C:870:ASN:HB2	2.00	0.43
40:E:236:PHE:HB3	40:E:257:LEU:HD21	2.00	0.43
41:F:102:ILE:O	41:F:106:TYR:N	2.51	0.43
46:1:442:VAL:HG13	46:1:446:MET:HB3	1.99	0.43
2:p:209:ASP:N	2:p:209:ASP:OD1	2.51	0.43
3:d:165:VAL:HG21	3:d:217:ALA:HB1	2.00	0.43
8:s:70:LYS:HD3	8:s:70:LYS:HA	1.81	0.43
9:t:113:TYR:OH	9:t:156:ALA:O	2.35	0.43
24:e:59:LYS:HA	24:e:59:LYS:HD2	1.78	0.43
38:A:479:ASP:HB2	38:A:502:ARG:HG2	2.00	0.43
39:C:513:LYS:HE3	39:C:513:LYS:HB2	1.84	0.43
46:1:8:ILE:HG13	46:1:75:LEU:HD22	1.99	0.43
3:d:206:SER:OG	3:d:224:THR:OG1	2.31	0.43
18:R:76:GLY:H	48:D:83:VAL:HG23	1.83	0.43
20:2:1314:U:H5''	20:2:1315:U:H5	1.83	0.43
20:2:1613:G:OP2	27:o:39:ALA:N	2.51	0.43
37:B:293:LEU:HA	37:B:362:GLY:HA2	2.00	0.43
39:C:573:ILE:HG21	39:C:589:MET:HB2	2.00	0.43
39:C:859:LEU:HD13	42:H:247:MET:HG2	1.99	0.43
44:L:479:LEU:HG	44:L:489:GLN:HB3	2.00	0.43
14:y:69:ILE:HD13	14:y:69:ILE:HA	1.86	0.43
18:R:47:PHE:HB3	18:R:50:ALA:HB2	1.99	0.43
20:2:57:U:O2	20:2:88:G:N2	2.43	0.43
20:2:1261:C:O2	20:2:1618:C:N4	2.51	0.43
27:o:41:GLN:NE2	27:o:113:GLY:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A:175:HIS:ND1	38:A:232:THR:OG1	2.45	0.43
46:1:88:CYS:SG	46:1:89:ALA:N	2.92	0.43
20:2:1566:G:N7	29:x:101:ARG:NH2	2.59	0.43
20:2:1578:U:O2'	23:b:5:ILE:O	2.34	0.43
20:2:1623:A:C8	28:k:132:ARG:HB3	2.54	0.43
26:v:20:GLU:O	26:v:24:THR:OG1	2.35	0.43
26:v:32:ALA:HB3	26:v:110:VAL:HB	2.00	0.43
34:U:119:ARG:HE	34:U:119:ARG:HB2	1.62	0.43
38:A:167:ASN:HB3	38:A:170:VAL:HG22	1.99	0.43
39:C:443:CYS:SG	39:C:444:ILE:N	2.92	0.43
39:C:499:VAL:O	39:C:503:TYR:N	2.45	0.43
39:C:515:ASP:OD1	39:C:515:ASP:N	2.47	0.43
39:C:645:LEU:HD13	48:D:42:VAL:HG11	2.01	0.43
39:C:759:GLU:HA	39:C:762:ASN:HB2	2.00	0.43
41:F:242:TYR:O	41:F:246:ARG:N	2.43	0.43
45:M:218:PHE:HB3	45:M:320:MET:HE2	2.01	0.43
46:1:117:SER:OG	46:1:171:GLN:OE1	2.36	0.43
48:D:418:GLY:HA2	48:D:421:ILE:HG22	2.00	0.43
20:2:1310:U:OP1	26:v:36:ARG:NH1	2.39	0.43
20:2:1652:G:O6	20:2:1672:U:O4	2.36	0.43
28:k:67:VAL:O	28:k:71:MET:CB	2.66	0.43
39:C:635:ASP:OD1	39:C:635:ASP:N	2.45	0.43
43:K:51:LEU:HD13	43:K:88:MET:HB3	2.00	0.43
44:L:187:ILE:HG13	44:L:191:ILE:HG13	2.00	0.43
44:L:370:LEU:HA	44:L:373:ILE:HB	2.01	0.43
48:D:419:ALA:O	48:D:423:THR:OG1	2.33	0.43
5:q:100:ARG:HG2	5:q:102:ILE:HG12	2.00	0.43
20:2:464:A:O4'	46:1:567:ARG:NH2	2.51	0.43
20:2:1864:U:O2'	20:2:1866:A:N7	2.52	0.43
39:C:760:LYS:O	39:C:764:LYS:N	2.51	0.43
16:j:54:LYS:HG2	16:j:70:VAL:HG12	2.01	0.43
20:2:1294:G:H2'	20:2:1295:A:H8	1.84	0.43
20:2:1660:C:OP2	33:l:32:ARG:NH1	2.51	0.43
25:u:2:LEU:H	25:u:2:LEU:HG	1.57	0.43
38:A:9:GLU:HG3	38:A:46:ILE:HG12	2.00	0.43
38:A:105:LYS:HD3	38:A:188:TYR:HE1	1.83	0.43
38:A:454:ARG:NH1	45:M:309:GLU:OE1	2.39	0.43
39:C:740:ALA:HB2	39:C:755:PHE:HB2	2.01	0.43
42:H:324:ASN:O	42:H:328:GLN:NE2	2.46	0.43
48:D:220:ILE:HD11	48:D:222:ARG:HE	1.84	0.43
8:s:45:ILE:HG22	8:s:64:VAL:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:2:1630:A:H5''	28:k:37:GLY:H	1.84	0.43
24:e:153:LEU:HB3	24:e:189:ALA:HA	2.01	0.43
35:V:174:VAL:HG12	35:V:188:HIS:HB2	2.00	0.43
39:C:320:LYS:N	39:C:323:GLU:OE1	2.51	0.43
44:L:262:ARG:HD3	44:L:283:LEU:HG	2.01	0.43
3:d:190:SER:O	3:d:190:SER:OG	2.31	0.43
10:c:32:ILE:HD11	10:c:40:LYS:HG2	2.00	0.43
13:i:133:THR:HA	13:i:134:PRO:HD3	1.93	0.43
20:2:1545:A:H4'	22:g:74:GLY:HA2	1.99	0.43
25:u:35:LEU:HD13	25:u:40:VAL:HG21	2.00	0.43
27:o:91:GLY:N	27:o:107:ILE:O	2.48	0.43
30:h:74:SER:O	30:h:74:SER:OG	2.36	0.43
42:H:222:SER:OG	42:H:223:ALA:N	2.52	0.43
42:H:274:LYS:HD3	42:H:277:TYR:HB3	2.01	0.43
44:L:400:ARG:HH21	44:L:411:GLU:HG2	1.84	0.43
35:V:153:CYS:SG	35:V:155:ARG:NH2	2.92	0.42
38:A:177:ILE:HD12	38:A:177:ILE:HA	1.90	0.42
38:A:245:LEU:HD23	38:A:245:LEU:HA	1.87	0.42
39:C:872:ARG:HB3	42:H:261:ASN:HD21	1.83	0.42
40:E:169:LEU:HD13	40:E:192:LEU:HA	2.01	0.42
42:H:159:GLN:HG2	42:H:238:HIS:CE1	2.54	0.42
46:1:174:ASP:OD1	46:1:174:ASP:N	2.50	0.42
13:i:96:LYS:HD2	13:i:132:VAL:HG11	2.01	0.42
20:2:1407:U:O2'	22:g:11:GLN:NE2	2.44	0.42
20:2:1412:C:H2'	20:2:1413:G:H8	1.83	0.42
20:2:1598:G:H5''	31:P:80:ARG:HH11	1.83	0.42
23:b:10:LYS:NZ	30:h:111:GLU:OE2	2.52	0.42
39:C:732:SER:OG	39:C:733:MET:N	2.52	0.42
40:E:239:GLN:HB3	40:E:242:TYR:HD2	1.84	0.42
40:E:322:ASP:OD1	40:E:322:ASP:N	2.48	0.42
46:1:386:THR:HG23	46:1:389:ILE:HD11	2.01	0.42
48:D:270:GLN:O	48:D:277:PHE:N	2.44	0.42
16:j:11:ARG:NH1	20:2:399:C:O4'	2.53	0.42
20:2:1112:U:H3	20:2:1121:G:H1	1.67	0.42
20:2:1627:C:H2'	20:2:1628:C:H6	1.85	0.42
26:v:21:VAL:O	26:v:25:ALA:CB	2.68	0.42
39:C:117:LEU:HD11	39:C:141:LEU:HG	2.00	0.42
39:C:452:ASP:N	39:C:452:ASP:OD1	2.51	0.42
40:E:422:ILE:HD12	40:E:422:ILE:HA	1.90	0.42
46:1:559:LEU:HD23	46:1:562:LEU:HD12	2.00	0.42
3:d:91:SER:O	3:d:91:SER:OG	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:c:109:ARG:NH2	10:c:111:GLN:OE1	2.48	0.42
10:c:136:ARG:HH11	10:c:139:LYS:H	1.68	0.42
20:2:969:U:O2	20:2:971:G:N1	2.52	0.42
20:2:1621:U:OP2	20:2:1623:A:O2'	2.29	0.42
22:g:19:ALA:HB2	22:g:75:GLY:HA3	2.02	0.42
35:V:99:ARG:HD2	35:V:99:ARG:HA	1.94	0.42
35:V:268:ASP:OD1	35:V:268:ASP:N	2.51	0.42
39:C:783:ILE:HD12	39:C:783:ILE:HA	1.93	0.42
39:C:860:ALA:HB2	41:F:340:LEU:HD11	2.00	0.42
40:E:142:GLY:O	40:E:143:ASN:ND2	2.52	0.42
42:H:272:GLN:O	42:H:276:GLN:N	2.43	0.42
43:K:31:ARG:HA	43:K:31:ARG:HD3	1.89	0.42
46:1:486:ASP:HA	46:1:518:VAL:HB	2.00	0.42
10:c:91:LYS:H	10:c:91:LYS:HG2	1.68	0.42
11:n:11:GLN:HE21	11:n:11:GLN:HB3	1.64	0.42
17:z:44:LEU:HD23	17:z:55:ILE:HD11	2.02	0.42
29:x:76:THR:HG21	29:x:97:LYS:HG2	2.01	0.42
35:V:249:CYS:HB2	35:V:258:ILE:HA	2.02	0.42
43:K:125:MET:HE3	43:K:127:LEU:HB2	2.01	0.42
43:K:208:ASP:OD1	43:K:208:ASP:N	2.53	0.42
45:M:170:GLU:HA	45:M:173:VAL:HG12	2.01	0.42
48:D:233:PRO:O	48:D:237:LYS:N	2.52	0.42
2:p:77:ASP:OD1	38:A:10:ASN:ND2	2.53	0.42
14:y:27:LYS:HD3	14:y:27:LYS:HA	1.86	0.42
15:f:42:MET:HE2	15:f:42:MET:HB3	1.89	0.42
15:f:107:SER:HB3	20:2:860:G:H21	1.83	0.42
24:e:88:MET:HE2	24:e:88:MET:HB3	1.73	0.42
40:E:5:ASP:OD1	40:E:5:ASP:N	2.49	0.42
42:H:274:LYS:O	42:H:278:GLN:N	2.50	0.42
46:1:199:ILE:HD12	46:1:199:ILE:HA	1.88	0.42
48:D:169:GLU:HB3	48:D:521:SER:HB3	2.01	0.42
1:a:19:LEU:HD21	21:w:106:LEU:HD11	2.02	0.42
3:d:176:LYS:HA	3:d:176:LYS:HD2	1.89	0.42
3:d:179:THR:HG22	3:d:221:ASP:HB2	2.00	0.42
3:d:232:THR:O	3:d:232:THR:OG1	2.37	0.42
8:s:8:ILE:HG22	8:s:44:ASN:HB3	2.00	0.42
20:2:1779:G:H2'	20:2:1780:G:C4	2.55	0.42
44:L:534:LYS:O	44:L:538:ARG:NE	2.53	0.42
46:1:120:LEU:HB3	46:1:239:MET:HG2	2.01	0.42
46:1:124:ALA:HB2	46:1:239:MET:HE3	2.00	0.42
46:1:326:ASP:OD1	46:1:326:ASP:N	2.41	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:D:199:LEU:HA	48:D:355:SER:HB2	2.02	0.42
48:D:409:TRP:HE3	48:D:466:LEU:HD21	1.84	0.42
20:2:15:U:O2'	20:2:669:A:N6	2.53	0.42
20:2:594:A:N1	20:2:642:U:O2'	2.40	0.42
20:2:723:C:H2'	20:2:724:A:H8	1.85	0.42
20:2:1245:G:O2'	20:2:1492:U:OP1	2.31	0.42
20:2:1289:U:H4'	25:u:2:LEU:HD13	2.01	0.42
22:g:34:VAL:HA	22:g:70:VAL:HB	2.01	0.42
34:U:94:LYS:HA	34:U:94:LYS:HD2	1.78	0.42
43:K:72:LYS:O	43:K:75:THR:OG1	2.35	0.42
44:L:476:ALA:HA	44:L:479:LEU:HB2	2.01	0.42
48:D:222:ARG:NH2	48:D:325:GLN:OE1	2.53	0.42
2:p:163:GLN:HG3	2:p:204:ILE:HD13	2.02	0.42
10:c:139:LYS:HB2	10:c:139:LYS:HE3	1.84	0.42
17:z:122:LYS:HD3	20:2:84:A:H5''	2.02	0.42
24:e:98:GLU:OE1	31:P:101:SER:OG	2.38	0.42
25:u:7:ASN:ND2	25:u:38:LYS:O	2.53	0.42
35:V:74:ASP:OD1	35:V:74:ASP:N	2.53	0.42
35:V:270:LEU:HD23	35:V:310:TRP:CD2	2.55	0.42
39:C:784:GLN:HG2	39:C:813:LEU:HG	2.02	0.42
40:E:42:LEU:O	40:E:46:SER:N	2.41	0.42
46:1:325:ARG:HG2	46:1:327:ALA:H	1.85	0.42
48:D:510:LYS:NZ	48:D:514:LYS:O	2.42	0.42
20:2:1597:C:OP1	28:k:25:LYS:NZ	2.40	0.42
39:C:691:MET:HE2	39:C:691:MET:HB3	1.93	0.42
39:C:792:LEU:O	39:C:796:SER:OG	2.32	0.42
41:F:289:TYR:HE2	41:F:304:VAL:HG11	1.85	0.42
42:H:51:LYS:HA	42:H:51:LYS:HD3	1.78	0.42
8:s:73:GLN:HA	8:s:76:GLN:HB2	2.02	0.41
20:2:199:C:H5	20:2:202:G:H21	1.68	0.41
25:u:9:ILE:O	25:u:13:GLU:HB2	2.20	0.41
27:o:78:THR:N	27:o:95:GLY:O	2.43	0.41
37:B:521:LYS:HD3	37:B:521:LYS:HA	1.86	0.41
1:a:57:LYS:HD2	1:a:57:LYS:HA	1.87	0.41
9:t:108:PRO:HA	9:t:111:GLN:HB3	2.01	0.41
10:c:144:ILE:HG22	10:c:146:SER:H	1.83	0.41
15:f:27:ILE:HB	15:f:61:ILE:HB	2.02	0.41
23:b:227:LYS:N	35:V:185:LYS:O	2.53	0.41
26:v:93:LYS:HB3	26:v:101:ARG:HG3	2.02	0.41
39:C:502:ILE:HD12	39:C:502:ILE:HA	1.90	0.41
40:E:375:ILE:HG23	40:E:380:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:89:LYS:HD3	1:a:89:LYS:HA	1.79	0.41
9:t:143:LYS:HB3	9:t:143:LYS:HE3	1.89	0.41
15:f:32:LYS:N	20:2:686:U:OP1	2.53	0.41
20:2:874:G:H2'	20:2:875:A:H8	1.85	0.41
20:2:1562:C:H2'	20:2:1563:G:C8	2.56	0.41
20:2:1598:G:H1'	20:2:1599:U:H5	1.84	0.41
33:l:10:HIS:HD2	33:l:12:ARG:HH22	1.68	0.41
40:E:12:HIS:HD2	48:D:8:VAL:HG23	1.85	0.41
43:K:48:LEU:HD23	44:L:292:LYS:HG2	2.03	0.41
45:M:157:THR:HG23	45:M:159:GLU:H	1.85	0.41
46:1:384:GLY:CA	55:1:605:ATP:O2A	2.68	0.41
3:d:89:LYS:HA	3:d:89:LYS:HD2	1.87	0.41
20:2:1514:G:H2'	20:2:1515:G:C8	2.55	0.41
29:x:70:ALA:O	29:x:121:ARG:N	2.47	0.41
37:B:565:ILE:HA	37:B:581:HIS:HA	2.01	0.41
38:A:394:LEU:HD12	38:A:403:LEU:HD21	2.02	0.41
39:C:459:MET:HB2	39:C:459:MET:HE2	1.82	0.41
40:E:136:LYS:O	40:E:140:GLU:N	2.53	0.41
45:M:25:LYS:HE2	45:M:25:LYS:HB3	1.86	0.41
1:a:124:VAL:HG21	1:a:134:LEU:HD21	2.02	0.41
20:2:980:A:H2'	20:2:981:A:C8	2.55	0.41
24:e:26:ASP:OD1	24:e:26:ASP:N	2.54	0.41
35:V:82:SER:OG	35:V:83:TRP:N	2.53	0.41
38:A:450:ILE:O	38:A:491:LEU:N	2.49	0.41
40:E:339:PHE:HD1	40:E:339:PHE:HA	1.76	0.41
48:D:267:ILE:O	48:D:508:ILE:N	2.47	0.41
2:p:43:ASN:OD1	2:p:43:ASN:N	2.51	0.41
6:W:4:LYS:HZ1	20:2:1842:C:H5	1.67	0.41
20:2:1337:C:H2'	20:2:1338:G:C8	2.54	0.41
20:2:1452:A:H61	20:2:1473:G:H21	1.67	0.41
38:A:203:MET:HE3	38:A:203:MET:HB3	1.83	0.41
39:C:326:HIS:HB3	39:C:366:LEU:HB3	2.02	0.41
