



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 11:57 AM UTC

PDB ID : 8CH6 / pdb_00008ch6
EMDB ID : EMD-16658
Title : Structure of a late-stage activated spliceosome (BAqr) arrested with a dominant-negative Aquarius mutant (state B complex).
Authors : Cretu, C.; Schmitzova, J.; Pena, V.
Deposited on : 2023-02-07
Resolution : 5.90 Å (reported)
Based on initial models : 5Z57, 6FF7, 6FF4

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

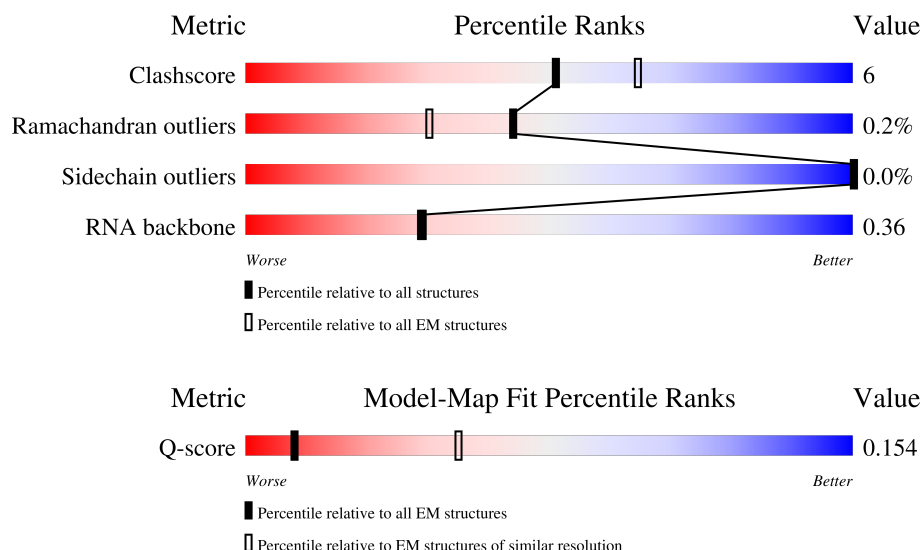
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.90 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	501 (5.40 - 6.40)

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	1	92	
1	i	92	
2	2	86	

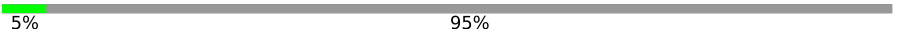
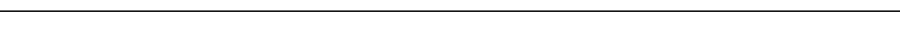
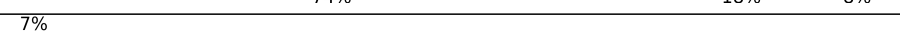
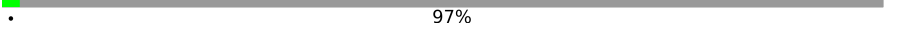
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Mol	Chain	Length	Quality of chain
2	h	86	
3	3	126	
3	j	126	
4	4	118	
4	l	118	
5	5	119	
5	k	119	
6	8	240	
6	n	240	
7	9	76	
7	m	76	
8	A	1217	
9	B	86	
10	C	1304	
11	D	110	
12	E	895	
13	F	424	
14	G	476	
15	H	793	
16	I	464	
17	J	501	
18	K	504	
18	M	504	
18	R	504	
18	v	504	

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Mol	Chain	Length	Quality of chain
19	L	619	 5% 95%
20	N	1041	 61% 15% 24%
21	O	514	 48% 14% 38%
22	P	802	 11% 35% 6% 59%
23	Q	229	 33% 10% 56%
24	S	225	 36% 60% 11% 29%
25	T	144	 81% 18% .
26	U	420	 55% 15% 30%
27	V	492	 51% 6% 42%
28	W	908	 47% . 49%
29	X	848	 27% . 72%
30	Y	536	 49% 7% 43%
31	Z	343	 26% . 72%
32	a	2335	 78% 15% 7%
33	b	972	 74% 18% 8%
34	c	2136	 7% 80% . 19%
35	d	106	 42% 41% 6% 12%
36	e	117	 45% 34% . 16%
37	f	188	 . 50% 19% . 27%
38	g	319	 11% 10% . 76%
39	o	357	 64% 20% 16%
40	p	166	 89% 7% .
41	q	2752	 . 97%
42	r	255	 . 64% 36%
43	s	225	 6% 72% . 27%

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Mol	Chain	Length	Quality of chain
44	t	285	14%83%
45	u	520	63%7%29%
46	w	301	69%5%26%
47	x	579	61%37%
48	y	1485	13%77%13%11%
49	z	855	19%76%19%

2 Entry composition

There are 53 unique types of molecules in this entry. The entry contains 119058 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	1	79	Total	C	N	O	0	0
			391	233	79	79		
1	i	70	Total	C	N	O	0	0
			346	206	70	70		

- Molecule 2 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	2	74	Total	C	N	O	0	0
			361	213	74	74		
2	h	66	Total	C	N	O	0	0
			322	190	66	66		

- Molecule 3 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	3	76	Total	C	N	O	0	0
			373	221	76	76		
3	j	68	Total	C	N	O	0	0
			335	199	68	68		

- Molecule 4 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	4	85	Total	C	N	O	0	0
			422	252	85	85		
4	l	68	Total	C	N	O	0	0
			337	201	68	68		

- Molecule 5 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	5	82	Total	C	N	O	0	0
			406	242	82	82		
5	k	78	Total	C	N	O	0	0
			388	232	78	78		

- Molecule 6 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	8	86	Total	C	N	O	0	0
			422	250	86	86		
6	n	64	Total	C	N	O	0	0
			315	187	64	64		

- Molecule 7 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	9	68	Total	C	N	O	0	0
			334	198	68	68		
7	m	63	Total	C	N	O	0	0
			309	183	63	63		

- Molecule 8 is a protein called Splicing factor 3B subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	A	1158	Total	C	N	O	0	0
			5714	3398	1158	1158		

- Molecule 9 is a protein called Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	B	70	Total	C	N	O	0	0
			350	210	70	70		

- Molecule 10 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C	815	Total	C	N	O	S	0	0
			5115	3242	928	930	15		

- Molecule 11 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D	89	Total	C	N	O	S	0	0
			649	399	117	120	13		

- Molecule 12 is a protein called Splicing factor 3B subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	198	Total	C	N	O	S	0	0
			1350	855	249	241	5		

- Molecule 13 is a protein called Splicing factor 3B subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	F	78	Total	C	N	O	0	0
			383	227	78	78		

- Molecule 14 is a protein called G-patch domain and KOW motifs-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	G	67	Total	C	N	O	0	0
			364	228	68	68		

- Molecule 15 is a protein called Splicing factor 3A subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	H	106	Total	C	N	O	0	0
			530	318	106	106		

- Molecule 16 is a protein called Splicing factor 3A subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	185	Total	C	N	O	S	0	0
			1034	620	215	197	2		

- Molecule 17 is a protein called Splicing factor 3A subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	J	410	Total	C	N	O	S	0	0
			2187	1326	431	426	4		

- Molecule 18 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	K	118	Total	C	N	O	S	0	0
			938	586	167	181	4		
18	M	125	Total	C	N	O	S	0	0
			988	618	176	190	4		
18	R	118	Total	C	N	O	S	0	0
			938	586	167	181	4		
18	v	125	Total	C	N	O	S	0	0
			988	618	176	190	4		

- Molecule 19 is a protein called BUD13 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	28	Total	C	N	O	S	0	0
			177	111	32	32	2		

- Molecule 20 is a protein called Putative pre-mRNA-splicing factor ATP-dependent RNA helicase DHX16.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	791	Total	C	N	O	S	0	0
			6147	3893	1089	1137	28		

- Molecule 21 is a protein called Pleiotropic regulator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	O	320	Total	C	N	O	S	0	0
			2517	1592	457	460	8		

- Molecule 22 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	P	330	Total	C	N	O	S	0	0
			2432	1522	446	454	10		

- Molecule 23 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Q	100	Total	C	N	O	S	0	0
			823	509	161	151	2		

- Molecule 24 is a protein called Pre-mRNA-splicing factor SPF27.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	S	159	Total	C	N	O	S	0	0
			1323	820	246	248	9		

- Molecule 25 is a protein called Protein BUD31 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	T	142	Total	C	N	O	S	0	0
			1176	741	216	208	11		

- Molecule 26 is a protein called Pre-mRNA-splicing factor RBM22.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	U	295	Total	C	N	O	S	0	0
			2080	1290	380	392	18		

- Molecule 27 is a protein called Peptidyl-prolyl cis-trans isomerase-like 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	V	285	Total	C	N	O	S	0	0
			1996	1252	338	396	10		

- Molecule 28 is a protein called Pre-mRNA-splicing factor CWC22 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	W	459	Total	C	N	O	S	0	0
			2921	1817	533	559	12		

- Molecule 29 is a protein called Crooked neck-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	X	241	Total	C	N	O	S	0	0
			1587	1017	298	270	2		

- Molecule 30 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Y	306	Total	C	N	O	S	0	0
			2250	1412	411	417	10		

- Molecule 31 is a protein called RING finger protein 113A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Z	95	Total	C	N	O	S	0	0
			607	378	109	117	3		

- Molecule 32 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	a	2183	Total	C	N	O	S	0	0
			16415	10472	2956	2922	65		

- Molecule 33 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	b	898	Total	C	N	O	S	0	0
			7046	4513	1172	1327	34		

- Molecule 34 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	c	1722	Total	C	N	O		0	0
			8530	5086	1722	1722			

- Molecule 35 is a RNA chain called RNU6-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	d	93	Total	C	N	O	P	0	0
			1989	889	364	643	93		

- Molecule 36 is a RNA chain called RNU5A-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	e	98	Total	C	N	O	P	0	0
			2070	926	347	699	98		

- Molecule 37 is a RNA chain called RNU2-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	f	137	Total	C	N	O	P	0	0
			2906	1298	501	970	137		

- Molecule 38 is a RNA chain called MINX-M3.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	g	76	Total	C	N	O	P	0	0
			1559	697	250	536	76		

- Molecule 39 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	o	299	Total	C	N	O	S	0	0
			2338	1470	410	445	13		

- Molecule 40 is a protein called Peptidyl-prolyl cis-trans isomerase-like 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	p	159	Total	C	N	O	0	0
			776	457	159	160		

- Molecule 41 is a protein called Serine/arginine repetitive matrix protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	q	74	Total	C	N	O	S	0	0
			461	285	89	85	2		

- Molecule 42 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	r	162	Total	C	N	O	0	0
			804	480	162	162		

- Molecule 43 is a protein called U2 small nuclear ribonucleoprotein B''.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	s	165	Total	C	N	O	0	0
			813	483	165	165		

- Molecule 44 is a protein called Pre-mRNA-splicing factor ISY1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	t	48	Total	C	N	O	S	0	0
			407	261	64	81	1		

- Molecule 45 is a protein called RING-type E3 ubiquitin-protein ligase PPIL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	u	367	Total	C	N	O	S	0	0
			1963	1181	382	399	1		

- Molecule 46 is a protein called Peptidyl-prolyl cis-trans isomerase E.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	w	224	Total	C	N	O		0	0
			1093	645	224	224			

- Molecule 47 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	x	362	Total	C	N	O		0	0
			1787	1063	362	362			

- Molecule 48 is a protein called Intron-binding protein aquarius.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	y	1327	Total	C	N	O	S	0	0
			10878	6988	1871	1965	54		

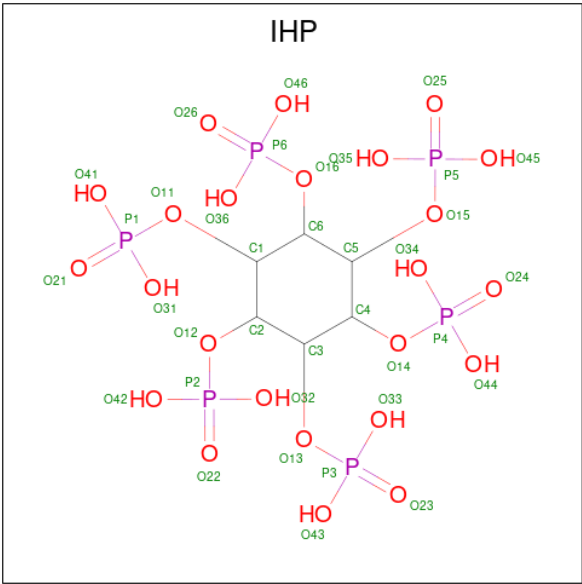
- Molecule 49 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	z	692	Total	C	N	O	S	0	0
			4511	2853	837	807	14		

- Molecule 50 is ZINC ION (CCD ID: ZN) (formula: Zn).