39:C:548:MET:HB2	39:C:548:MET:HE2	1.80	0.41
40:E:229:ARG:HA	40:E:232:ILE:HD12	2.03	0.41
42:H:274:LYS:HD3	42:H:274:LYS:HA	1.77	0.41
1:a:85:ARG:HH11	1:a:85:ARG:HD3	1.76	0.41
2:p:109:LYS:HD2	2:p:109:LYS:HA	1.86	0.41
34:U:107:LYS:HB2	34:U:117:LEU:HD13	2.03	0.41
41:F:172:TRP:HE1	41:F:187:HIS:CD2	2.38	0.41
42:H:249:ARG:HA	42:H:252:GLU:HB3	2.02	0.41
46:1:76:PRO:HB3	46:1:322:LEU:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:D:234:VAL:HB	48:D:342:PRO:HG3	2.02	0.41
2:p:71:LEU:HD12	2:p:71:LEU:HA	1.88	0.41
10:c:33:GLY:HA3	19:T:38:TYR:CG	2.56	0.41
17:z:117:VAL:HG11	17:z:125:VAL:HG21	2.02	0.41
23:b:172:VAL:HG22	23:b:185:LYS:HG2	2.02	0.41
24:e:19:LEU:HB3	24:e:23:TRP:HB2	2.03	0.41
26:v:121:LYS:O	26:v:125:GLU:HB2	2.21	0.41
40:E:130:THR:HA	40:E:133:ARG:HB2	2.03	0.41
40:E:279:LYS:HB2	40:E:279:LYS:HE2	1.86	0.41
44:L:410:GLU:OE1	44:L:452:GLN:NE2	2.54	0.41
46:1:4:LYS:HA	46:1:4:LYS:HD3	1.86	0.41
46:1:568:ARG:HG3	46:1:595:PHE:HE1	1.85	0.41
5:q:153:LEU:HG	7:r:216:ARG:HE	1.84	0.41
9:t:56:ARG:HA	9:t:56:ARG:HD3	1.89	0.41
10:c:122:SER:OG	20:2:527:C:OP1	2.34	0.41
13:i:53:ILE:HD13	13:i:90:ILE:HG13	2.01	0.41
20:2:1154:U:OP1	20:2:1155:U:O2'	2.31	0.41
20:2:1175:G:H1	20:2:1186:U:H3	1.69	0.41
22:g:34:VAL:N	22:g:37:ARG:O	2.53	0.41
24:e:157:GLY:O	24:e:160:GLU:N	2.54	0.41
28:k:8:LYS:HE3	28:k:60:THR:HG22	2.02	0.41
29:x:96:SER:HB2	29:x:99:VAL:HG12	2.02	0.41
35:V:45:LEU:HD12	35:V:53:GLY:HA3	2.01	0.41
38:A:317:ARG:HD2	38:A:317:ARG:HA	1.91	0.41
39:C:55:LYS:HB2	39:C:55:LYS:HE2	1.87	0.41
39:C:804:MET:HA	39:C:807:LEU:HB2	2.03	0.41
40:E:91:ILE:HA	40:E:94:MET:HG2	2.02	0.41
41:F:334:LEU:HD23	41:F:334:LEU:HA	1.93	0.41
43:K:99:ILE:HA	43:K:102:ILE:HG22	2.02	0.41
44:L:514:GLN:HE21	44:L:514:GLN:HB3	1.70	0.41
45:M:106:LEU:HD23	45:M:106:LEU:HA	1.94	0.41
45:M:215:PRO:HA	45:M:276:LYS:HE2	2.02	0.41
49:Y:2:ALA:HB1	49:Y:56:ALA:HB2	2.02	0.41
1:a:156:TYR:OH	14:y:61:ARG:NH1	2.54	0.41
20:2:532:C:H2'	20:2:533:A:H8	1.85	0.41
20:2:1455:A:OP1	21:w:5:ARG:NH2	2.53	0.41
24:e:77:MET:HE3	24:e:77:MET:HB2	1.90	0.41
24:e:192:LYS:HD2	24:e:192:LYS:HA	1.90	0.41
28:k:92:ASP:OD2	28:k:94:LYS:NZ	2.49	0.41
35:V:260:ASP:N	35:V:265:ILE:O	2.53	0.41
39:C:637:GLN:HE21	39:C:682:LEU:HG	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:C:854:ASN:HA	39:C:857:LEU:HB2	2.02	0.41
40:E:56:ASP:O	40:E:60:ASN:N	2.54	0.41
41:F:103:VAL:HG13	42:H:210:LEU:HD23	2.03	0.41
42:H:79:THR:OG1	42:H:113:ASP:OD2	2.39	0.41
42:H:338:LEU:HA	42:H:341:LEU:HD12	2.03	0.41
43:K:204:LYS:HE2	43:K:204:LYS:HB2	1.86	0.41
20:2:749:U:O4	20:2:792:C:N4	2.46	0.40
20:2:1596:U:OP2	31:P:85:ARG:NE	2.54	0.40
28:k:138:THR:O	28:k:141:ARG:NH1	2.55	0.40
29:x:11:GLN:NE2	29:x:62:ARG:HD2	2.36	0.40
31:P:68:ILE:HB	31:P:109:TYR:HB2	2.03	0.40
39:C:595:GLN:NE2	48:D:39:LEU:O	2.53	0.40
44:L:243:GLN:HA	44:L:246:VAL:HG22	2.02	0.40
44:L:405:ASP:HA	44:L:406:PRO:HD3	1.91	0.40
45:M:138:GLN:HE22	45:M:175:CYS:HB3	1.86	0.40
46:1:17:LYS:HA	46:1:18:PRO:HD3	1.93	0.40
48:D:31:GLN:HA	48:D:32:PRO:HD3	1.95	0.40
48:D:426:LYS:HA	48:D:426:LYS:HD2	1.90	0.40
1:a:147:LEU:O	1:a:165:ASN:ND2	2.50	0.40
9:t:42:ARG:NH1	20:2:1742:C:OP2	2.48	0.40
20:2:1523:C:OP1	28:k:142:ARG:NH1	2.54	0.40
20:2:1718:G:N2	20:2:1816:G:N7	2.68	0.40
20:2:1726:G:H2'	20:2:1727:G:C8	2.56	0.40
25:u:79:LEU:HD23	25:u:79:LEU:HA	1.90	0.40
28:k:51:ASP:OD1	28:k:51:ASP:N	2.54	0.40
40:E:31:ILE:HD12	40:E:31:ILE:HA	1.97	0.40
40:E:46:SER:O	40:E:73:LYS:NZ	2.44	0.40
40:E:171:GLY:O	40:E:175:SER:N	2.54	0.40
42:H:276:GLN:HA	42:H:279:GLN:HG2	2.03	0.40
44:L:401:MET:HB2	44:L:402:GLN:HE21	1.86	0.40
2:p:38:MET:N	2:p:38:MET:SD	2.94	0.40
3:d:71:LYS:HE2	3:d:71:LYS:HB3	1.88	0.40
8:s:65:PRO:O	8:s:69:LEU:N	2.55	0.40
9:t:31:ARG:NH1	20:2:380:G:OP1	2.54	0.40
9:t:48:VAL:HG11	9:t:54:LYS:HD2	2.03	0.40
12:m:4:MET:SD	12:m:124:ARG:NH1	2.94	0.40
20:2:1166:G:O6	20:2:1193:U:O4	2.38	0.40
32:S:9:ILE:HD12	32:S:59:LEU:HA	2.02	0.40
39:C:867:VAL:O	39:C:871:GLU:N	2.51	0.40
40:E:385:ASP:O	40:E:389:GLY:N	2.49	0.40
42:H:40:GLN:HG3	42:H:77:GLU:HA	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:K:33:VAL:HG21	43:K:65:VAL:HG13	2.03	0.40
43:K:135:GLU:OE2	43:K:139:ARG:NH2	2.54	0.40
48:D:221:LYS:HD3	48:D:221:LYS:HA	1.90	0.40
5:q:202:PRO:HB2	11:n:42:LEU:HD23	2.04	0.40
14:y:3:ASN:OD1	14:y:3:ASN:N	2.51	0.40
20:2:97:U:O2	20:2:434:G:N2	2.54	0.40
20:2:1589:A:N3	20:2:1653:U:O2'	2.49	0.40
25:u:47:LYS:HA	25:u:47:LYS:HD3	1.76	0.40
38:A:402:LYS:HE3	38:A:406:ARG:HD2	2.02	0.40
41:F:243:ASP:HA	41:F:246:ARG:HG2	2.02	0.40
41:F:334:LEU:HD11	42:H:337:ASN:HB2	2.04	0.40
5:q:188:ASN:ND2	20:2:808:A:OP1	2.46	0.40
9:t:13:LYS:HG3	11:n:137:THR:HG21	2.03	0.40
9:t:54:LYS:NZ	9:t:181:GLN:OE1	2.39	0.40
16:j:67:ARG:HH11	16:j:67:ARG:HD3	1.73	0.40
18:R:2:PRO:HB2	18:R:3:LEU:H	1.74	0.40
20:2:1468:C:H2'	20:2:1469:A:C8	2.56	0.40
20:2:1499:U:H2'	20:2:1500:G:H8	1.86	0.40
20:2:1627:C:H5''	29:x:41:LYS:HB2	2.03	0.40
29:x:21:PHE:HD1	29:x:24:LYS:HE2	1.86	0.40
39:C:477:ALA:O	39:C:481:ALA:N	2.54	0.40
39:C:517:LYS:HE2	39:C:517:LYS:HB2	1.96	0.40
40:E:38:LEU:HD22	40:E:57:VAL:HG13	2.02	0.40
41:F:90:ARG:HD3	41:F:90:ARG:HA	1.88	0.40
44:L:487:ARG:HD3	44:L:488:ILE:HD13	2.03	0.40
46:1:386:THR:HA	46:1:389:ILE:HG12	2.03	0.40
46:1:417:SER:O	46:1:417:SER:OG	2.37	0.40
48:D:408:ASP:O	48:D:412:LYS:N	2.47	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	214/216 (99%)	214 (100%)	0	0	100	100
2	p	209/211 (99%)	209 (100%)	0	0	100	100
3	d	214/216 (99%)	214 (100%)	0	0	100	100
4	Q	99/101 (98%)	99 (100%)	0	0	100	100
5	q	253/255 (99%)	250 (99%)	3 (1%)	0	100	100
6	W	22/24 (92%)	22 (100%)	0	0	100	100
7	r	220/222 (99%)	220 (100%)	0	0	100	100
8	s	165/181 (91%)	165 (100%)	0	0	100	100
9	t	195/205 (95%)	195 (100%)	0	0	100	100
10	c	178/180 (99%)	178 (100%)	0	0	100	100
11	n	131/144 (91%)	131 (100%)	0	0	100	100
12	m	147/149 (99%)	147 (100%)	0	0	100	100
13	i	123/125 (98%)	123 (100%)	0	0	100	100
14	y	80/82 (98%)	80 (100%)	0	0	100	100
15	f	127/129 (98%)	126 (99%)	1 (1%)	0	100	100
16	j	137/139 (99%)	135 (98%)	2 (2%)	0	100	100
17	z	120/122 (98%)	120 (100%)	0	0	100	100
18	R	80/82 (98%)	80 (100%)	0	0	100	100
19	T	40/44 (91%)	40 (100%)	0	0	100	100
21	w	124/130 (95%)	124 (100%)	0	0	100	100
22	g	136/138 (99%)	134 (98%)	2 (2%)	0	100	100
23	b	222/224 (99%)	221 (100%)	1 (0%)	0	100	100
24	e	187/189 (99%)	185 (99%)	2 (1%)	0	100	100
25	u	93/95 (98%)	93 (100%)	0	0	100	100
26	v	107/116 (92%)	107 (100%)	0	0	100	100
27	o	117/119 (98%)	117 (100%)	0	0	100	100
28	k	138/140 (99%)	138 (100%)	0	0	100	100
29	x	139/141 (99%)	139 (100%)	0	0	100	100
30	h	96/98 (98%)	96 (100%)	0	0	100	100
31	P	68/70 (97%)	68 (100%)	0	0	100	100
32	S	59/61 (97%)	59 (100%)	0	0	100	100
33	l	52/54 (96%)	52 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	U	53/62 (86%)	53 (100%)	0	0	100	100
35	V	290/309 (94%)	287 (99%)	3 (1%)	0	100	100
36	I	301/316 (95%)	301 (100%)	0	0	100	100
37	B	528/566 (93%)	528 (100%)	0	0	100	100
38	A	682/722 (94%)	682 (100%)	0	0	100	100
39	C	615/743 (83%)	613 (100%)	2 (0%)	0	100	100
40	E	406/429 (95%)	406 (100%)	0	0	100	100
41	F	267/269 (99%)	266 (100%)	1 (0%)	0	100	100
42	H	289/318 (91%)	289 (100%)	0	0	100	100
43	K	215/217 (99%)	215 (100%)	0	0	100	100
44	L	370/372 (100%)	366 (99%)	4 (1%)	0	100	100
45	M	330/362 (91%)	330 (100%)	0	0	100	100
46	1	572/595 (96%)	570 (100%)	2 (0%)	0	100	100
47	N	89/91 (98%)	88 (99%)	1 (1%)	0	100	100
48	D	441/527 (84%)	441 (100%)	0	0	100	100
49	Y	76/78 (97%)	76 (100%)	0	0	100	100
50	G	68/258 (26%)	68 (100%)	0	0	100	100
50	J	71/258 (28%)	71 (100%)	0	0	100	100
All	All	9955/10894 (91%)	9931 (100%)	24 (0%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	180/180 (100%)	177 (98%)	3 (2%)	53	67
2	p	192/192 (100%)	189 (98%)	3 (2%)	55	68
3	d	182/182 (100%)	180 (99%)	2 (1%)	65	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	Q	88/88 (100%)	87 (99%)	1 (1%)	65	73
5	q	220/220 (100%)	219 (100%)	1 (0%)	81	81
6	W	23/23 (100%)	23 (100%)	0	100	100
7	r	193/193 (100%)	191 (99%)	2 (1%)	68	74
8	s	155/163 (95%)	153 (99%)	2 (1%)	61	71
9	t	174/178 (98%)	174 (100%)	0	100	100
10	c	160/160 (100%)	159 (99%)	1 (1%)	78	79
11	n	125/132 (95%)	125 (100%)	0	100	100
12	m	130/130 (100%)	129 (99%)	1 (1%)	73	76
13	i	98/98 (100%)	98 (100%)	0	100	100
14	y	66/66 (100%)	65 (98%)	1 (2%)	57	69
15	f	112/112 (100%)	112 (100%)	0	100	100
16	j	111/111 (100%)	109 (98%)	2 (2%)	51	67
17	z	106/106 (100%)	106 (100%)	0	100	100
18	R	74/74 (100%)	73 (99%)	1 (1%)	59	70
19	T	35/35 (100%)	35 (100%)	0	100	100
21	w	111/118 (94%)	110 (99%)	1 (1%)	70	74
22	g	114/114 (100%)	112 (98%)	2 (2%)	51	67
23	b	188/188 (100%)	185 (98%)	3 (2%)	55	68
24	e	159/159 (100%)	154 (97%)	5 (3%)	35	57
25	u	86/86 (100%)	85 (99%)	1 (1%)	63	72
26	v	94/98 (96%)	91 (97%)	3 (3%)	34	56
27	o	107/107 (100%)	106 (99%)	1 (1%)	70	74
28	k	122/122 (100%)	120 (98%)	2 (2%)	55	68
29	x	111/111 (100%)	110 (99%)	1 (1%)	70	74
30	h	91/91 (100%)	91 (100%)	0	100	100
31	P	62/62 (100%)	61 (98%)	1 (2%)	55	68
32	S	54/54 (100%)	52 (96%)	2 (4%)	30	54
33	l	47/47 (100%)	47 (100%)	0	100	100
34	U	51/55 (93%)	51 (100%)	0	100	100
35	V	256/268 (96%)	251 (98%)	5 (2%)	48	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	B	90/508 (18%)	86 (96%)	4 (4%)	25	49
38	A	546/667 (82%)	540 (99%)	6 (1%)	65	73
39	C	554/662 (84%)	544 (98%)	10 (2%)	51	67
40	E	380/393 (97%)	376 (99%)	4 (1%)	65	73
41	F	237/237 (100%)	230 (97%)	7 (3%)	36	57
42	H	269/290 (93%)	264 (98%)	5 (2%)	50	66
43	K	192/192 (100%)	191 (100%)	1 (0%)	81	81
44	L	342/342 (100%)	336 (98%)	6 (2%)	51	67
45	M	305/324 (94%)	301 (99%)	4 (1%)	61	71
46	1	506/523 (97%)	497 (98%)	9 (2%)	51	67
47	N	77/78 (99%)	77 (100%)	0	100	100
48	D	398/473 (84%)	390 (98%)	8 (2%)	48	65
All	All	7973/8812 (90%)	7862 (99%)	111 (1%)	57	70

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	97	THR
1	a	107	THR
1	a	140	VAL
2	p	79	VAL
2	p	125	VAL
2	p	153	THR
3	d	132	ASP
3	d	248	TYR
4	Q	63	VAL
5	q	247	THR
7	r	162	LEU
7	r	180	VAL
8	s	66	VAL
8	s	134	VAL
10	c	151	LEU
12	m	60	VAL
14	y	9	VAL
16	j	85	VAL
16	j	112	VAL
18	R	53	VAL
21	w	41	ILE

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Mol	Chain	Res	Type
22	g	12	VAL
22	g	102	GLU
23	b	86	LEU
23	b	176	LEU
23	b	198	ILE
24	e	26	ASP
24	e	30	ILE
24	e	128	ILE
24	e	168	THR
24	e	187	SER
25	u	2	LEU
26	v	103	VAL
26	v	106	CYS
26	v	123	VAL
27	o	116	LEU
28	k	81	ASP
28	k	136	THR
29	x	35	ASP
31	P	72	VAL
32	S	38	THR
32	S	43	ILE
35	V	23	THR
35	V	70	VAL
35	V	111	VAL
35	V	113	PHE
35	V	166	VAL
37	B	489	ILE
37	B	493	VAL
37	B	513	VAL
37	B	559	VAL
38	A	311	THR
38	A	336	THR
38	A	407	VAL
38	A	446	ILE
38	A	459	VAL
38	A	462	VAL
39	C	324	ILE
39	C	378	ILE
39	C	379	ILE
39	C	413	PHE
39	C	440	VAL
39	C	444	ILE

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Mol	Chain	Res	Type
39	C	470	VAL
39	C	633	LEU
39	C	709	MET
39	C	726	LEU
40	E	173	LEU
40	E	219	LEU
40	E	339	PHE
40	E	342	GLU
41	F	116	VAL
41	F	119	THR
41	F	146	VAL
41	F	219	THR
41	F	223	VAL
41	F	230	VAL
41	F	322	ASP
42	H	36	VAL
42	H	110	VAL
42	H	133	LEU
42	H	233	LEU
42	H	243	LEU
43	K	90	ASP
44	L	187	ILE
44	L	244	LEU
44	L	293	VAL
44	L	346	THR
44	L	501	VAL
44	L	503	THR
45	M	63	VAL
45	M	82	LEU
45	M	117	THR
45	M	119	VAL
46	1	11	VAL
46	1	55	CYS
46	1	241	ASP
46	1	269	ILE
46	1	272	VAL
46	1	305	VAL
46	1	416	ILE
46	1	493	ASP
46	1	543	THR
48	D	234	VAL
48	D	272	VAL