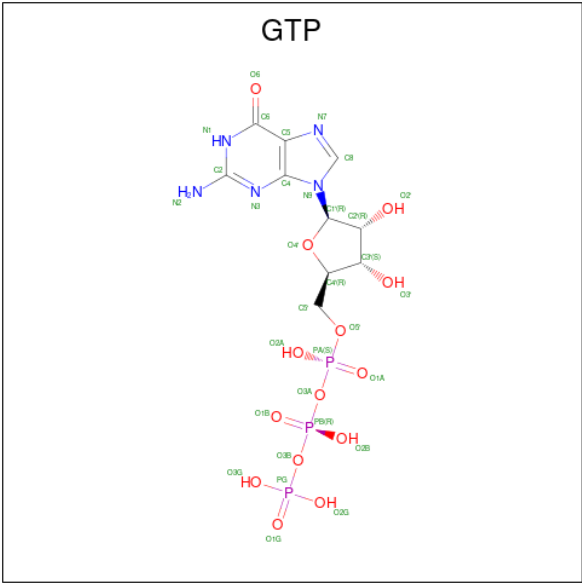
Mol	Chain	Residues	Atoms		AltConf
50	D	3	Total	Zn	0
			3	3	
50	I	1	Total	Zn	0
			1	1	
50	J	1	Total	Zn	0
			1	1	
50	T	3	Total	Zn	0
			3	3	
50	U	3	Total	Zn	0
			3	3	
50	Z	1	Total	Zn	0
			1	1	

- Molecule 51 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
51	a	1	Total	C	O	P	0
			36	6	24	6	

- Molecule 52 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
52	b	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 53 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

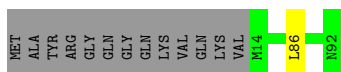
Mol	Chain	Residues	Atoms		AltConf
53	b	1	Total 1	Mg 1	0
53	d	6	Total 6	Mg 6	0

3 Residue-property plots [i](#)

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: Small nuclear ribonucleoprotein E

Chain 1:  85% 14%



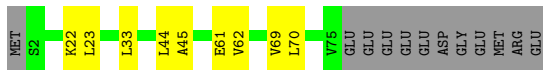
- Molecule 1: Small nuclear ribonucleoprotein E

Chain i:  72% 24%



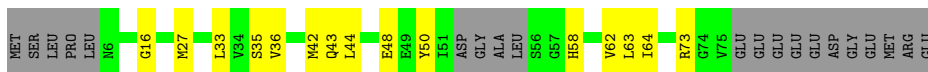
- Molecule 2: Small nuclear ribonucleoprotein F

Chain 2:  76% 10% 14%



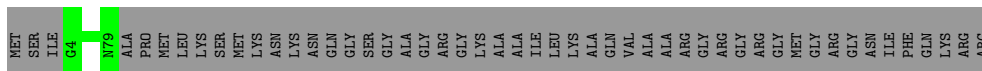
- Molecule 2: Small nuclear ribonucleoprotein F

Chain h:  59% 17% 23%

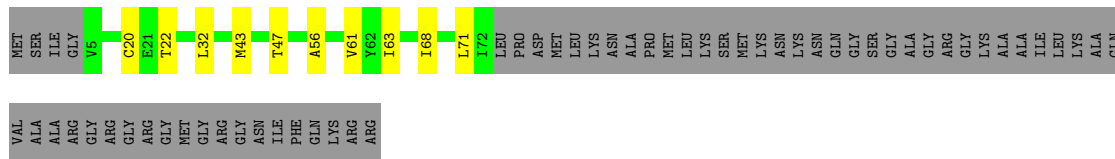


- Molecule 3: Small nuclear ribonucleoprotein Sm D3

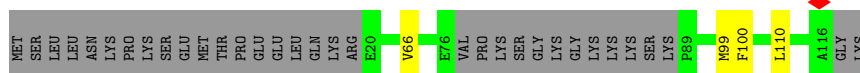
Chain 3:  60% 40%



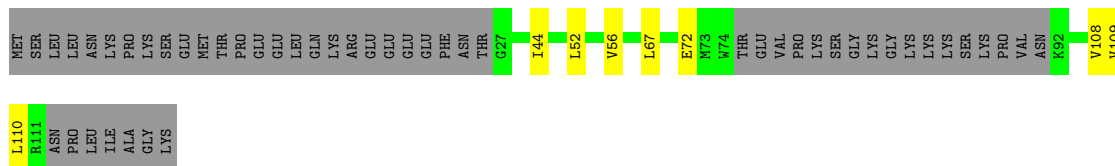
- Molecule 3: Small nuclear ribonucleoprotein Sm D3



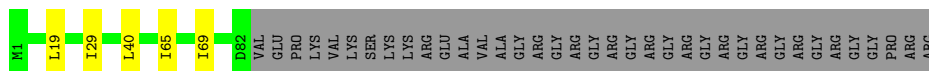
- Molecule 4: Small nuclear ribonucleoprotein Sm D2



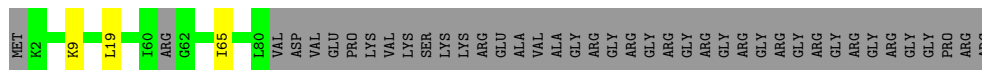
- Molecule 4: Small nuclear ribonucleoprotein Sm D2



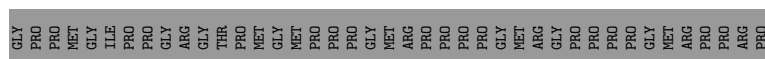
- Molecule 5: Small nuclear ribonucleoprotein Sm D1



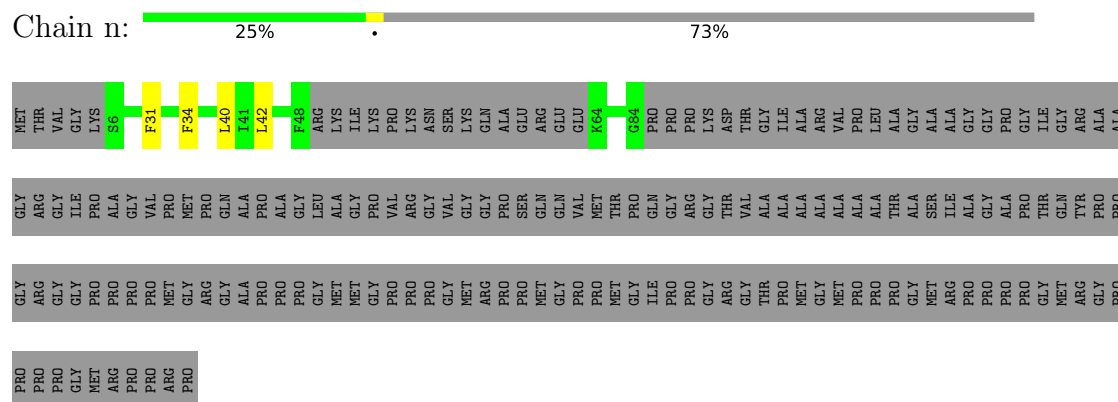
- Molecule 5: Small nuclear ribonucleoprotein Sm D1



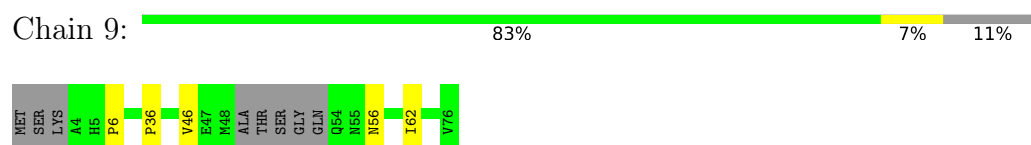
- Molecule 6: Small nuclear ribonucleoprotein-associated proteins B and B'



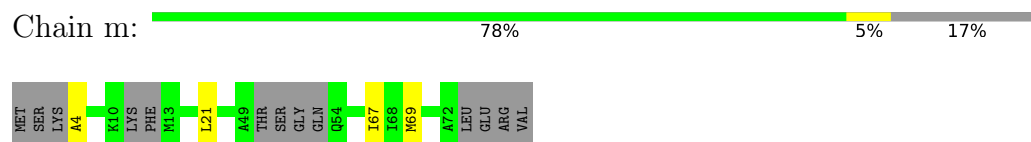
- Molecule 6: Small nuclear ribonucleoprotein-associated proteins B and B'



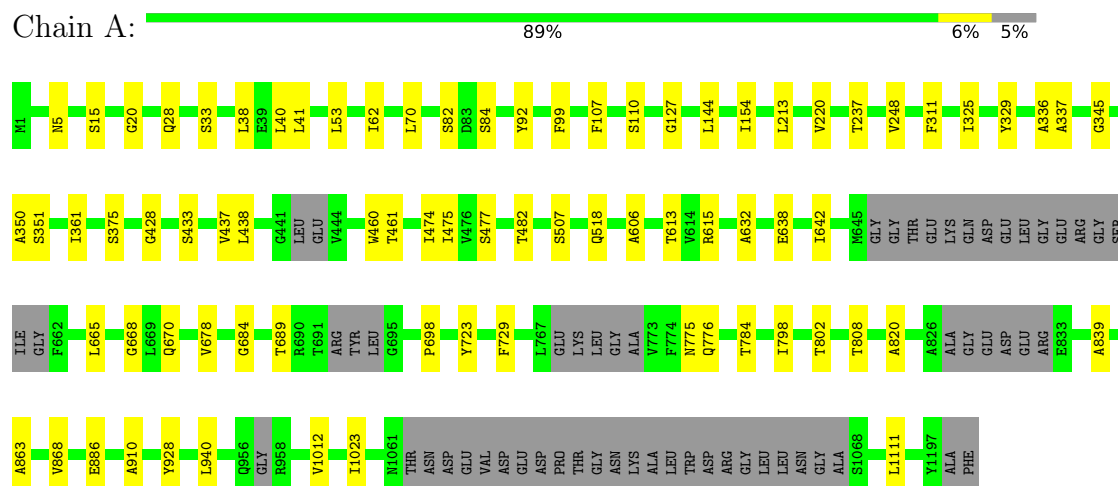
- Molecule 7: Small nuclear ribonucleoprotein G



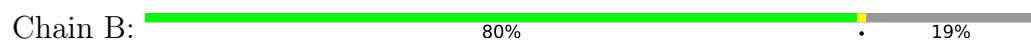
- Molecule 7: Small nuclear ribonucleoprotein G



- Molecule 8: Splicing factor 3B subunit 3



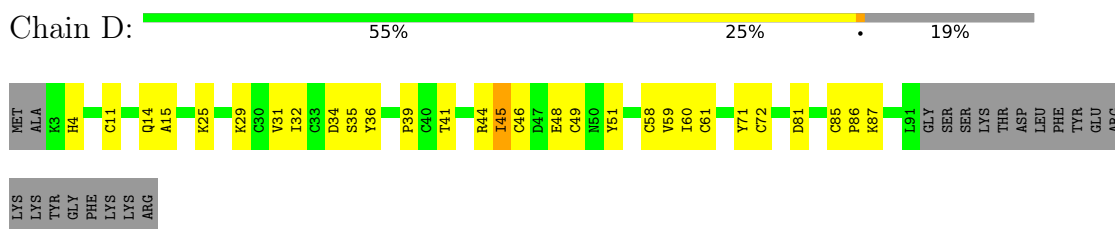
- Molecule 9: Splicing factor 3B subunit 5



- Molecule 10: Splicing factor 3B subunit 1



- Molecule 11: PHD finger-like domain-containing protein 5A



- Molecule 12: Splicing factor 3B subunit 2



- Molecule 13: Splicing factor 3B subunit 4

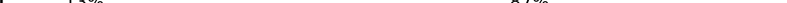
[illegible]

- Molecule 14: G-patch domain and KOW motifs-containing protein.