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Mol	Chain	Res	Type
48	D	288	LEU
48	D	291	VAL
48	D	368	ASP
48	D	468	THR
48	D	491	LEU
48	D	520	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (176) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	9	GLN
1	a	50	ASN
1	a	110	ASN
2	p	40	ASN
2	p	92	GLN
2	p	157	GLN
2	p	160	GLN
2	p	202	GLN
4	Q	25	ASN
4	Q	72	HIS
5	q	17	HIS
5	q	50	ASN
5	q	98	ASN
5	q	112	HIS
5	q	209	HIS
5	q	216	ASN
5	q	224	ASN
7	r	13	GLN
7	r	56	ASN
7	r	59	GLN
8	s	73	GLN
8	s	91	HIS
8	s	165	ASN
9	t	7	ASN
9	t	35	ASN
9	t	64	ASN
9	t	111	GLN
9	t	146	GLN
9	t	165	GLN
9	t	167	GLN
10	c	39	ASN
10	c	132	GLN

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Mol	Chain	Res	Type
10	c	177	ASN
11	n	11	GLN
11	n	13	GLN
11	n	39	ASN
12	m	90	HIS
13	i	38	ASN
13	i	79	GLN
13	i	113	GLN
15	f	64	ASN
15	f	98	GLN
15	f	113	HIS
16	j	46	HIS
16	j	61	GLN
17	z	22	GLN
18	R	83	GLN
19	T	22	GLN
19	T	44	ASN
19	T	58	ASN
21	w	26	ASN
21	w	31	ASN
21	w	56	HIS
22	g	24	HIS
22	g	142	GLN
23	b	179	GLN
24	e	74	ASN
24	e	82	ASN
24	e	95	HIS
24	e	148	ASN
24	e	149	GLN
24	e	203	ASN
25	u	7	ASN
25	u	32	HIS
25	u	42	ASN
25	u	77	GLN
26	v	82	ASN
27	o	98	ASN
27	o	103	ASN
28	k	42	HIS
28	k	73	ASN
28	k	105	ASN
28	k	120	HIS
28	k	135	HIS

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Mol	Chain	Res	Type
29	x	11	GLN
29	x	128	GLN
30	h	81	GLN
31	P	46	ASN
31	P	106	GLN
33	l	3	HIS
33	l	26	ASN
35	V	20	GLN
35	V	117	ASN
35	V	196	ASN
35	V	311	GLN
37	B	497	GLN
37	B	518	HIS
37	B	520	GLN
38	A	10	ASN
38	A	16	ASN
38	A	47	HIS
38	A	73	GLN
38	A	236	GLN
38	A	247	GLN
38	A	316	GLN
38	A	432	GLN
38	A	433	ASN
38	A	434	ASN
38	A	550	HIS
38	A	551	GLN
38	A	586	ASN
39	C	62	ASN
39	C	365	ASN
39	C	460	GLN
39	C	478	GLN
39	C	575	HIS
39	C	637	GLN
39	C	713	GLN
39	C	717	GLN
39	C	784	GLN
39	C	819	HIS
39	C	845	HIS
39	C	870	ASN
40	E	49	ASN
40	E	121	HIS
40	E	143	ASN

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Mol	Chain	Res	Type
40	E	210	GLN
40	E	252	HIS
40	E	335	ASN
40	E	361	ASN
40	E	377	ASN
40	E	403	GLN
41	F	280	GLN
41	F	332	ASN
42	H	52	HIS
42	H	86	GLN
42	H	100	GLN
42	H	109	HIS
42	H	114	HIS
42	H	121	GLN
42	H	207	ASN
42	H	238	HIS
42	H	244	GLN
42	H	255	GLN
42	H	270	GLN
42	H	271	GLN
42	H	336	GLN
42	H	352	ASN
43	K	25	ASN
43	K	36	GLN
43	K	47	ASN
43	K	55	GLN
43	K	76	ASN
43	K	91	GLN
43	K	101	GLN
43	K	119	GLN
43	K	151	GLN
43	K	152	HIS
44	L	195	GLN
44	L	243	GLN
44	L	363	GLN
44	L	364	ASN
44	L	402	GLN
44	L	452	GLN
44	L	529	HIS
45	M	79	GLN
45	M	138	GLN
45	M	258	ASN

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Mol	Chain	Res	Type
45	M	259	ASN
45	M	302	GLN
45	M	346	GLN
46	1	154	ASN
46	1	175	GLN
46	1	213	ASN
46	1	572	ASN
46	1	588	GLN
46	1	593	ASN
47	N	48	GLN
48	D	10	GLN
48	D	31	GLN
48	D	178	GLN
48	D	270	GLN
48	D	322	ASN
48	D	397	ASN
48	D	427	ASN
48	D	469	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
20	2	1710/1720 (99%)	525 (30%)	10 (0%)

All (525) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
20	2	2	A
20	2	6	G
20	2	25	A
20	2	41	G
20	2	44	U
20	2	45	A
20	2	46	A
20	2	47	G
20	2	49	C
20	2	56	G
20	2	60	A
20	2	62	G
20	2	64	A
20	2	65	C

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Mol	Chain	Res	Type
20	2	67	C
20	2	68	A
20	2	69	C
20	2	71	G
20	2	72	C
20	2	74	G
20	2	76	U
20	2	79	A
20	2	92	A
20	2	99	A
20	2	103	A
20	2	112	U
20	2	113	G
20	2	114	G
20	2	115	U
20	2	126	G
20	2	128	U
20	2	129	C
20	2	130	G
20	2	143	U
20	2	147	A
20	2	149	A
20	2	155	G
20	2	163	U
20	2	170	A
20	2	175	A
20	2	178	C
20	2	182	C
20	2	187	G
20	2	190	G
20	2	195	C
20	2	196	C
20	2	197	U
20	2	198	U
20	2	199	C
20	2	200	G
20	2	202	G
20	2	204	G
20	2	206	G
20	2	207	G
20	2	208	G
20	2	220	U

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Mol	Chain	Res	Type
20	2	222	U
20	2	223	C
20	2	291	G
20	2	305	U
20	2	307	G
20	2	308	G
20	2	309	G
20	2	312	G
20	2	313	A
20	2	332	G
20	2	333	G
20	2	344	U
20	2	345	U
20	2	346	C
20	2	347	G
20	2	362	C
20	2	364	A
20	2	368	U
20	2	369	C
20	2	370	G
20	2	381	C
20	2	384	U
20	2	385	G
20	2	386	C
20	2	399	C
20	2	400	C
20	2	408	A
20	2	409	C
20	2	418	A
20	2	421	G
20	2	435	A
20	2	438	G
20	2	439	A
20	2	445	A
20	2	448	A
20	2	449	A
20	2	450	C
20	2	451	G
20	2	455	A
20	2	461	U
20	2	464	A
20	2	465	A

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Mol	Chain	Res	Type
20	2	472	C
20	2	474	G
20	2	482	G
20	2	483	C
20	2	487	U
20	2	488	U
20	2	492	C
20	2	493	A
20	2	494	C
20	2	500	A
20	2	501	C
20	2	508	A
20	2	509	G
20	2	523	A
20	2	525	A
20	2	529	A
20	2	537	C
20	2	538	U
20	2	539	C
20	2	541	U
20	2	542	U
20	2	543	C
20	2	544	G
20	2	546	G
20	2	547	G
20	2	548	C
20	2	549	C
20	2	551	U
20	2	556	U
20	2	559	G
20	2	560	A
20	2	564	A
20	2	568	C
20	2	570	C
20	2	574	A
20	2	576	A
20	2	587	A
20	2	588	G
20	2	589	G
20	2	591	U
20	2	593	C
20	2	594	A

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Mol	Chain	Res	Type
20	2	600	G
20	2	603	C
20	2	604	A
20	2	606	G
20	2	607	U
20	2	608	C
20	2	609	U
20	2	614	C
20	2	615	C
20	2	617	G
20	2	623	G
20	2	627	U
20	2	628	A
20	2	629	A
20	2	630	U
20	2	639	C
20	2	640	A
20	2	643	A
20	2	644	G
20	2	655	A
20	2	660	C
20	2	662	G
20	2	666	U
20	2	668	A
20	2	669	A
20	2	671	A
20	2	672	A
20	2	673	G
20	2	675	U
20	2	684	G
20	2	687	C
20	2	690	G
20	2	691	G
20	2	698	G
20	2	707	C
20	2	709	G
20	2	710	C
20	2	713	C
20	2	714	G
20	2	716	G
20	2	717	G
20	2	719	G

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Mol	Chain	Res	Type
20	2	723	C
20	2	727	G
20	2	733	C
20	2	734	C
20	2	735	C
20	2	739	C
20	2	749	U
20	2	750	C
20	2	751	G
20	2	752	G
20	2	792	C
20	2	793	G
20	2	794	A
20	2	796	G
20	2	798	G
20	2	799	U
20	2	801	U
20	2	810	A
20	2	811	A
20	2	816	A
20	2	821	G
20	2	822	U
20	2	823	U
20	2	824	C
20	2	827	A
20	2	830	A
20	2	847	A
20	2	869	A
20	2	870	A
20	2	871	U
20	2	872	A
20	2	873	G
20	2	874	G
20	2	878	G
20	2	881	G
20	2	883	U
20	2	884	C
20	2	885	U
20	2	886	A
20	2	887	U
20	2	888	U
20	2	889	U

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Mol	Chain	Res	Type
20	2	890	U
20	2	891	G
20	2	892	U
20	2	893	U
20	2	894	G
20	2	895	G
20	2	897	U
20	2	898	U
20	2	899	U
20	2	901	G
20	2	902	G
20	2	903	A
20	2	907	G
20	2	908	A
20	2	909	G
20	2	912	C
20	2	913	A
20	2	919	A
20	2	920	A
20	2	921	G
20	2	922	A
20	2	930	C
20	2	933	G
20	2	938	A
20	2	943	U
20	2	952	G
20	2	953	C
20	2	961	G
20	2	963	A
20	2	970	G
20	2	971	G
20	2	973	C
20	2	989	C
20	2	990	A
20	2	992	A
20	2	997	A
20	2	1008	A
20	2	1017	U
20	2	1023	A
20	2	1026	C
20	2	1027	A
20	2	1029	G

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Mol	Chain	Res	Type
20	2	1030	A
20	2	1045	U
20	2	1049	A
20	2	1053	C
20	2	1054	G
20	2	1056	U
20	2	1058	A
20	2	1060	A
20	2	1061	U
20	2	1064	C
20	2	1082	A
20	2	1083	A
20	2	1085	C
20	2	1087	A
20	2	1096	G
20	2	1097	G
20	2	1109	C
20	2	1113	A
20	2	1114	U
20	2	1115	U
20	2	1116	C
20	2	1117	C
20	2	1118	C
20	2	1120	U
20	2	1138	C
20	2	1143	A
20	2	1149	A
20	2	1153	C
20	2	1154	U
20	2	1155	U
20	2	1156	U
20	2	1157	G
20	2	1166	G
20	2	1168	G
20	2	1170	A
20	2	1171	G
20	2	1181	A
20	2	1188	A
20	2	1194	A
20	2	1195	A
20	2	1207	G
20	2	1208	A

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Mol	Chain	Res	Type
20	2	1210	G
20	2	1211	G
20	2	1215	C
20	2	1216	C
20	2	1221	G
20	2	1224	G
20	2	1229	G
20	2	1236	G
20	2	1237	C
20	2	1240	A
20	2	1242	U
20	2	1248	U
20	2	1249	C
20	2	1250	A
20	2	1251	A
20	2	1253	A
20	2	1256	G
20	2	1257	G
20	2	1258	A
20	2	1259	A
20	2	1260	A
20	2	1263	U
20	2	1264	C
20	2	1265	A
20	2	1271	C
20	2	1273	C
20	2	1274	G
20	2	1275	G
20	2	1277	C
20	2	1280	G
20	2	1285	G
20	2	1286	G
20	2	1287	A
20	2	1289	U
20	2	1293	A
20	2	1295	A
20	2	1297	U
20	2	1299	A
20	2	1301	A
20	2	1302	G
20	2	1306	U
20	2	1313	A

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Mol	Chain	Res	Type
20	2	1315	U
20	2	1317	C
20	2	1321	G
20	2	1322	G
20	2	1328	G
20	2	1330	G
20	2	1341	C
20	2	1342	U
20	2	1352	G
20	2	1354	G
20	2	1355	C
20	2	1358	U
20	2	1362	U
20	2	1363	C
20	2	1369	A
20	2	1371	U
20	2	1372	U
20	2	1378	A
20	2	1381	G
20	2	1382	A
20	2	1397	U
20	2	1398	G
20	2	1401	A
20	2	1402	A
20	2	1403	C
20	2	1405	A
20	2	1428	G
20	2	1429	G
20	2	1430	C
20	2	1447	G
20	2	1449	G
20	2	1452	A
20	2	1454	A
20	2	1462	U
20	2	1463	U
20	2	1464	C
20	2	1466	G
20	2	1473	G
20	2	1475	G
20	2	1477	U
20	2	1478	U
20	2	1480	A

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Mol	Chain	Res	Type
20	2	1484	A
20	2	1489	A
20	2	1490	G
20	2	1493	C
20	2	1497	G
20	2	1498	A
20	2	1499	U
20	2	1506	A
20	2	1507	G
20	2	1508	A
20	2	1519	U
20	2	1520	G
20	2	1521	C
20	2	1522	A
20	2	1531	A
20	2	1533	A
20	2	1536	G
20	2	1544	C
20	2	1547	C
20	2	1548	G
20	2	1551	U
20	2	1552	G
20	2	1553	C
20	2	1554	C
20	2	1556	A
20	2	1558	C
20	2	1559	C
20	2	1560	U
20	2	1568	C
20	2	1575	G
20	2	1578	U
20	2	1580	A
20	2	1582	C
20	2	1584	G
20	2	1585	U
20	2	1587	G
20	2	1588	A
20	2	1599	U
20	2	1601	A
20	2	1603	G
20	2	1604	G
20	2	1606	G

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Mol	Chain	Res	Type
20	2	1620	A
20	2	1621	U
20	2	1623	A
20	2	1624	U
20	2	1629	C
20	2	1632	G
20	2	1634	A
20	2	1636	G
20	2	1637	A
20	2	1648	G
20	2	1654	G
20	2	1660	C
20	2	1661	A
20	2	1664	A
20	2	1665	G
20	2	1669	G
20	2	1671	G
20	2	1677	U
20	2	1680	G
20	2	1683	C
20	2	1686	G
20	2	1694	U
20	2	1695	A
20	2	1697	A
20	2	1700	C
20	2	1702	G
20	2	1718	G
20	2	1720	U
20	2	1721	U
20	2	1722	G
20	2	1723	G
20	2	1725	U
20	2	1726	G
20	2	1730	U
20	2	1733	U
20	2	1742	C
20	2	1744	G
20	2	1751	C
20	2	1752	C
20	2	1753	C
20	2	1755	C
20	2	1756	C

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Mol	Chain	Res	Type
20	2	1757	G
20	2	1758	G
20	2	1759	G
20	2	1760	G
20	2	1772	C
20	2	1773	C
20	2	1774	C
20	2	1777	G
20	2	1778	C
20	2	1780	G
20	2	1781	A
20	2	1783	C
20	2	1784	G
20	2	1785	C
20	2	1787	G
20	2	1791	A
20	2	1799	G
20	2	1800	A
20	2	1805	G
20	2	1806	A
20	2	1808	U
20	2	1810	U
20	2	1811	C
20	2	1814	G
20	2	1816	G
20	2	1820	G
20	2	1821	U
20	2	1822	A
20	2	1823	A
20	2	1824	A
20	2	1825	A
20	2	1826	G
20	2	1829	G
20	2	1831	A
20	2	1834	A
20	2	1835	A
20	2	1837	G
20	2	1838	U
20	2	1848	U
20	2	1849	A
20	2	1851	A
20	2	1857	G

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Mol	Chain	Res	Type
20	2	1861	G
20	2	1862	G
20	2	1863	A
20	2	1865	C
20	2	1866	A
20	2	1867	U
20	2	1869	A

All (10) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
20	2	332	G
20	2	367	U
20	2	368	U
20	2	550	C
20	2	912	C
20	2	1060	A
20	2	1292	C
20	2	1474	A
20	2	1581	C
20	2	1807	C

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 5 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
53	ADP	1	603	54	28,29,29	1.41	4 (14%)	43,45,45	1.82	10 (23%)
52	SF4	1	602	-	0,12,12	-	-	-	-	-
55	ATP	1	605	54	32,33,33	1.39	4 (12%)	48,52,52	1.77	9 (18%)
52	SF4	1	601	-	0,12,12	-	-	-	-	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	SF4	1	602	-	-	-	0/6/5/5
53	ADP	1	603	54	-	5/16/32/32	0/3/3/3
55	ATP	1	605	54	-	2/22/38/38	0/3/3/3
52	SF4	1	601	-	-	-	0/6/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1	605	ATP	C5-C4	4.74	1.47	1.39
53	1	603	ADP	C5-C4	4.71	1.47	1.39
55	1	605	ATP	C5-C6	2.75	1.48	1.41
53	1	603	ADP	C5-C6	2.73	1.48	1.41
55	1	605	ATP	C8-N7	2.41	1.36	1.31
53	1	603	ADP	C8-N7	2.35	1.36	1.31
53	1	603	ADP	C5-N7	-2.29	1.34	1.39
55	1	605	ATP	C5-N7	-2.23	1.35	1.39

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	1	605	ATP	C5-C4-N3	-5.86	118.64	126.72
53	1	603	ADP	C5-C4-N3	-5.77	118.78	126.72
53	1	603	ADP	N3-C4-N9	4.62	135.02	127.17
55	1	605	ATP	N3-C4-N9	4.55	134.91	127.17
55	1	605	ATP	C2-N3-C4	3.73	120.94	111.83
53	1	603	ADP	C2-N3-C4	3.65	120.75	111.83
55	1	605	ATP	C4-C5-N7	-3.54	106.54	110.58
53	1	603	ADP	C4-C5-N7	-3.48	106.61	110.58
55	1	605	ATP	N3-C2-N1	-3.20	123.74	128.58
53	1	603	ADP	N3-C2-N1	-3.20	123.75	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	1	603	ADP	C4-N9-C8	2.78	108.65	105.74
53	1	603	ADP	C5-N7-C8	2.56	107.47	103.45
55	1	605	ATP	C5-N7-C8	2.54	107.44	103.45
55	1	605	ATP	C4-N9-C8	2.53	108.39	105.74
55	1	605	ATP	C3'-C2'-C1'	2.47	106.13	101.46
55	1	605	ATP	C6-C5-N7	2.14	136.22	132.09
53	1	603	ADP	C3'-C2'-C1'	2.09	105.41	101.46
53	1	603	ADP	C6-C5-N7	2.04	136.03	132.09
53	1	603	ADP	N9-C8-N7	-2.02	111.06	113.94

There are no chirality outliers.

All (7) torsion outliers are listed below:

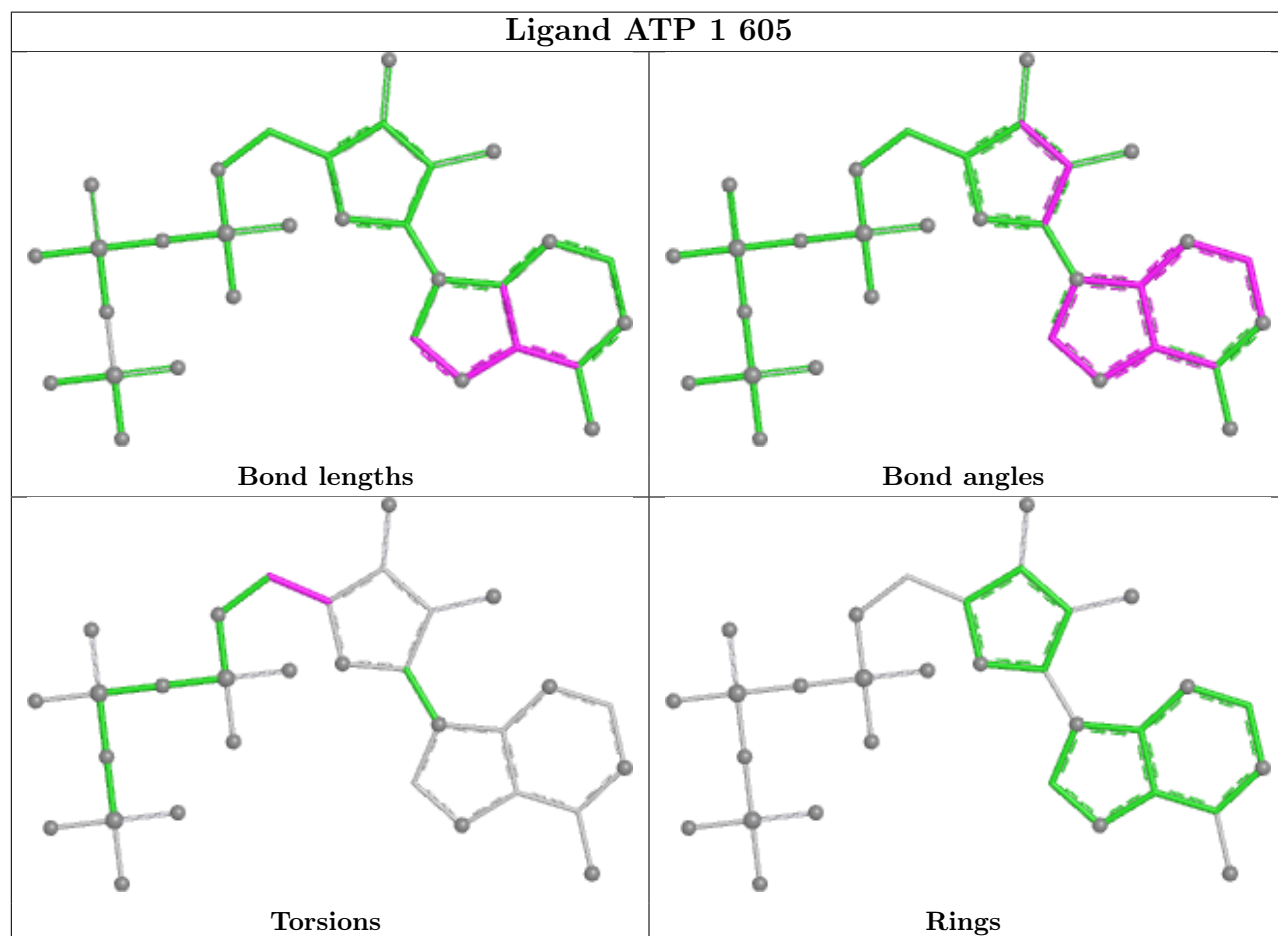
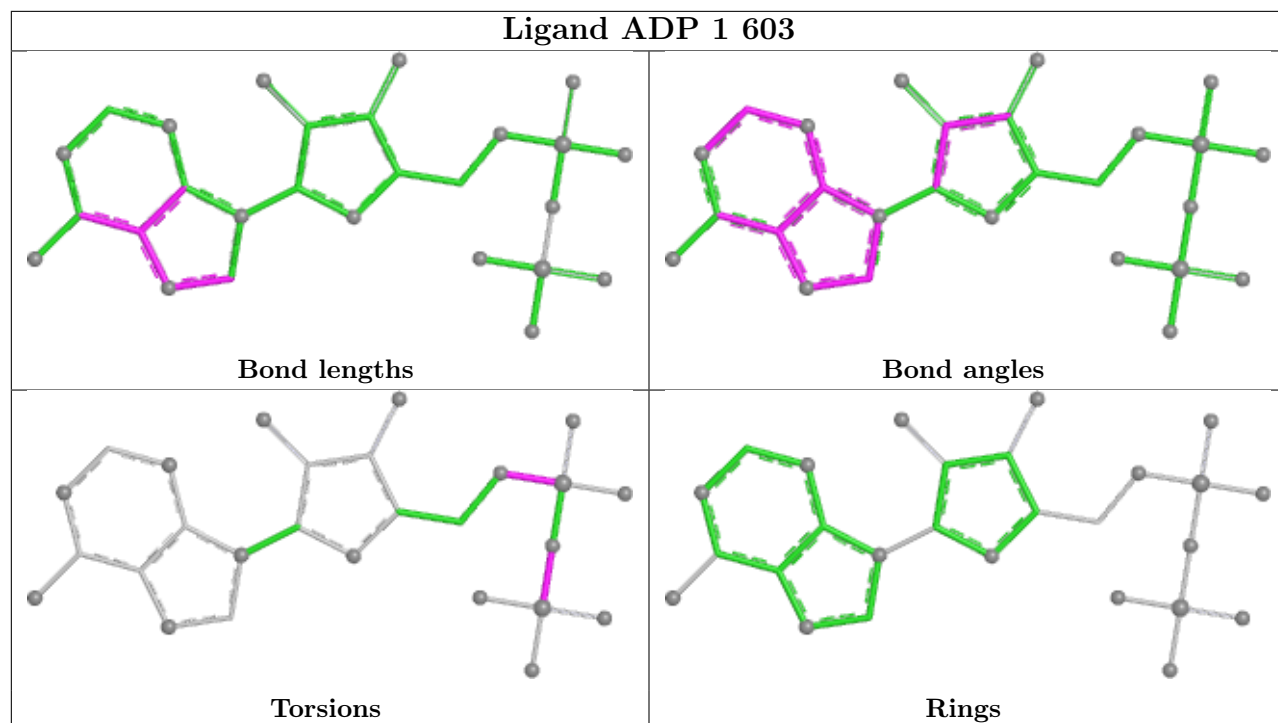
Mol	Chain	Res	Type	Atoms
53	1	603	ADP	C5'-O5'-PA-O1A
53	1	603	ADP	C5'-O5'-PA-O2A
53	1	603	ADP	C5'-O5'-PA-O3A
55	1	605	ATP	O4'-C4'-C5'-O5'
53	1	603	ADP	PA-O3A-PB-O2B
53	1	603	ADP	PA-O3A-PB-O3B
55	1	605	ATP	C3'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
53	1	603	ADP	2	0
55	1	605	ATP	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
39	C	1
8	s	1
11	n	1
20	2	1
19	T	1
40	E	1
15	f	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	149:ASN	C	320:LYS	N	53.70
1	s	12:ASN	C	18:GLU	N	15.89
1	n	23:VAL	C	33:LEU	N	14.18
1	2	739:C	O3'	747:U	P	13.90
1	T	45:VAL	C	54:GLY	N	10.18
1	E	95:PHE	C	99:GLU	N	10.11
1	f	93:LEU	C	94:LEU	N	1.19