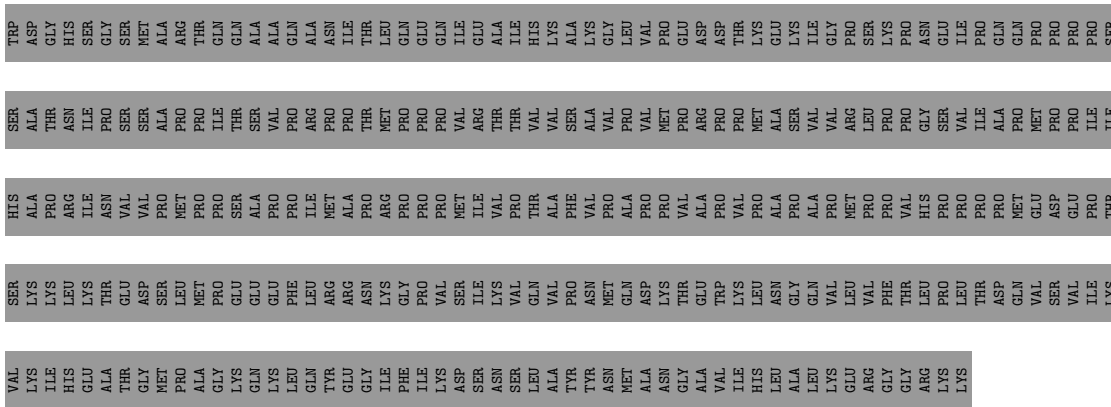
Chain G: 14% 86%

[illegible]

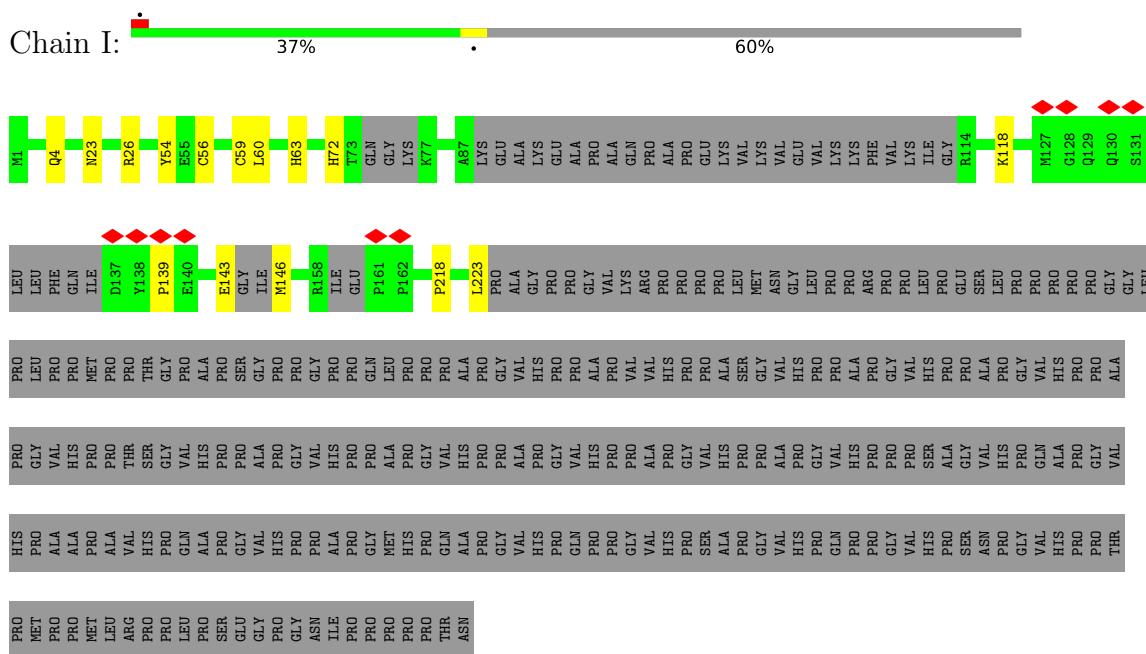
- Molecule 15: Splicing factor 3A subunit 1

Chain H:  13% 87%

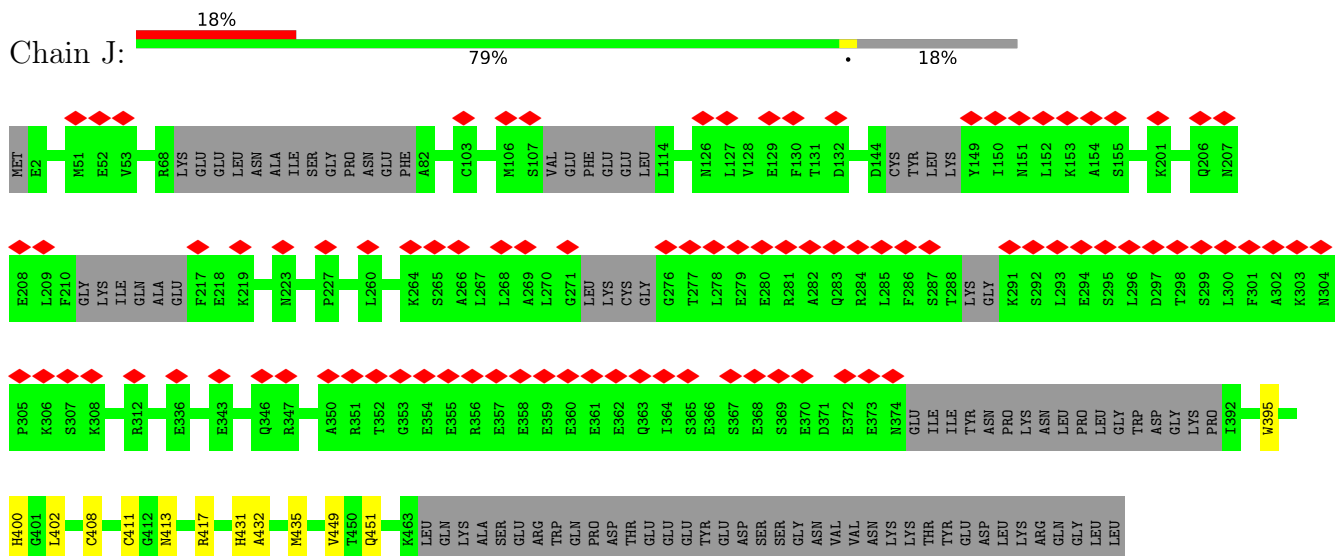
ARG	ASP	ARG	ASP	PRO	THR	GLU	LEU	THR	ALA	GLN	GLN	ARG	ALA	THR	MET
ASP	ARG	ASP	ASP	PRO	THR	GLU	PHE	S227	GLN	GLN	THR	ARG	ARG	ALA	PRO
ILE	ILE	GLN	GLU	VAL	VAL	VAL	K230	K230	THR	GLN	GLN	GLY	GLY	GLY	ALA
VAL	ILE	VAL	GLU	VAL	VAL	GLU	GLU	K231	GLN	GLN	GLN	PHE	GLU	VAL	GLN
LYS	VAL	VAL	SER	VAL	VAL	SER	ALA	GLU	LEU	LEU	LEU	GLU	GLU	ALA	GLN
GLN	GLN	ARG	ASP	ASP	GLU	GLU	GLU	GLU	PRO	PRO	PRO	ALA	VAL	VAL	ALA
SER	LYS	ARG	GLU	GLU	GLU	GLU	GLU	GLU	GLN	GLN	GLN	ARG	ARG	PRO	PRO
ASP	ASP	ASP	GLU	GLU	GLU	GLU	ASP	R237	VAL	VAL	VAL	ARG	ILE	PRO	PRO
ASP	GLU	ASP	ASP	ASP	ASP	ASP	GLU	K249	GLN	GLN	GLN	GLN	GLN	PRO	PRO
VAL	VAL	PRO	LYS	LYS	LYS	GLN	GLU	ALA	ALA	VAL	VAL	GLU	GLU	PRO	PRO
THR	THR	ALA	ALA	ALA	LYS	GLU	PHE	GLU	ILE	ILE	ILE	ASN	ASN	GLN	GLN
PRO	PRO	SER	LYS	LYS	GLU	ALA	GLU	GLU	GLN	GLN	GLU	ASN	ASN	GLU	GLU
GLY	GLY	LYS	GLU	PRO	PRO	GLU	GLU	GLU	PRO	PRO	THR	PRO	THR	THR	GLU
LEU	LEU	PRO	GLU	PRO	PRO	PRO	GLU	ARG	VAL	VAL	VAL	ASN	GLN	GLN	GLN
PRO	PRO	PRO	PRO	PRO	PRO	SER	GLU	R257	PHE	PRO	PRO	PHE	PHE	THR	PRO
SER	SER	ALA	SER	ALA	ALA	SER	GLU	GLU	LEU	PRO	PRO	LEU	LEU	GLU	GLU
SER	SER	ALA	GLN	ALA	ALA	LEU	GLU	V285	ASN	GLU	GLU	ASN	ASN	GLU	GLU
LEU	LEU	ALA	ASP	PRO	PRO	ASP	PHE	GLU	PRO	PRO	PRO	PRO	ALA	GLU	GLU
LYS	LYS	ASP	GLN	ASP	ASP	GLN	GLU	GLU	ALA	ALA	ALA	ASP	ASP	GLU	GLU
GLN	GLN	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLN	GLN	PHE	GLU	GLU	GLU	GLU
LEU	LEU	ALA	TYR	TYR	ALA	GLN	PRO	ALA	TYR	TYR	TYR	PRO	PRO	LYS	LYS
GLU	GLU	LEU	LEU	LEU	VAL	VAL	GLU	GLU	ASN	GLN	GLU	THR	THR	GLU	GLU
ARG	ARG	VAL	SER	SER	VAL	GLN	GLU	GLU	ASN	ASN	PHE	THR	THR	LYS	LYS
ARG	ARG	VAL	SER	VAL	VAL	GLN	GLU	GLU	ALA	ALA	PHE	ALA	ALA	ASP	ASP
THR	THR	PRO	PRO	PRO	PRO	GLN	GLY	GLY	ILE	ILE	ILE	TYR	TYR	SER	SER
ASP	ASP	ILE	ILE	ILE	ILE	MET	ASN	ASN	ALA	ALA	ALA	TYR	TYR	ALA	ALA
PHE	PHE	GLY	GLY	GLY	GLY	ASP	PHE	PHE	ASP	ASP	ASP	ARG	ARG	SER	SER
GLY	GLY	GLY	GLY	GLY	GLY	GLY	PRO	PRO	LYS	LYS	LYS	HIS	HIS	LYS	LYS
VAL	VAL	VAL	SER	VAL	VAL	SER	PRO	PRO	VAL	VAL	VAL	VAL	VAL	VAL	VAL
GLU	GLU	GLU	ASP	PRO	PRO	ASP	THR	THR	ILE	ILE	ILE	GLU	GLU	PRO	PRO
THR	THR	ALA	SER	ALA	ALA	GLU	GLU	PRO	S160	S160	S160	PHE	PHE	VAL	VAL
ILE	ILE	ILE	LYS	LYS	LYS	GLU	GLU	GLU	R176	R176	R176	LYS	LYS	ILE	ILE
GLY	GLY	GLY	MET	MET	GLY	GLY	GLY	GLY	ASN	ASN	ASN	GLY	GLY	TYR	TYR
LYS	LYS	GLN	GLN	GLN	GLY	GLN	LEU	LEU	GLY	GLY	GLY	ALA	ALA	PRO	PRO
LYS	LYS	GLU	GLU	GLU	LYS	LYS	ALA	ALA	R179	R179	R179	ALA	ALA	PRO	PRO
ILE	ILE	HIS	VAL	VAL	VAL	VAL	ARG	ARG	Q180	Q180	Q180	GLN	GLN	PRO	PRO
MET	MET	ARG	PRO	PRO	PRO	PRO	ILE	ILE	K188	K188	K188	GLU	GLU	VAL	VAL
GLY	GLY	ARG	PRO	PRO	PRO	PRO	LEU	LEU	E189	E189	E189	PRO	PRO	GLU	GLU