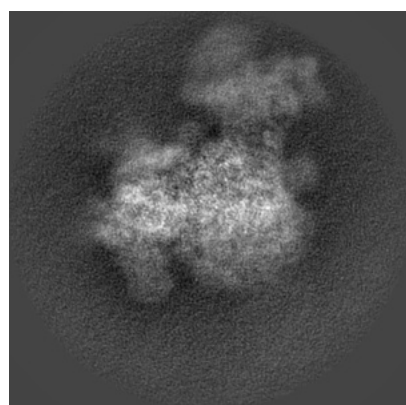
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11458. These allow visual inspection of the internal detail of the map and identification of artifacts.

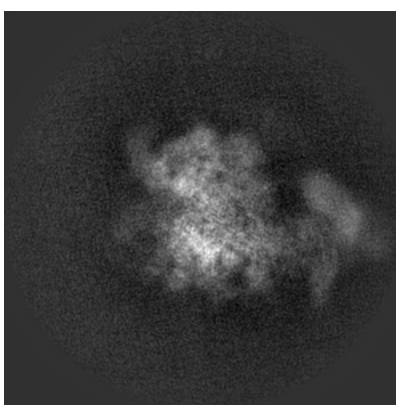
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

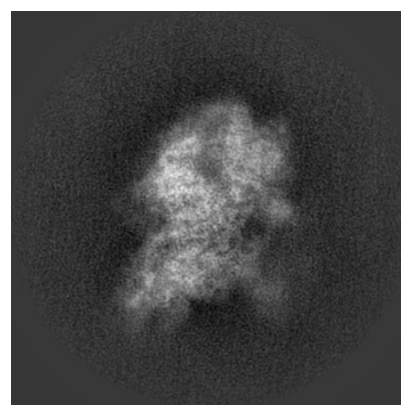
6.1.1 Primary map



X



Y

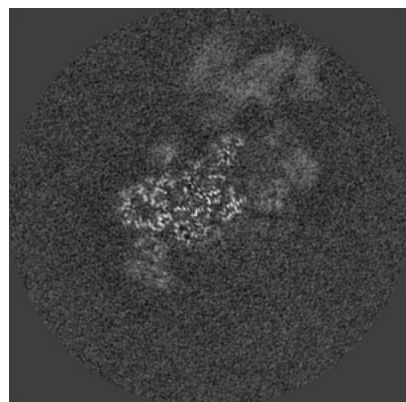


Z

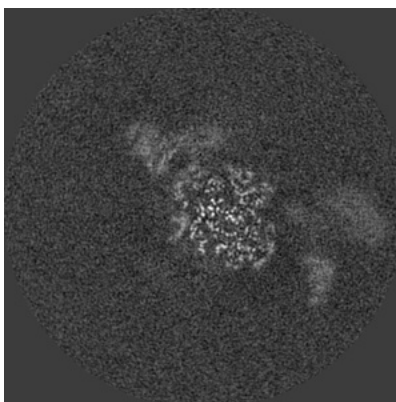
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

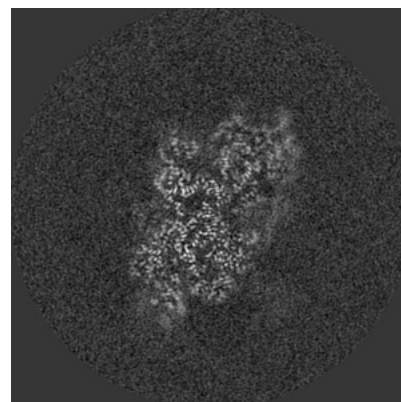
6.2.1 Primary map



X Index: 200



Y Index: 200

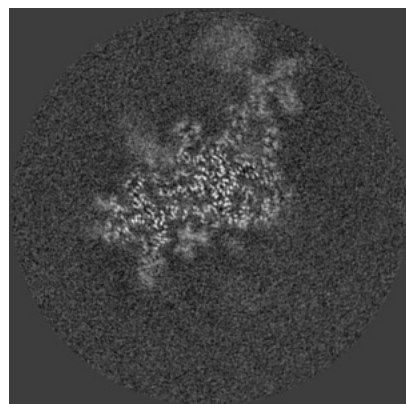


Z Index: 200

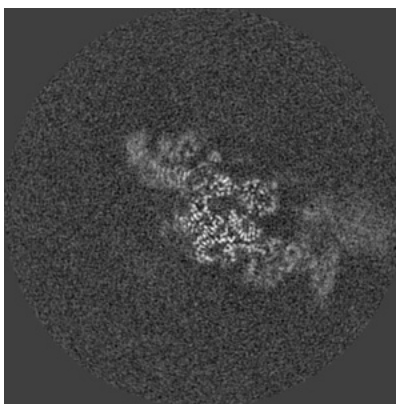
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

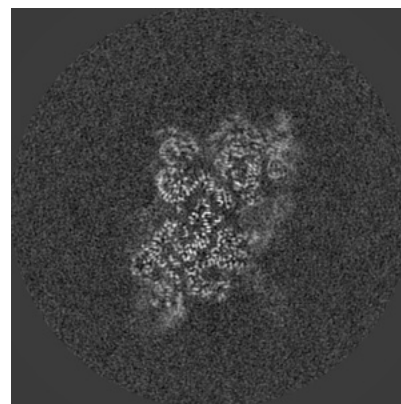
6.3.1 Primary map



X Index: 166



Y Index: 218

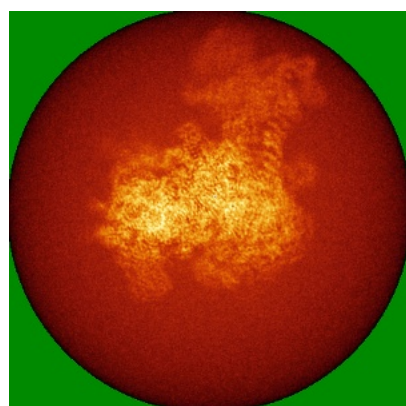


Z Index: 202

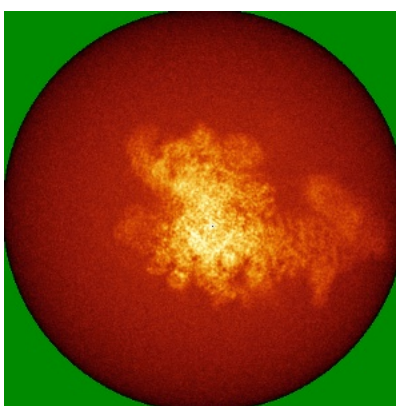
The images above show the largest variance slices of the map in three orthogonal directions.

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

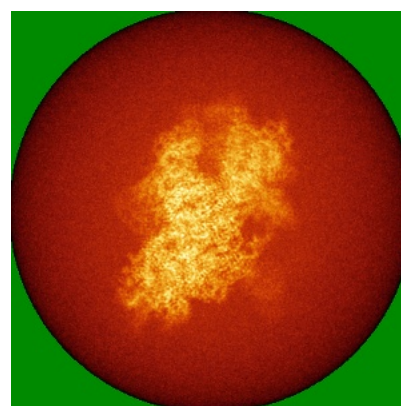
6.4.1 Primary map



X



Y

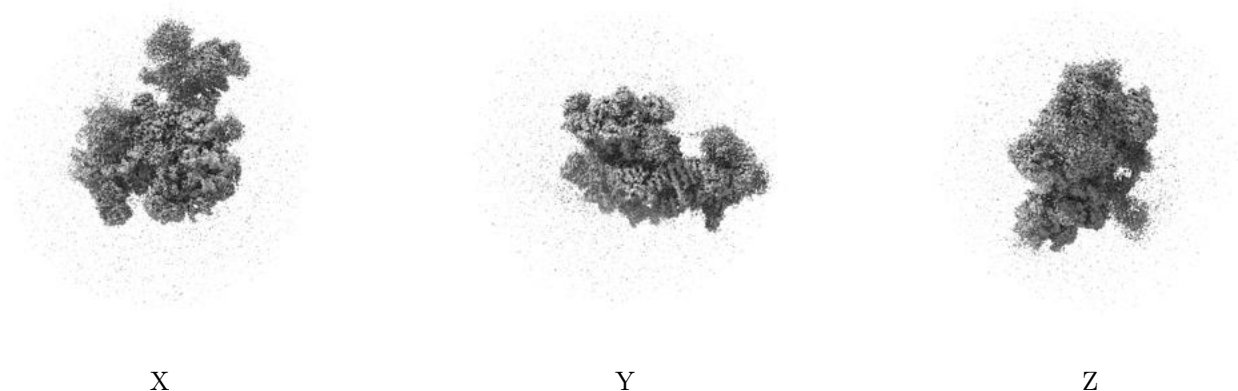


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

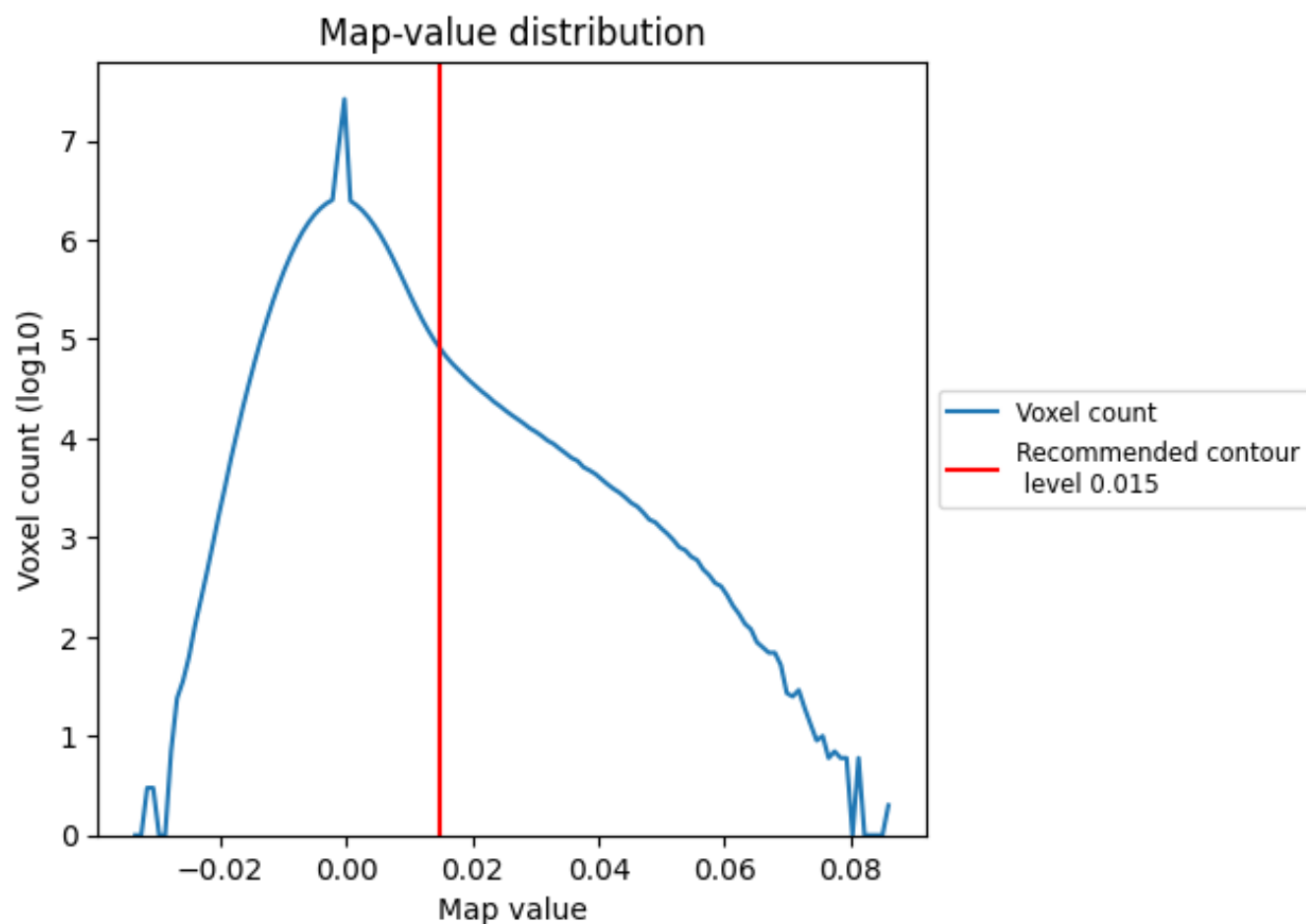
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

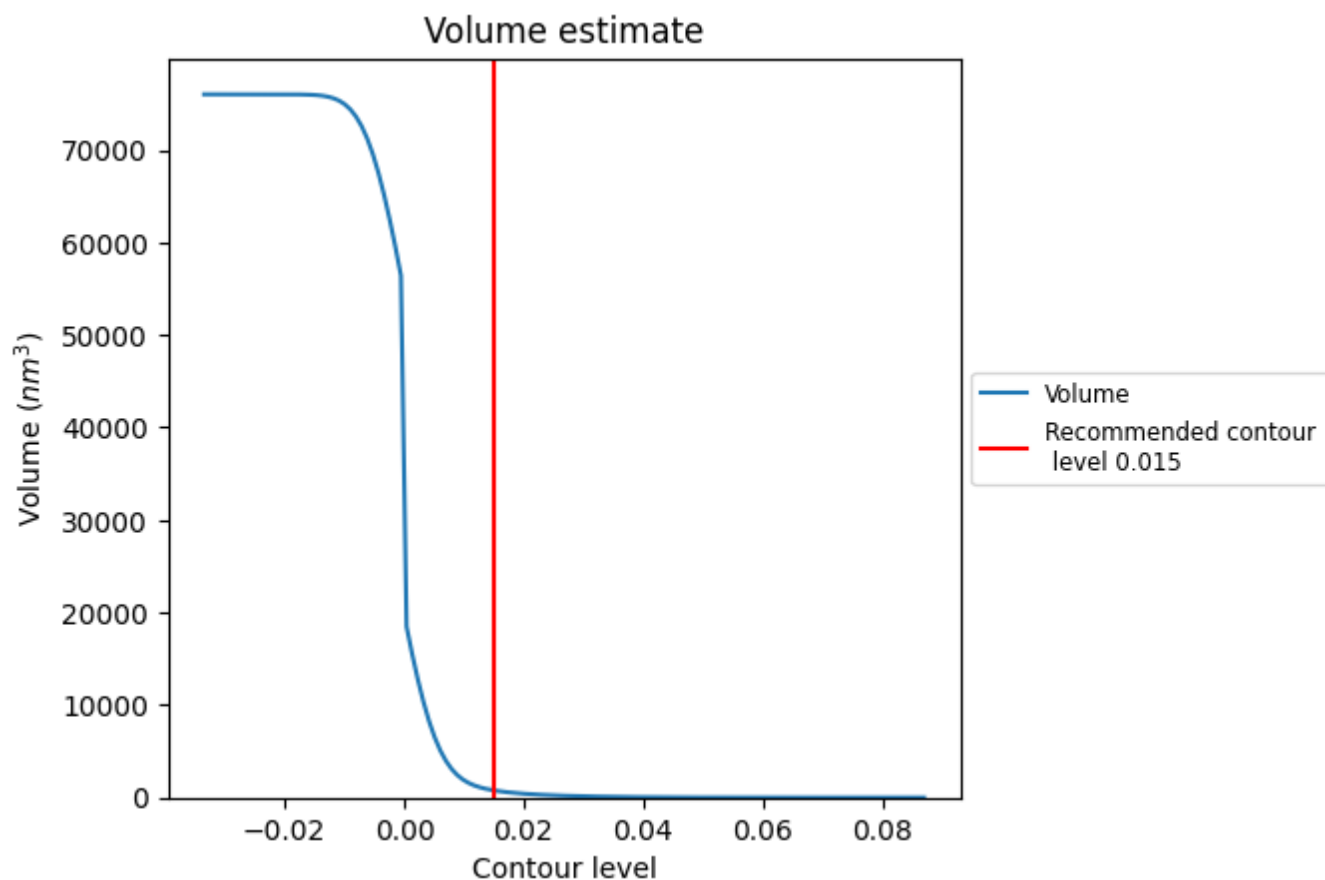
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

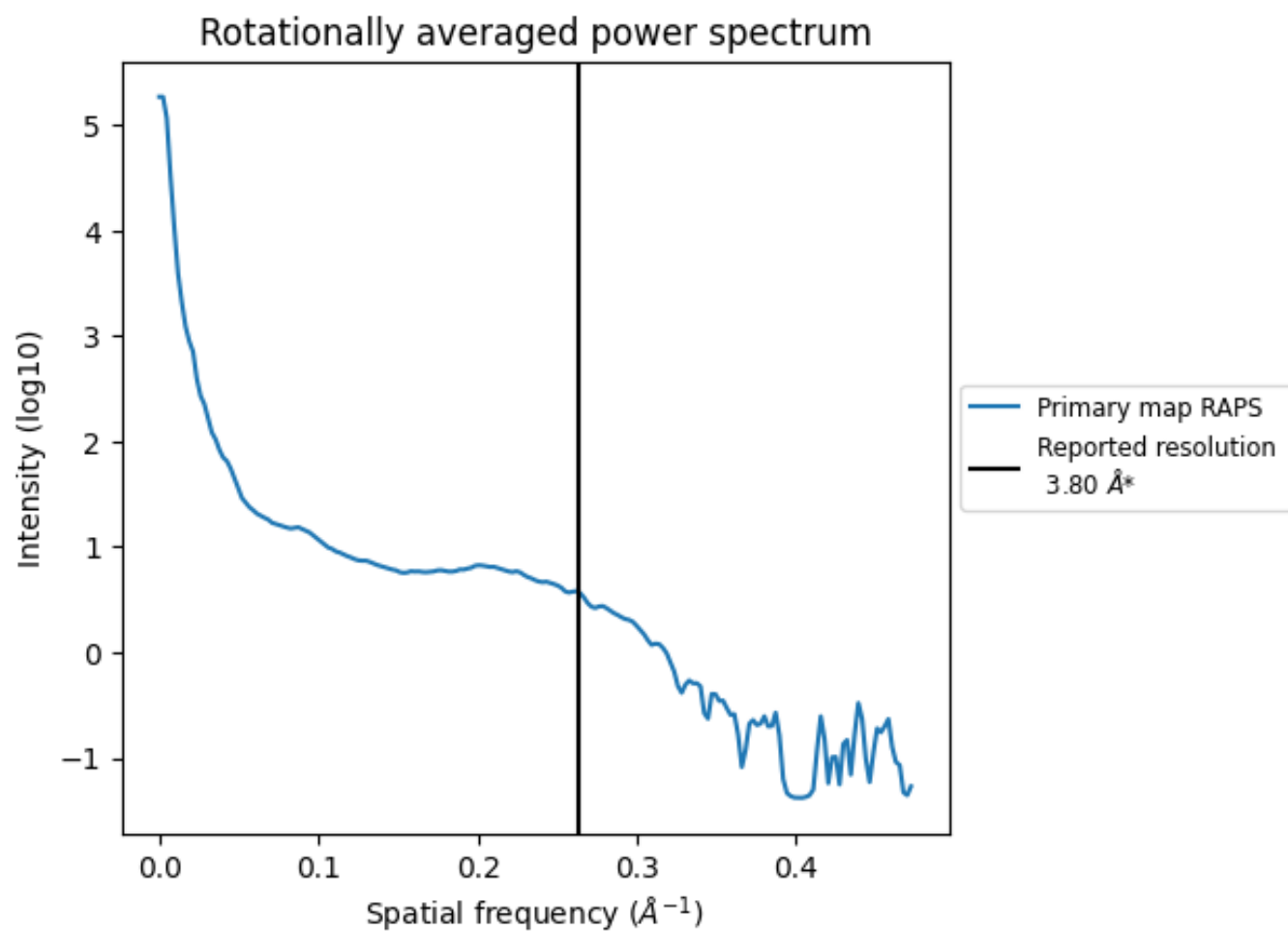
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 779 nm³; this corresponds to an approximate mass of 704 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 ⓘ