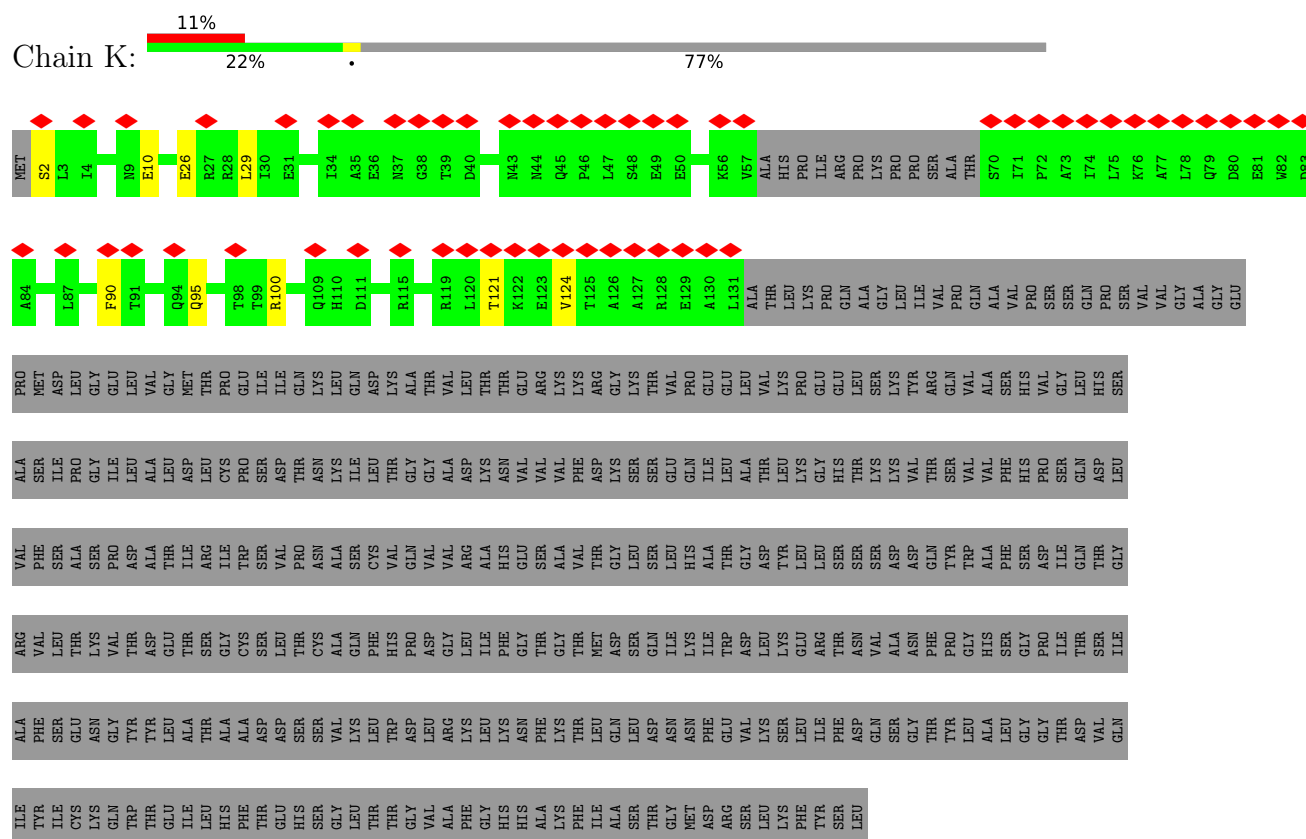
- Molecule 16: Splicing factor 3A subunit 2



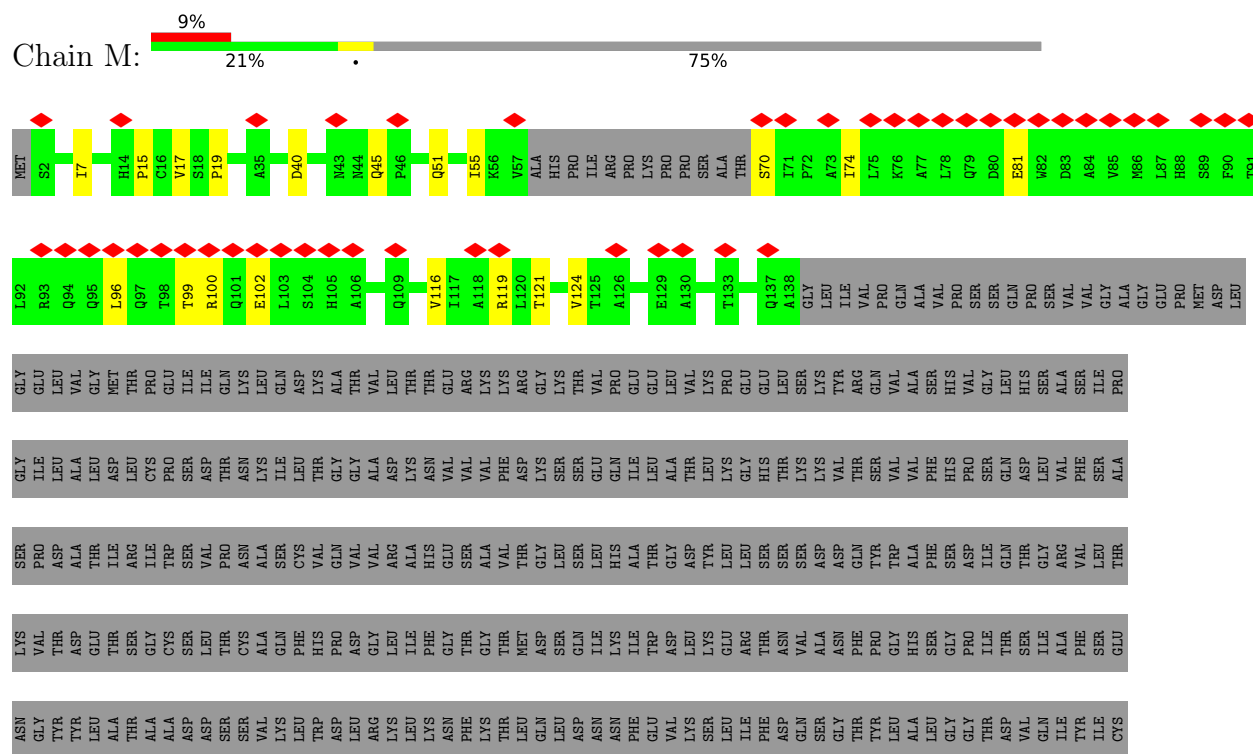
- Molecule 17: Splicing factor 3A subunit 3



• Molecule 18: Pre-mRNA-processing factor 19

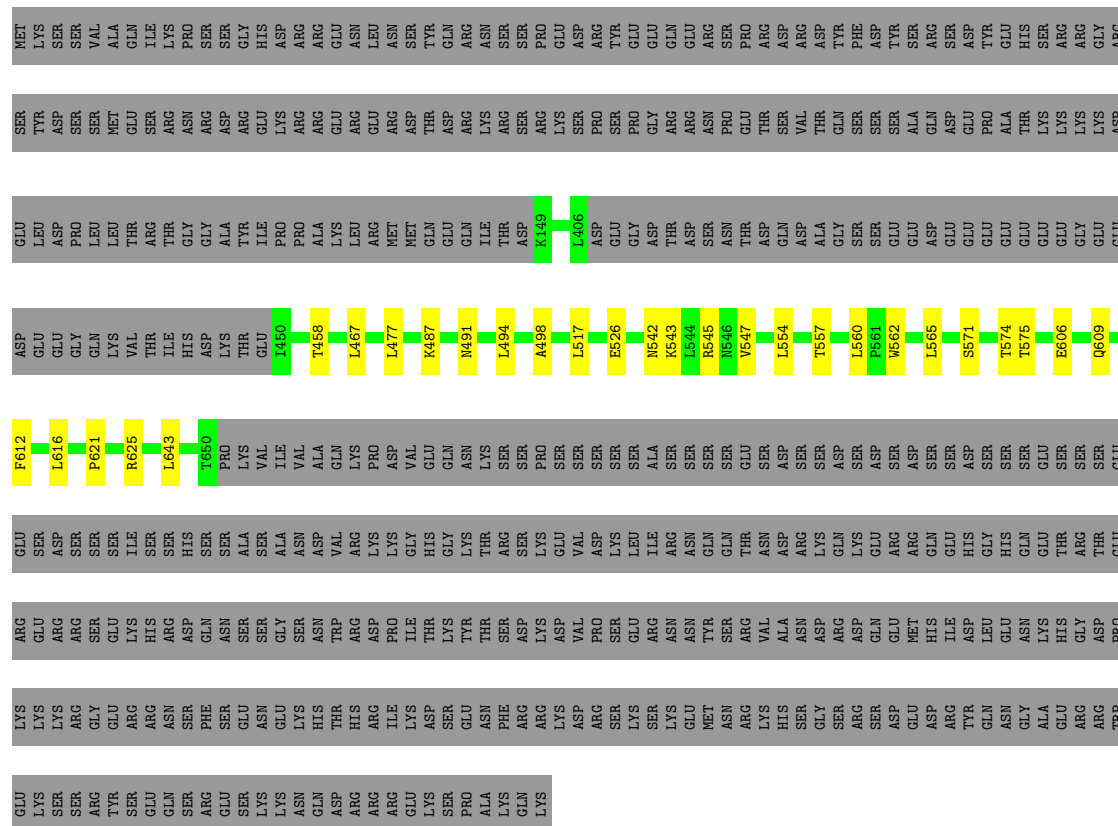


• Molecule 18: Pre-mRNA-processing factor 19

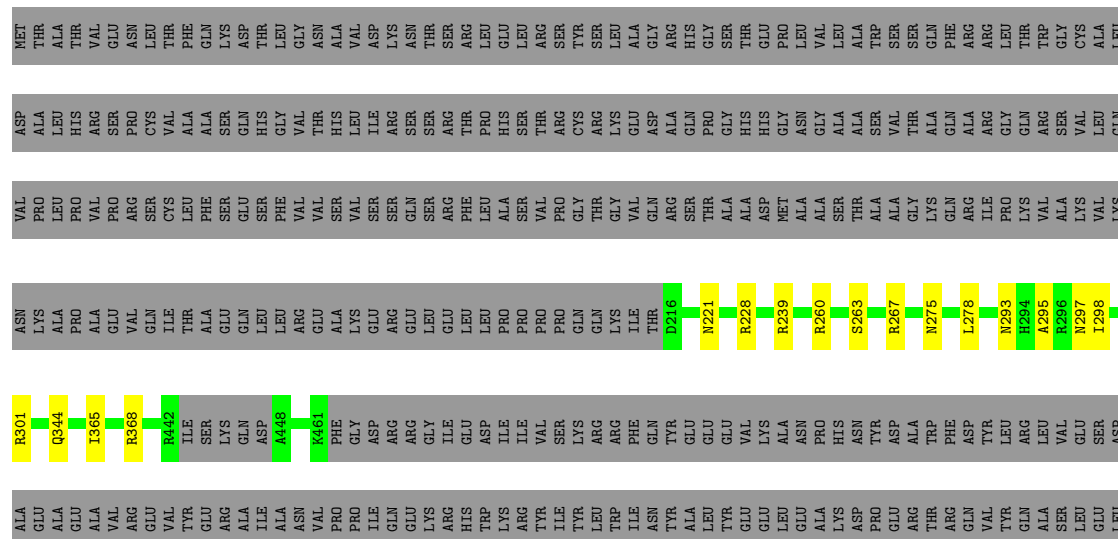




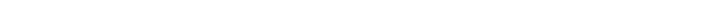
Chain W: 47% 0% 49%

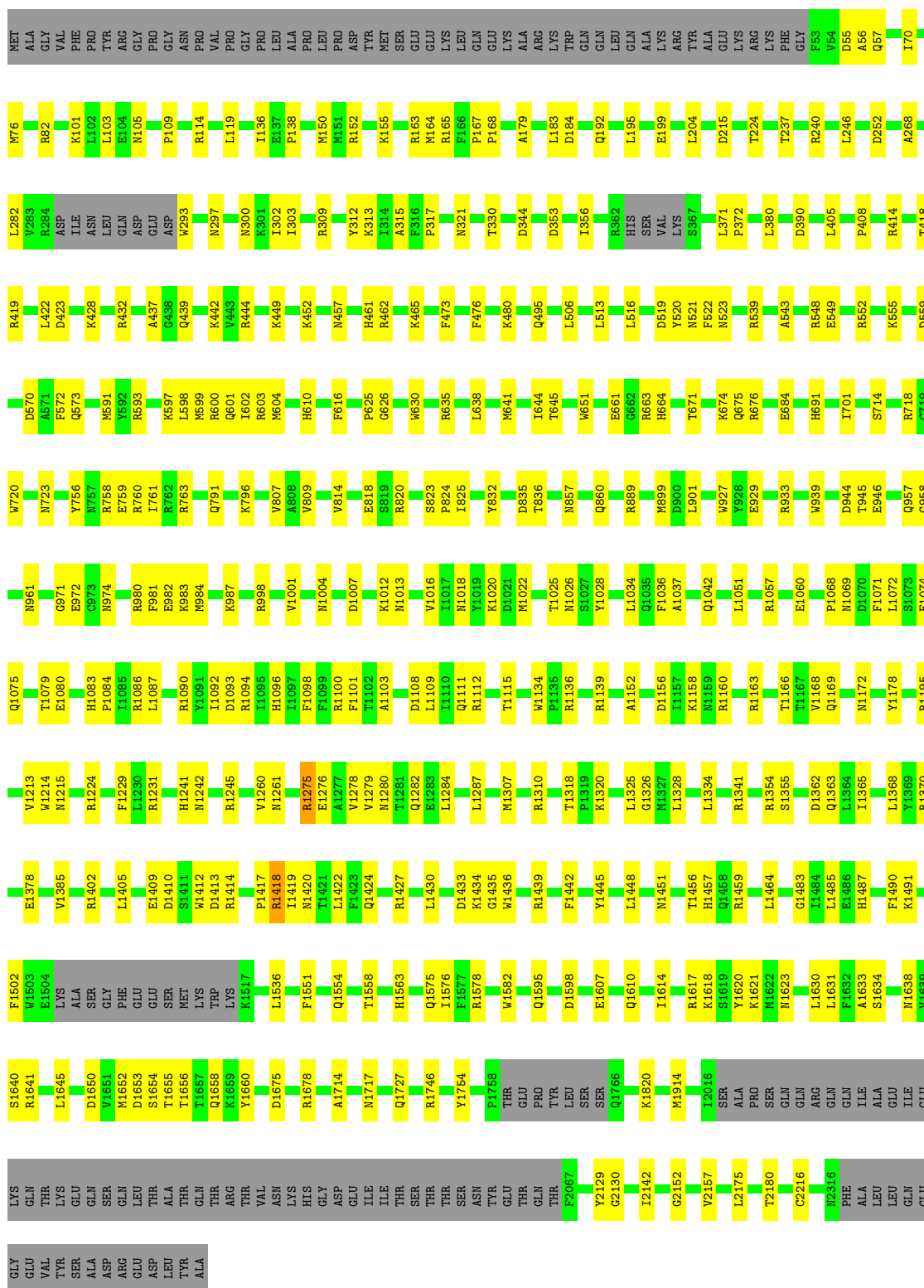


Chain X: 27% . 72%

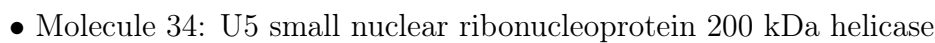




Chain a:  78% 15% 7%

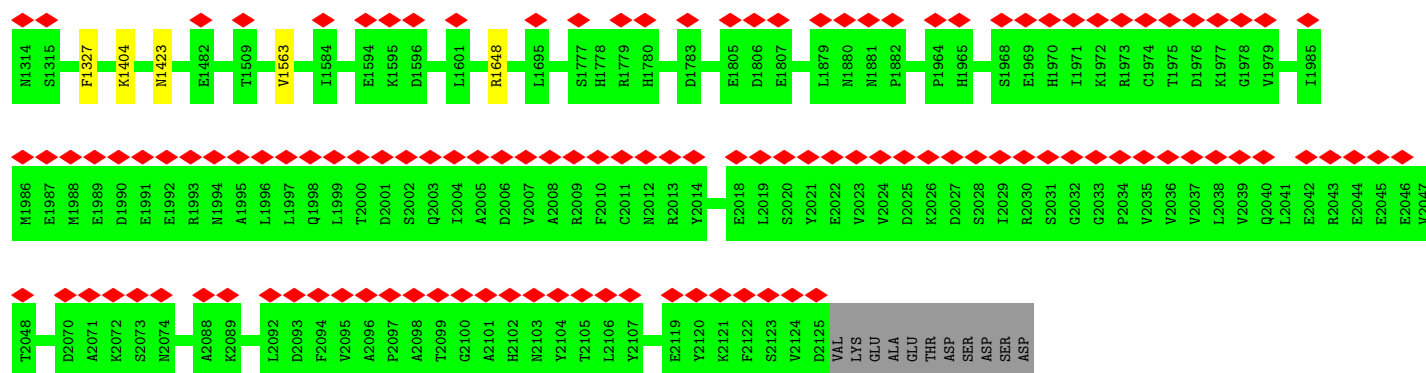


Response	Percentage
U.S. is responsible	74%
U.S. is not responsible	18%
Don't know	8%

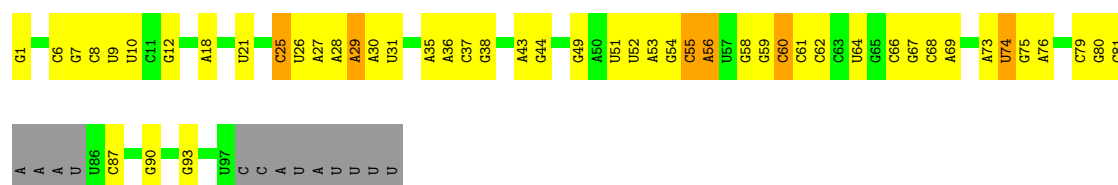


Chain c:

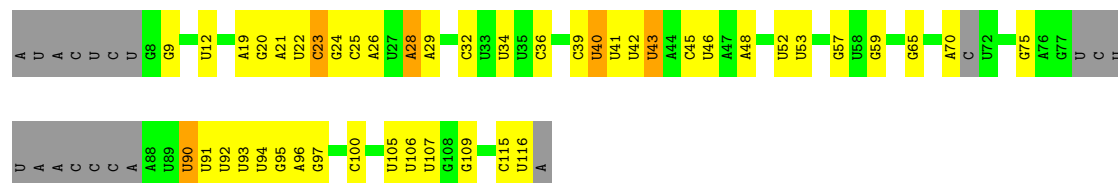




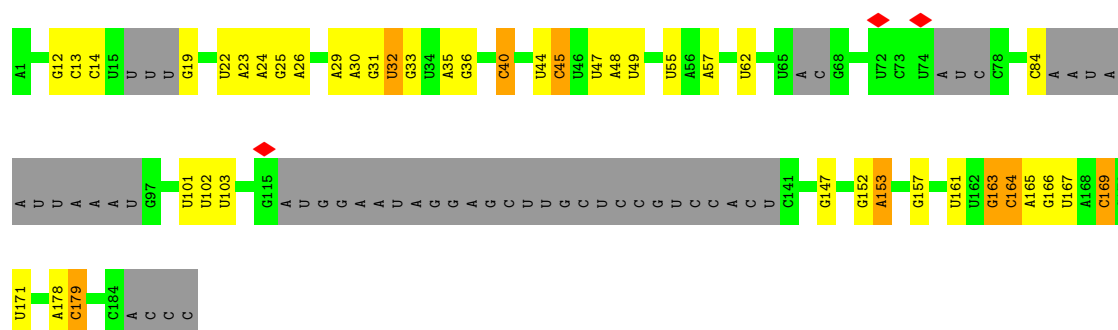
• Molecule 35: RNU6-1



• Molecule 36: RNU5A-1

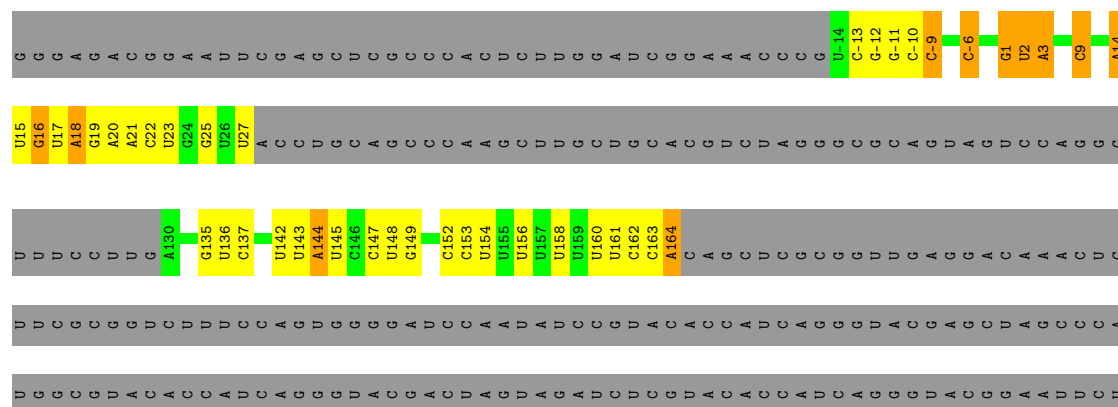


• Molecule 37: RNU2-1



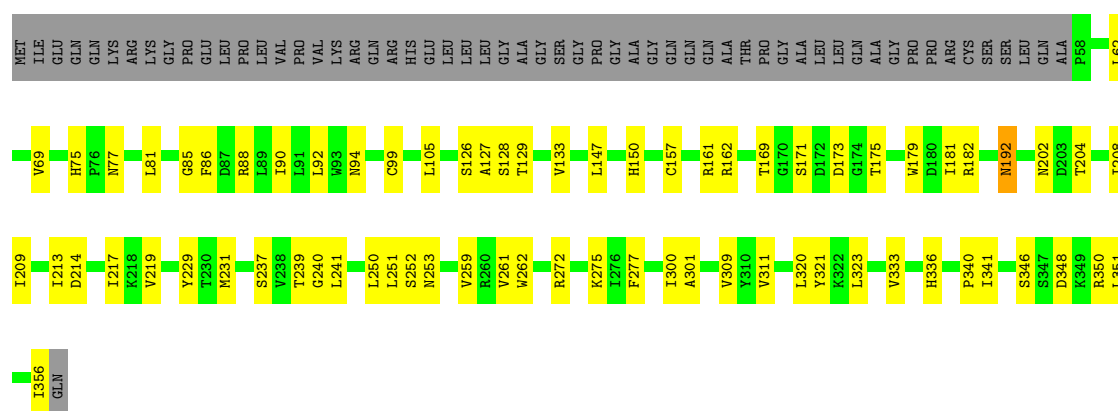
• Molecule 38: MINX-M3





• Molecule 39: U5 small nuclear ribonucleoprotein 40 kDa protein

Chain o: 64% 20% 16%



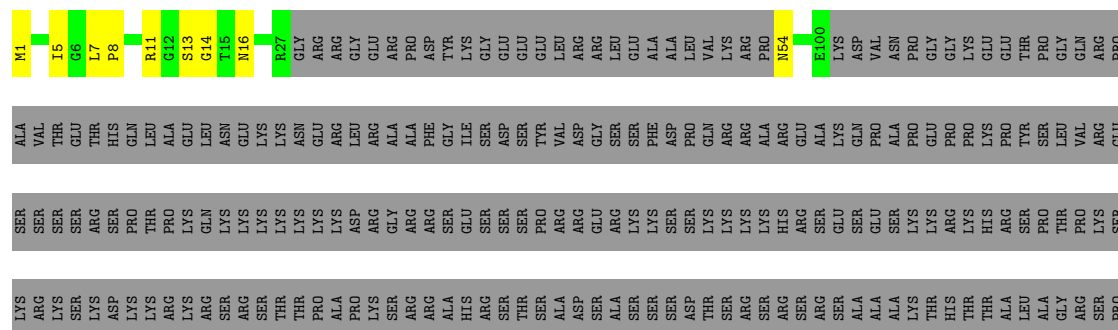
• Molecule 40: Peptidyl-prolyl cis-trans isomerase-like 1

Chain p: 89% 7% .