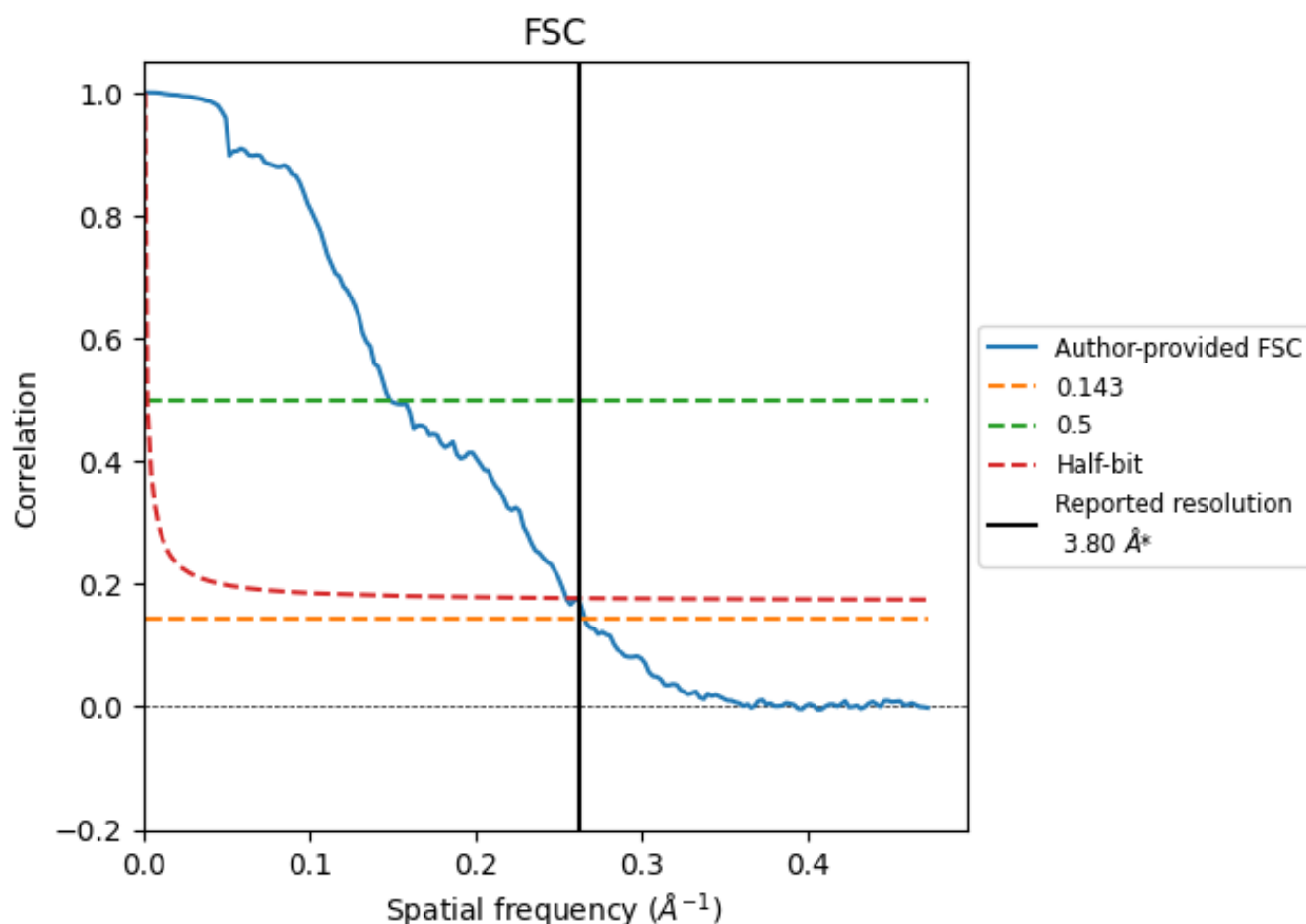


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

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 0.263 Å⁻¹

8.2 Resolution estimates [i](#)

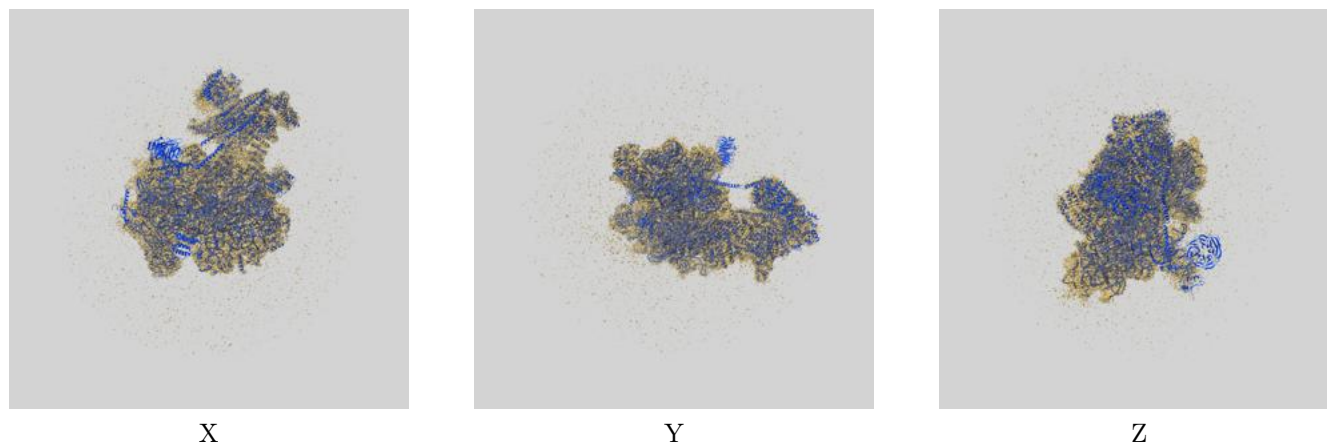
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.76	6.74	3.93
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

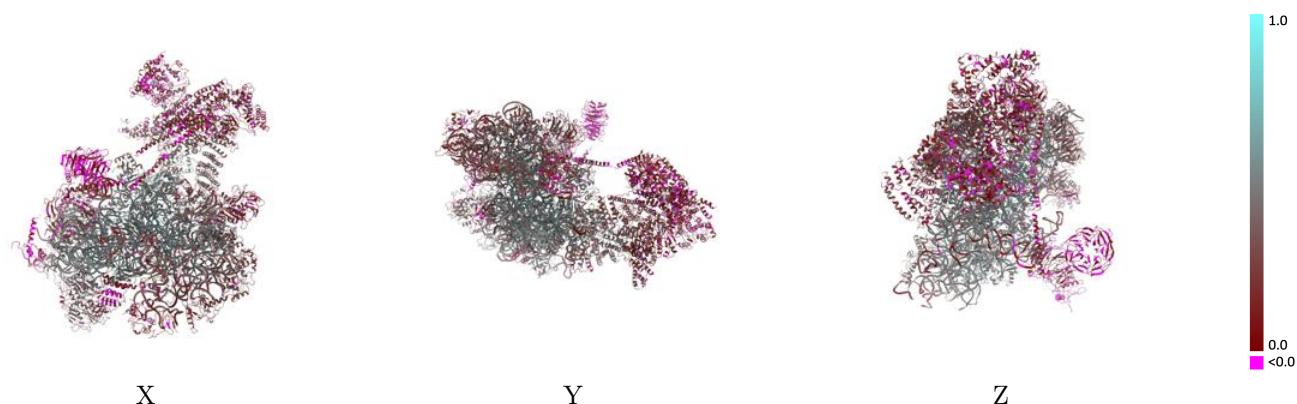
This section contains information regarding the fit between EMDB map EMD-11458 and PDB model 6ZVJ. Per-residue inclusion information can be found in [section 3](#) on [page 16](#).

9.1 Map-model overlay [i](#)



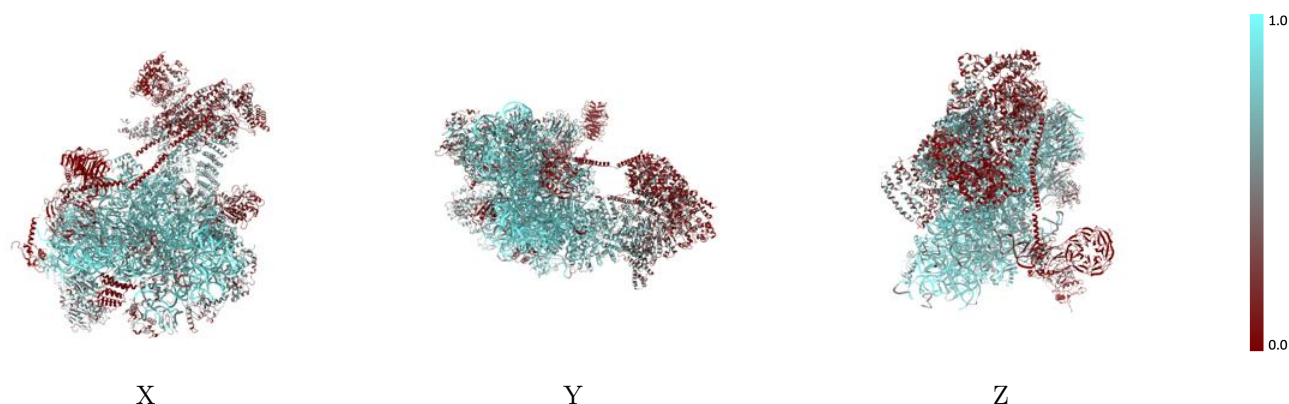
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



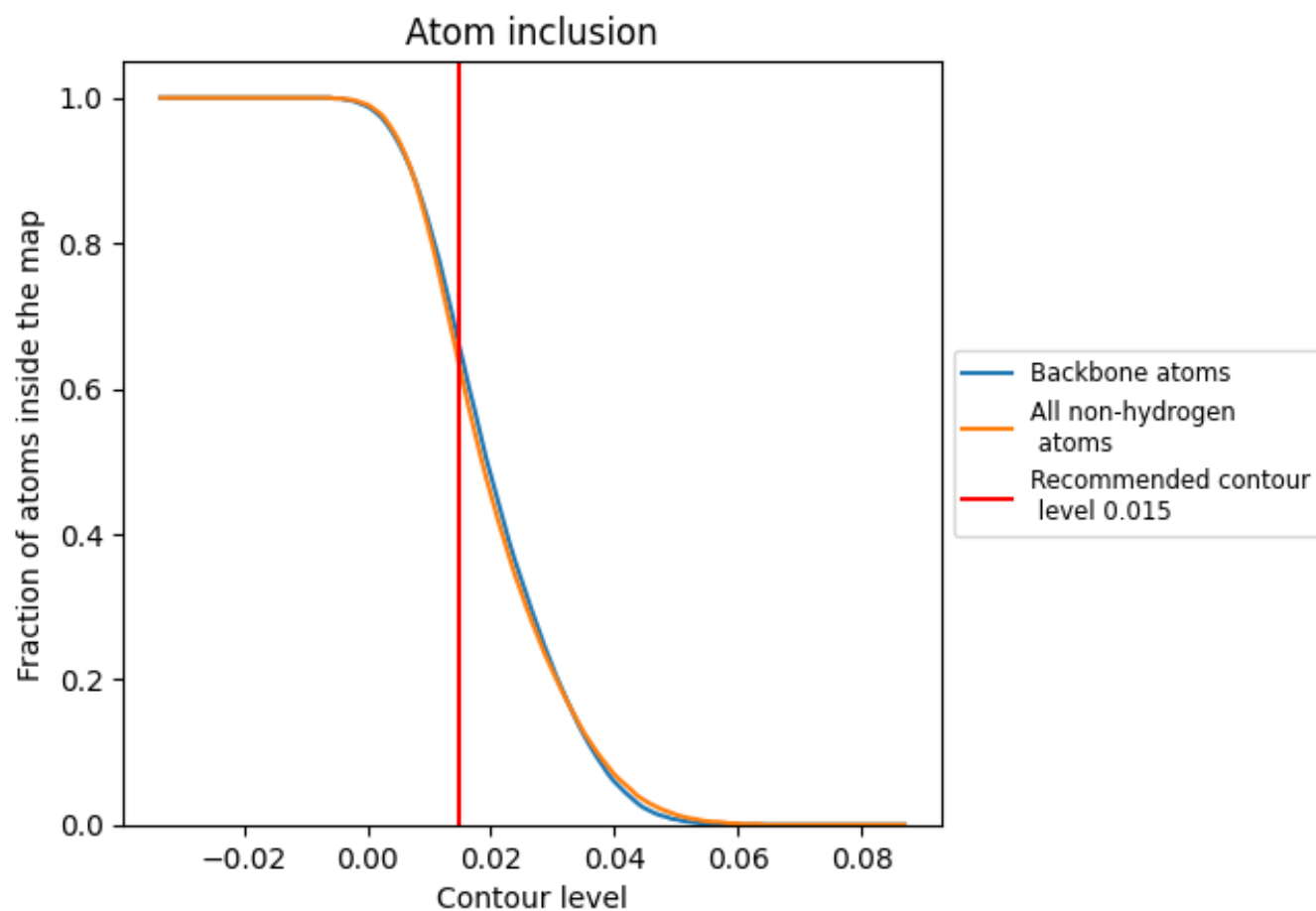
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 63% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6280	 0.3650
1	 0.5520	 0.3700
2	 0.8920	 0.4510
A	 0.4590	 0.2820
B	 0.1580	 0.1870
C	 0.5260	 0.3210
D	 0.2240	 0.2230
E	 0.3830	 0.2210
F	 0.2050	 0.1790
G	 0.0230	 0.0940
H	 0.1980	 0.1700
I	 0.0010	 0.0250
J	 0.0050	 0.1020
K	 0.1220	 0.1540
L	 0.1220	 0.1220
M	 0.2460	 0.1820
N	 0.1230	 0.2020
P	 0.5120	 0.2920
Q	 0.7680	 0.4840
R	 0.7810	 0.4910
S	 0.5020	 0.3380
T	 0.7730	 0.4720
U	 0.4220	 0.2280
V	 0.5930	 0.3130
W	 0.6380	 0.4350
Y	 0.3330	 0.2290
a	 0.7940	 0.4990
b	 0.6250	 0.3870
c	 0.7990	 0.4990
d	 0.8000	 0.5040
e	 0.6180	 0.3680
f	 0.8380	 0.5370
g	 0.6820	 0.4140
h	 0.6050	 0.3840
i	 0.7780	 0.4680



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Chain	Atom inclusion	Q-score
j	 0.7930	 0.5160
k	 0.5290	 0.3190
l	 0.7530	 0.4120
m	 0.8010	 0.4880
n	 0.8240	 0.5230
o	 0.4410	 0.2630
p	 0.7850	 0.4830
q	 0.8290	 0.5100
r	 0.7600	 0.4440
s	 0.7230	 0.4310
t	 0.8090	 0.4720
u	 0.5380	 0.3070
v	 0.3850	 0.2290
w	 0.6980	 0.4320
x	 0.6420	 0.3460
y	 0.7940	 0.4940
z	 0.8030	 0.4900