• Molecule 41: Serine/arginine repetitive matrix protein 2

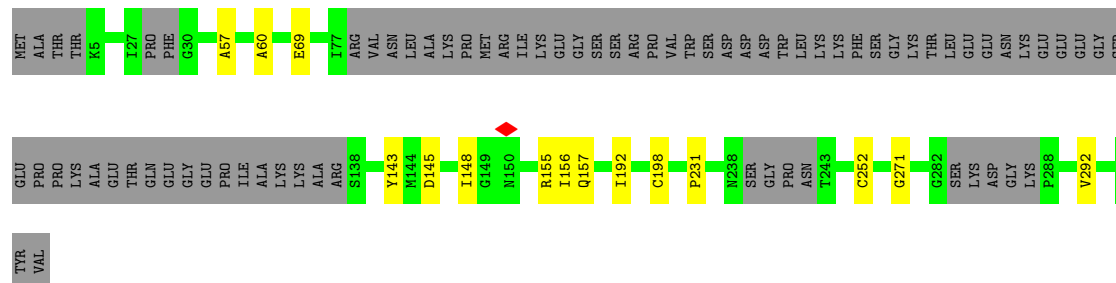
Chain q: 97%



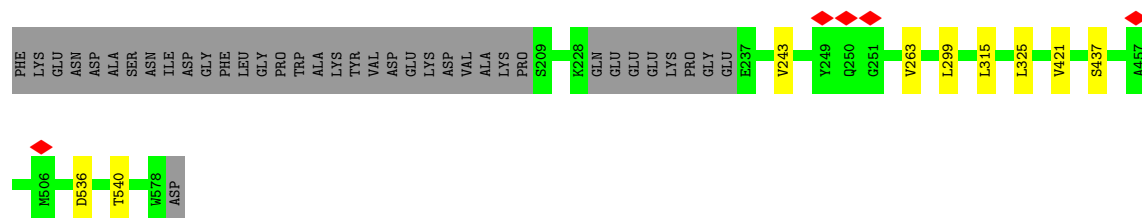
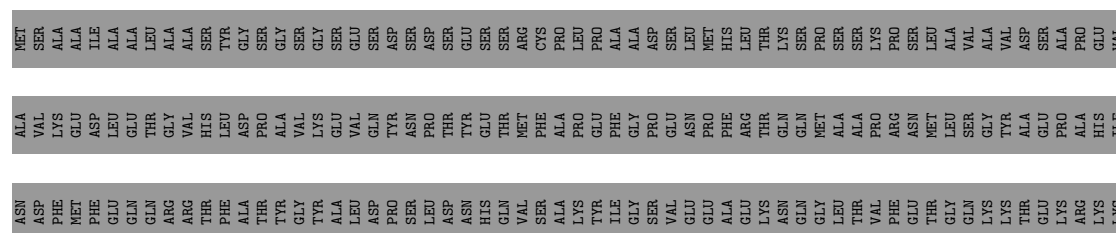




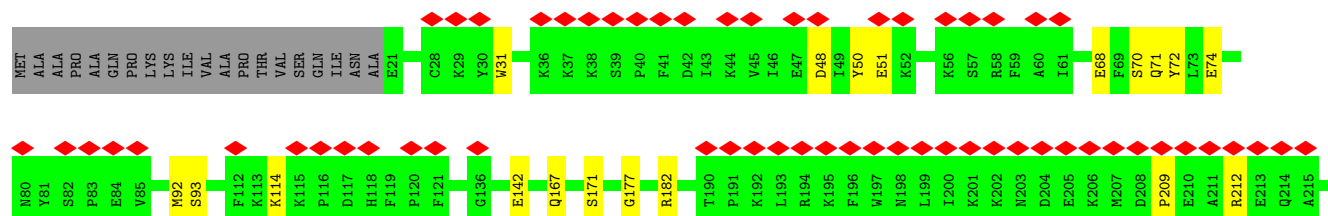
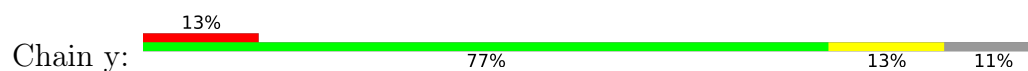
- Molecule 46: Peptidyl-prolyl cis-trans isomerase E



- Molecule 47: Pre-mRNA-processing factor 17



- Molecule 48: Intron-binding protein aquarius



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	12395	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 ($e^-/\text{\AA}^2$)	45.47	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.059	Depositor
Minimum map value	-0.010	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	546.0, 546.0, 546.0	wwPDB
Map dimensions	520, 520, 520	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	0.17	0/390	0.48	0/542
1	i	0.16	0/344	0.46	0/476
2	2	0.15	0/360	0.41	0/497
2	h	0.14	0/320	0.42	0/440
3	3	0.13	0/372	0.47	0/515
3	j	0.18	0/334	0.50	0/463
4	4	0.17	0/420	0.45	0/583
4	l	0.16	0/335	0.44	0/464
5	5	0.24	0/405	0.42	0/563
5	k	0.15	0/387	0.42	0/537
6	8	0.16	0/421	0.45	0/583
6	n	0.15	0/313	0.40	0/432
7	9	0.14	0/332	0.39	0/458
7	m	0.16	0/306	0.46	0/420
8	A	0.15	0/5706	0.41	0/7930
9	B	0.12	0/351	0.39	0/489
10	C	0.24	1/5209 (0.0%)	0.55	0/7211
11	D	0.20	0/660	0.68	2/893 (0.2%)
12	E	0.18	0/1383	0.49	0/1887
13	F	0.14	0/382	0.46	0/529
14	G	0.25	0/370	0.62	0/513
15	H	0.11	0/524	0.44	0/724
16	I	0.19	0/1037	0.47	0/1420
17	J	0.15	0/2195	0.48	0/3036
18	K	0.22	0/953	0.53	0/1295
18	M	0.23	0/1004	0.60	2/1365 (0.1%)
18	R	0.19	0/953	0.49	0/1295
18	v	0.21	0/1004	0.52	0/1365
19	L	0.22	0/178	0.57	0/240
20	N	0.25	0/6267	0.62	0/8491
21	O	0.22	0/2586	0.55	0/3527
22	P	0.19	0/2463	0.53	0/3317

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
23	Q	0.23	0/836	0.62	0/1117
24	S	0.22	0/1342	0.69	1/1804 (0.1%)
25	T	0.23	0/1202	0.61	0/1611
26	U	0.24	0/2118	0.61	3/2881 (0.1%)
27	V	0.19	0/2026	0.53	0/2760
28	W	0.19	0/2954	0.50	0/4033
29	X	0.18	0/1623	0.48	0/2240
30	Y	0.19	0/2290	0.54	0/3103
31	Z	0.16	0/618	0.54	0/845
32	a	0.20	0/16807	0.53	5/22895 (0.0%)
33	b	0.22	0/7206	0.56	2/9800 (0.0%)
34	c	0.15	0/8529	0.41	0/11891
35	d	0.17	0/2225	0.34	0/3464
36	e	0.18	0/2307	0.36	0/3584
37	f	0.14	0/3239	0.26	0/5031
38	g	0.17	0/1734	0.37	0/2691
39	o	0.21	0/2392	0.54	0/3242
40	p	0.14	0/775	0.39	0/1070
41	q	0.22	0/466	0.58	0/639
42	r	0.18	0/803	0.51	0/1119
43	s	0.14	0/810	0.43	0/1122
44	t	0.25	0/414	0.58	0/555
45	u	0.18	0/1969	0.51	2/2722 (0.1%)
46	w	0.15	0/1087	0.41	0/1497
47	x	0.16	0/1785	0.47	0/2482
48	y	0.20	0/11144	0.48	2/15101 (0.0%)
49	z	0.24	1/4593 (0.0%)	0.60	2/6317 (0.0%)
All	All	0.20	2/121558 (0.0%)	0.50	21/168116 (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
11	D	0	1
20	N	0	1
24	S	0	2
39	o	0	1
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	729	LYS	C-N	5.80	1.39	1.33
49	z	341	ARG	C-N	5.06	1.40	1.34

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	M	70	SER	CA-C-N	7.03	124.67	120.24
18	M	70	SER	C-N-CA	7.03	124.67	120.24
32	a	519	ASP	CA-C-N	6.25	133.48	121.54
32	a	519	ASP	C-N-CA	6.25	133.48	121.54
32	a	192	GLN	N-CA-C	5.74	117.62	110.91
24	S	82	LEU	CA-CB-CG	5.36	135.04	116.30
33	b	56	GLU	CA-C-N	5.28	131.48	121.97
33	b	56	GLU	C-N-CA	5.28	131.48	121.97
48	y	661	PRO	CA-C-N	5.28	131.63	121.54
48	y	661	PRO	C-N-CA	5.28	131.63	121.54
45	u	239	ALA	CA-C-N	5.17	131.42	121.54
45	u	239	ALA	C-N-CA	5.17	131.42	121.54
26	U	133	PRO	CA-C-N	5.17	131.28	121.97
26	U	133	PRO	C-N-CA	5.17	131.28	121.97
26	U	63	MET	CB-CG-SD	5.16	128.19	112.70
11	D	60	ILE	CA-C-N	5.08	131.24	121.54
11	D	60	ILE	C-N-CA	5.08	131.24	121.54
49	z	190	SER	CA-C-N	5.05	131.18	121.54
49	z	190	SER	C-N-CA	5.05	131.18	121.54
32	a	1418	ARG	CA-C-N	5.03	131.02	121.97
32	a	1418	ARG	C-N-CA	5.03	131.02	121.97

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	D	45	ILE	Peptide
20	N	504	GLU	Peptide
24	S	77	GLN	Peptide
24	S	89	LEU	Peptide
39	o	192	ASN	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	391	0	163	1	0
1	i	346	0	144	3	0
2	2	361	0	158	5	0
2	h	322	0	138	10	0
3	3	373	0	163	0	0
3	j	335	0	148	6	0
4	4	422	0	175	3	0
4	l	337	0	139	6	0
5	5	406	0	170	3	0
5	k	388	0	164	2	0
6	8	422	0	177	1	0
6	n	315	0	134	2	0
7	9	334	0	143	3	0
7	m	309	0	135	3	0
8	A	5714	0	2549	42	0
9	B	350	0	167	0	0
10	C	5115	0	4128	46	0
11	D	649	0	597	17	0
12	E	1350	0	1111	21	0
13	F	383	0	173	4	0
14	G	364	0	226	2	0
15	H	530	0	218	1	0
16	I	1034	0	621	7	0
17	J	2187	0	1161	10	0
18	K	938	0	938	8	0
18	M	988	0	994	13	0
18	R	938	0	938	10	0
18	v	988	0	994	8	0
19	L	177	0	140	0	0
20	N	6147	0	5981	103	0
21	O	2517	0	2466	52	0
22	P	2432	0	2205	38	0
23	Q	823	0	779	22	0
24	S	1323	0	1311	16	0
25	T	1176	0	1178	19	0
26	U	2080	0	1803	47	0
27	V	1996	0	1727	22	0
28	W	2921	0	2168	14	0
29	X	1587	0	1176	14	0
30	Y	2250	0	2095	34	0
31	Z	607	0	402	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	a	16415	0	14878	232	0
33	b	7046	0	7030	111	0
34	c	8530	0	3747	10	0
35	d	1989	0	1006	23	0
36	e	2070	0	1046	19	0
37	f	2906	0	1473	13	0
38	g	1559	0	794	22	0
39	o	2338	0	2275	43	0
40	p	776	0	358	8	0
41	q	461	0	354	6	0
42	r	804	0	350	0	0
43	s	813	0	366	2	0
44	t	407	0	393	6	0
45	u	1963	0	1065	22	0
46	w	1093	0	497	8	0
47	x	1787	0	780	3	0
48	y	10878	0	10826	108	0
49	z	4511	0	3545	22	0
50	D	3	0	0	0	0
50	I	1	0	0	0	0
50	J	1	0	0	0	0
50	T	3	0	0	0	0
50	U	3	0	0	0	0
50	Z	1	0	0	0	0
51	a	36	0	6	2	0
52	b	32	0	12	0	0
53	b	1	0	0	0	0
53	d	6	0	0	0	0
All	All	119058	0	91198	1113	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 (1113) 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)
25:T:139:CYS:SG	25:T:142:CYS:HB3	1.98	1.02
26:U:24:CYS:SG	26:U:81:CYS:HB2	2.12	0.90
32:a:972:GLU:HA	32:a:1101:PHE:O	1.72	0.90
36:e:90:U:HO2'	7:m:4:ALA:N	1.75	0.84
39:o:217:ILE:O	39:o:231:MET:HB3	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:1405:LEU:O	32:a:1409:GLU:HB2	1.80	0.81
27:V:65:SER:HG	27:V:77:PHE:N	1.80	0.80
33:b:441:PRO:O	33:b:445:ALA:HB2	1.82	0.79
26:U:27:CYS:HB3	26:U:84:CYS:SG	2.26	0.75
11:D:46:CYS:SG	11:D:85:CYS:HB2	2.26	0.75
22:P:48:ALA:O	22:P:52:GLU:HB2	1.87	0.73
39:o:240:GLY:O	39:o:252:SER:HA	1.91	0.71
20:N:504:GLU:O	20:N:508:GLU:HB3	1.91	0.70
26:U:179:CYS:HB3	26:U:183:HIS:NE2	2.06	0.70
33:b:500:THR:HA	33:b:544:VAL:O	1.92	0.69
27:V:95:SER:HA	27:V:124:THR:O	1.94	0.67
39:o:241:LEU:HA	39:o:251:LEU:O	1.95	0.67
16:I:54:TYR:HB2	16:I:63:HIS:HB2	1.77	0.66
17:J:411:CYS:HB3	17:J:431:HIS:ND1	2.10	0.66
17:J:411:CYS:CB	17:J:431:HIS:HD1	2.10	0.64
48:y:92:MET:HE2	48:y:142:GLU:HB2	1.80	0.64
25:T:117:CYS:SG	25:T:118:ILE:N	2.70	0.63
37:f:161:U:H2'	37:f:163:G:H21	1.63	0.62
17:J:408:CYS:O	17:J:413:ASN:HA	1.99	0.62
20:N:644:VAL:HA	20:N:670:VAL:O	1.99	0.62
30:Y:240:LYS:O	30:Y:244:GLU:HB2	2.00	0.62
20:N:988:GLU:HB3	20:N:998:ARG:HB2	1.81	0.62
24:S:133:ASN:HA	24:S:136:LYS:HB2	1.81	0.62
48:y:521:GLU:HB3	48:y:536:ARG:HB2	1.82	0.62
33:b:531:TRP:HB2	33:b:551:LEU:HB2	1.80	0.61
33:b:684:LYS:HB3	33:b:795:VAL:HB	1.83	0.61
30:Y:301:LYS:HB3	45:u:203:GLU:HB2	1.82	0.61
26:U:39:GLU:HB2	26:U:54:VAL:HB	1.83	0.61
32:a:1136:ARG:HD3	32:a:1139:ARG:HE	1.66	0.61
32:a:958:GLY:HA3	32:a:1072:LEU:HD13	1.83	0.61
25:T:105:CYS:SG	25:T:117:CYS:HB3	2.41	0.60
22:P:216:PHE:O	29:X:267:ARG:NH1	2.35	0.60
33:b:475:MET:HA	33:b:565:ILE:O	2.00	0.60
21:O:272:CYS:HB3	21:O:282:ARG:HB2	1.84	0.60
32:a:756:TYR:HB3	32:a:760:ARG:HH21	1.67	0.60
17:J:411:CYS:HB3	17:J:431:HIS:HD1	1.63	0.59
48:y:209:PRO:HA	48:y:212:ARG:HB3	1.83	0.59
24:S:179:ARG:HH22	18:v:119:ARG:HH21	1.50	0.59
13:F:39:VAL:HA	13:F:61:PHE:HA	1.85	0.59
23:Q:187:ARG:HE	27:V:118:TYR:HB2	1.67	0.59
20:N:615:LEU:HD12	20:N:621:ILE:HG13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:O:270:VAL:HB	21:O:284:TYR:HB2	1.85	0.59
21:O:477:LEU:O	21:O:488:VAL:HA	2.03	0.59
48:y:356:VAL:HG23	49:z:276:ARG:HH21	1.66	0.58
20:N:455:ARG:HG3	38:g:156:U:H5''	1.85	0.58
39:o:309:VAL:HB	39:o:323:LEU:HB2	1.85	0.58
8:A:336:ALA:HA	8:A:351:SER:HA	1.85	0.58
26:U:64:ARG:NH2	38:g:19:G:OP2	2.36	0.58
20:N:873:LEU:H	20:N:880:VAL:HG22	1.69	0.58
30:Y:217:LYS:HB3	35:d:60:C:H4'	1.86	0.58
39:o:62:LEU:HB2	39:o:351:LEU:HB2	1.85	0.58
22:P:226:ASP:HB2	29:X:297:ASN:HD21	1.68	0.57
32:a:832:TYR:HB3	32:a:835:ASP:HB3	1.86	0.57
32:a:165:ARG:NH1	32:a:1623:ASN:OD1	2.37	0.57
48:y:1269:ASP:HA	48:y:1298:ARG:HB2	1.87	0.57
39:o:340:PRO:HB2	39:o:356:ILE:HB	1.86	0.57
20:N:481:ILE:HA	20:N:500:MET:HE3	1.86	0.57
30:Y:178:ARG:HH11	30:Y:194:GLN:HB3	1.70	0.57
25:T:12:PRO:HB2	25:T:74:LEU:HD22	1.86	0.57
22:P:756:LYS:HG3	24:S:170:MET:HE1	1.85	0.56
18:R:19:PRO:HD2	18:R:47:LEU:HD11	1.87	0.56
20:N:765:LEU:HD22	20:N:822:PRO:HG3	1.86	0.56
21:O:195:LYS:HE2	21:O:490:ARG:HH21	1.68	0.56
39:o:259:VAL:HB	39:o:277:PHE:HB2	1.85	0.56
10:C:1244:CYS:SG	10:C:1245:ARG:NH1	2.79	0.56
20:N:251:LEU:HD11	20:N:273:LYS:HB3	1.87	0.56
20:N:752:VAL:O	20:N:757:ARG:NH1	2.39	0.56
18:M:81:GLU:HB3	18:R:71:ILE:HG12	1.88	0.56
21:O:210:ILE:HG12	21:O:221:THR:HG22	1.87	0.56
32:a:1675:ASP:HB3	32:a:1678:ARG:HE	1.70	0.56
32:a:1576:ILE:O	32:a:1746:ARG:NH1	2.39	0.56
23:Q:33:ARG:NH1	36:e:32:C:OP1	2.39	0.56
8:A:461:THR:HA	8:A:474:ILE:HA	1.88	0.56
20:N:232:ARG:HD2	27:V:237:PRO:HG3	1.88	0.56
20:N:700:TYR:HB2	20:N:707:GLU:HG3	1.86	0.56
32:a:603:ARG:NH2	38:g:-6:C:N3	2.53	0.56
32:a:980:ARG:HH21	32:a:984:MET:HE1	1.70	0.56
22:P:221:ALA:O	29:X:301:ARG:NH1	2.38	0.56
26:U:24:CYS:O	26:U:28:LEU:HB2	2.06	0.56
32:a:927:TRP:HB3	32:a:1434:LYS:HB2	1.88	0.56
2:h:16:GLY:N	2:h:33:LEU:O	2.39	0.56
47:x:315:LEU:O	47:x:325:LEU:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:D:29:LYS:HE2	11:D:34:ASP:HB3	1.87	0.55
26:U:84:CYS:O	26:U:201:ARG:NH2	2.39	0.55
26:U:133:PRO:HD2	26:U:137:LEU:HD22	1.88	0.55
32:a:1214:TRP:NE1	32:a:1276:GLU:OE1	2.39	0.55
32:a:1018:ASN:HA	32:a:1022:MET:O	2.05	0.55
8:A:437:VAL:O	8:A:776:GLN:HA	2.06	0.55
20:N:656:GLN:HA	20:N:659:ILE:HD12	1.87	0.55
48:y:705:MET:HE1	48:y:816:PRO:HB2	1.88	0.55
18:K:26:GLU:HB3	18:K:29:LEU:HB2	1.88	0.55
20:N:344:ARG:HH21	32:a:1069:ASN:HA	1.72	0.55
20:N:511:LEU:HB3	20:N:514:TYR:HB2	1.88	0.55
20:N:649:ALA:O	20:N:906:ARG:NH2	2.40	0.55
21:O:314:ILE:HB	21:O:324:HIS:HB2	1.88	0.55
27:V:14:ILE:HG12	27:V:129:VAL:HG22	1.87	0.55
32:a:971:GLY:HA3	32:a:1103:ALA:HB2	1.89	0.55
21:O:305:THR:HG1	21:O:315:TRP:HE1	1.55	0.55
32:a:1413:ASP:O	32:a:1418:ARG:NH1	2.40	0.55
33:b:166:CYS:O	33:b:536:ARG:NH2	2.40	0.55
48:y:365:LEU:HB3	48:y:408:VAL:HG22	1.88	0.55
48:y:848:ARG:NH1	48:y:1055:LYS:O	2.40	0.55
25:T:120:ARG:NH1	25:T:142:CYS:SG	2.78	0.55
8:A:820:ALA:HA	8:A:839:ALA:HB1	1.89	0.55
48:y:565:ILE:HG12	48:y:592:VAL:HG22	1.87	0.55
48:y:1230:TYR:OH	48:y:1277:ARG:NH1	2.40	0.55
11:D:4:HIS:NE2	11:D:32:ILE:O	2.40	0.55
18:M:116:VAL:HG13	18:M:119:ARG:HH21	1.71	0.55
20:N:416:GLN:HG3	20:N:417:VAL:HG13	1.88	0.55
32:a:405:LEU:O	33:b:413:ARG:NH2	2.40	0.55
34:c:912:ASN:HA	34:c:978:ASN:HA	1.89	0.55
33:b:154:HIS:O	33:b:158:ARG:NH2	2.41	0.54
48:y:852:VAL:HG22	48:y:1037:MET:HB2	1.89	0.54
21:O:195:LYS:NZ	21:O:491:GLU:O	2.41	0.54
3:j:32:LEU:HA	3:j:43:MET:HA	1.90	0.54
20:N:612:LEU:HB3	20:N:689:VAL:HG22	1.89	0.54
20:N:612:LEU:O	20:N:689:VAL:HA	2.06	0.54
28:W:467:LEU:O	32:a:1370:ARG:NH1	2.40	0.54
12:E:508:ARG:HH11	12:E:513:GLY:H	1.56	0.54
20:N:453:PRO:HG3	20:N:524:GLU:HG3	1.89	0.54
35:d:38:G:O6	38:g:9:C:N4	2.41	0.54
48:y:71:GLN:NE2	48:y:74:GLU:OE2	2.41	0.54
26:U:168:TRP:O	26:U:185:LYS:NZ	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:1424:GLN:O	32:a:1427:ARG:NH1	2.36	0.54
33:b:853:ARG:NH1	33:b:879:ASP:O	2.41	0.54
40:p:96:GLY:H	40:p:116:LEU:HA	1.73	0.54
48:y:582:PRO:O	48:y:586:GLN:HB2	2.07	0.54
21:O:381:HIS:O	30:Y:134:ARG:NH2	2.41	0.54
26:U:78:LYS:NZ	26:U:202:TYR:O	2.41	0.54
33:b:559:ILE:O	33:b:612:LYS:NZ	2.41	0.54
5:k:19:LEU:HA	5:k:65:ILE:HA	1.90	0.54
12:E:530:ARG:HH22	12:E:578:TRP:HB3	1.73	0.54
39:o:86:PHE:O	39:o:88:ARG:NH1	2.41	0.54
26:U:162:PRO:O	26:U:182:ARG:NE	2.38	0.54
45:u:55:THR:HA	45:u:88:LEU:HA	1.90	0.53
48:y:916:GLN:NE2	48:y:921:VAL:O	2.41	0.53
21:O:485:THR:OG1	21:O:487:LYS:NZ	2.41	0.53
26:U:288:PHE:HA	26:U:300:VAL:H	1.73	0.53
32:a:1645:LEU:O	32:a:1727:GLN:NE2	2.41	0.53
33:b:151:GLU:O	33:b:158:ARG:NH2	2.41	0.53
7:9:46:VAL:HA	7:9:56:ASN:HA	1.90	0.53
20:N:343:ALA:HA	32:a:1074:PHE:H	1.72	0.53
32:a:380:LEU:N	33:b:354:ARG:O	2.41	0.53
41:q:13:SER:OG	41:q:14:GLY:N	2.42	0.53
8:A:15:SER:N	8:A:33:SER:O	2.42	0.53
10:C:1068:ALA:O	10:C:1074:ARG:NH1	2.41	0.53
10:C:1190:ALA:O	10:C:1194:HIS:ND1	2.41	0.53
20:N:559:ARG:HH22	20:N:782:ASP:HB3	1.72	0.53
32:a:548:ARG:NH1	32:a:549:GLU:OE2	2.42	0.53
39:o:75:HIS:ND1	39:o:77:ASN:OD1	2.39	0.53
21:O:356:LEU:HB2	21:O:366:VAL:HB	1.91	0.53
32:a:1261:ASN:OD1	32:a:1320:LYS:NZ	2.42	0.53
10:C:940:LEU:HD23	10:C:948:ARG:HB3	1.89	0.53
32:a:330:THR:OG1	33:b:177:ARG:NH1	2.42	0.53
32:a:1042:GLN:O	32:a:1090:ARG:NH2	2.42	0.53
33:b:605:ASP:OD1	33:b:608:ARG:NH2	2.41	0.53
48:y:914:ARG:NH1	48:y:973:TYR:O	2.42	0.53
20:N:460:SER:OG	20:N:464:ARG:NH1	2.41	0.53
20:N:648:TYR:HB2	20:N:651:LEU:HB2	1.91	0.53
35:d:31:U:H3	38:g:15:U:H3	1.57	0.53
27:V:7:THR:HG22	27:V:156:ILE:HG12	1.89	0.53
32:a:215:ASP:N	32:a:215:ASP:OD1	2.42	0.53
32:a:372:PRO:O	33:b:358:LYS:NZ	2.41	0.53
32:a:671:THR:O	32:a:676:ARG:NH1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:b:222:SER:O	33:b:448:LYS:NZ	2.39	0.53
48:y:71:GLN:OE1	48:y:1285:ARG:NH2	2.42	0.53
11:D:41:THR:HB	11:D:71:TYR:HB2	1.91	0.53
32:a:825:ILE:HB	32:a:1001:VAL:HG12	1.91	0.53
45:u:293:LEU:HA	45:u:400:VAL:HA	1.91	0.53
20:N:945:ALA:HA	20:N:1011:VAL:HG21	1.91	0.52
21:O:189:GLN:NE2	21:O:440:ASP:OD1	2.42	0.52
21:O:376:ARG:NH2	32:a:691:HIS:O	2.43	0.52
22:P:779:GLU:HA	22:P:782:LYS:HD2	1.91	0.52
27:V:96:MET:HB3	27:V:124:THR:HB	1.90	0.52
32:a:957:GLN:O	32:a:961:ASN:ND2	2.43	0.52
27:V:7:THR:HA	27:V:156:ILE:HA	1.91	0.52
33:b:162:ASP:OD1	33:b:162:ASP:N	2.43	0.52
48:y:866:ILE:HA	48:y:869:LEU:HD12	1.90	0.52
48:y:1027:LEU:HA	48:y:1031:GLU:HB3	1.91	0.52
10:C:942:ASN:O	10:C:948:ARG:NH1	2.42	0.52
10:C:1062:LEU:HD22	10:C:1077:THR:HG23	1.91	0.52
31:Z:203:LYS:HB3	38:g:2:U:H2'	1.90	0.52
32:a:539:ARG:NH2	35:d:64:U:O2	2.41	0.52
33:b:947:VAL:HG12	33:b:949:ILE:H	1.74	0.52
48:y:68:GLU:OE1	48:y:1285:ARG:NH1	2.43	0.52
49:z:98:CYS:HA	49:z:101:ARG:HB2	1.91	0.52
12:E:515:ARG:NH1	37:f:40:C:OP1	2.43	0.52
20:N:752:VAL:HG13	20:N:757:ARG:HH11	1.75	0.52
26:U:26:THR:HG22	26:U:155:PRO:HA	1.91	0.52
32:a:419:ARG:NH2	32:a:423:ASP:O	2.42	0.52
35:d:53:A:H61	37:f:22:U:H3	1.58	0.52
10:C:1062:LEU:HA	10:C:1065:LEU:HB2	1.92	0.52
10:C:1106:ARG:O	10:C:1109:ARG:NH1	2.43	0.52
17:J:395:TRP:N	37:f:45:C:O2	2.41	0.52
32:a:600:ARG:NH1	32:a:601:GLN:OE1	2.43	0.52
33:b:240:GLU:OE2	33:b:292:TYR:OH	2.27	0.52
20:N:960:ARG:NH1	20:N:961:THR:O	2.43	0.52
22:P:211:ASN:OD1	29:X:228:ARG:NH1	2.40	0.52
30:Y:103:ARG:NH1	30:Y:107:SER:O	2.43	0.52
30:Y:145:GLU:OE2	30:Y:148:ARG:NH1	2.43	0.52
32:a:317:PRO:HA	32:a:321:ASN:HD22	1.75	0.52
34:c:1225:VAL:O	34:c:1234:LEU:N	2.42	0.52
10:C:1019:ARG:O	10:C:1019:ARG:NH1	2.43	0.52
24:S:73:LEU:HD23	24:S:76:ARG:HH22	1.74	0.52
32:a:457:ASN:ND2	36:e:28:A:OP2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:b:171:LEU:HB2	33:b:174:GLU:HG3	1.91	0.52
33:b:914:LYS:HD3	33:b:931:ARG:HH22	1.74	0.52
33:b:947:VAL:HB	33:b:950:SER:HB2	1.90	0.52
6:n:31:PHE:HA	6:n:42:LEU:HA	1.92	0.52
39:o:90:ILE:HB	39:o:105:LEU:HB2	1.91	0.52
48:y:813:GLY:HA2	48:y:819:THR:HG21	1.90	0.52
14:G:120:GLU:O	20:N:184:ARG:NH2	2.43	0.52
21:O:282:ARG:NH1	23:Q:38:HIS:O	2.42	0.52
32:a:70:ILE:HG13	32:a:495:GLN:HG2	1.91	0.52
32:a:309:ARG:HD3	32:a:312:TYR:HE2	1.74	0.52
32:a:1554:GLN:NE2	32:a:1558:THR:O	2.43	0.52
32:a:1638:ASN:ND2	32:a:1653:ASP:OD1	2.43	0.52
30:Y:408:ASP:HA	32:a:1402:ARG:HH21	1.75	0.52
32:a:1215:ASN:O	32:a:1224:ARG:NH1	2.43	0.52
20:N:479:TYR:HE2	20:N:484:GLU:HB3	1.75	0.51
21:O:306:CYS:HB2	21:O:333:VAL:HB	1.93	0.51
27:V:42:ILE:HG23	27:V:53:THR:HB	1.92	0.51
27:V:266:ILE:HA	27:V:288:PHE:HA	1.92	0.51
32:a:1134:TRP:O	32:a:1139:ARG:NH1	2.43	0.51
32:a:1412:TRP:O	32:a:1420:ASN:ND2	2.43	0.51
48:y:1061:MET:HE2	48:y:1093:MET:HE1	1.91	0.51
17:J:402:LEU:HD13	17:J:417:ARG:HH21	1.75	0.51
22:P:777:GLN:OE1	24:S:185:TRP:NE1	2.44	0.51
23:Q:52:GLU:O	23:Q:56:ASN:ND2	2.43	0.51
39:o:192:ASN:ND2	39:o:214:ASP:OD2	2.40	0.51
39:o:209:ILE:HG22	39:o:241:LEU:HD13	1.93	0.51
39:o:311:VAL:O	39:o:320:LEU:N	2.43	0.51
44:t:152:MET:HE3	49:z:142:ILE:HG13	1.92	0.51
48:y:31:TRP:NE1	48:y:70:SER:OG	2.43	0.51
8:A:606:ALA:HA	8:A:615:ARG:O	2.10	0.51
20:N:948:PHE:O	20:N:1016:TYR:OH	2.27	0.51
18:R:15:PRO:HG2	18:R:55:ILE:HB	1.91	0.51
33:b:738:ASP:N	33:b:738:ASP:OD1	2.43	0.51
2:2:22:LYS:O	2:2:70:LEU:N	2.44	0.51
8:A:107:PHE:O	11:D:14:GLN:NE2	2.43	0.51
20:N:754:GLU:OE1	20:N:757:ARG:NH2	2.44	0.51
22:P:226:ASP:O	30:Y:84:ASN:N	2.44	0.51
32:a:521:ASN:OD1	32:a:555:LYS:NZ	2.44	0.51
10:C:1056:MET:HE3	12:E:559:PRO:HB2	1.92	0.51
20:N:863:HIS:ND1	32:a:836:THR:OG1	2.37	0.51
21:O:345:ILE:HB	21:O:357:TRP:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:O:349:SER:OG	21:O:350:HIS:N	2.43	0.51
26:U:32:PRO:HA	30:Y:195:ARG:HG2	1.93	0.51
28:W:562:TRP:HA	28:W:565:LEU:HD13	1.92	0.51
35:d:29:A:N6	38:g:16:G:O3'	2.44	0.51
20:N:835:SER:OG	20:N:836:CYS:N	2.43	0.51
26:U:26:THR:O	26:U:160:ASN:ND2	2.44	0.51
30:Y:65:PRO:HB3	40:p:90:LEU:HA	1.93	0.51
30:Y:311:GLN:HG2	30:Y:314:ARG:HH12	1.75	0.51
33:b:770:PHE:HA	33:b:816:VAL:HG21	1.92	0.51
45:u:321:PHE:HA	45:u:332:GLY:HA2	1.91	0.51
8:A:70:LEU:HA	8:A:127:GLY:HA3	1.92	0.51
10:C:1017:LEU:HD13	10:C:1050:VAL:HG21	1.92	0.51
16:I:4:GLN:OE1	36:e:40:U:N3	2.43	0.51
26:U:50:ARG:HH22	26:U:118:THR:HG22	1.75	0.51
35:d:67:G:H1	36:e:43:U:H4'	1.75	0.51
48:y:226:ILE:HG23	48:y:279:LEU:HD13	1.93	0.51
48:y:803:THR:HG21	48:y:1135:ALA:HB3	1.93	0.51
8:A:798:ILE:HA	8:A:868:VAL:HA	1.93	0.51
10:C:925:VAL:HA	10:C:928:TYR:HD2	1.76	0.51
11:D:48:GLU:HA	11:D:51:TYR:HB3	1.93	0.51
22:P:71:LEU:HD11	22:P:100:TYR:HB2	1.93	0.51
32:a:972:GLU:O	32:a:1100:ARG:NH1	2.43	0.51
33:b:771:GLN:O	33:b:775:ARG:HB2	2.10	0.51
10:C:1078:VAL:HG22	10:C:1115:ALA:HB2	1.93	0.51
45:u:242:SER:HA	45:u:263:ALA:HA	1.93	0.51
48:y:563:PHE:HB2	48:y:657:MET:HB3	1.93	0.51
48:y:1355:ILE:HG23	48:y:1360:GLN:HB3	1.93	0.51
10:C:813:PRO:O	10:C:817:HIS:ND1	2.44	0.51
20:N:653:SER:HG	30:Y:389:SER:HG	1.59	0.51
21:O:261:LEU:HB3	21:O:273:TRP:HB2	1.93	0.51
21:O:307:SER:OG	21:O:308:ARG:N	2.41	0.51
27:V:21:ARG:NH1	27:V:81:GLU:O	2.43	0.51
34:c:1308:PRO:HA	34:c:1327:PHE:HA	1.92	0.51
39:o:126:SER:O	39:o:133:VAL:HA	2.11	0.51
48:y:848:ARG:NH2	48:y:1028:LEU:O	2.44	0.51
8:A:928:TYR:HA	8:A:940:LEU:H	1.76	0.50
20:N:331:GLU:HA	20:N:334:LEU:HB2	1.93	0.50
20:N:696:LYS:NZ	38:g:153:C:OP1	2.44	0.50
22:P:19:LEU:HD23	22:P:54:LEU:HD22	1.93	0.50
28:W:487:LYS:O	28:W:491:ASN:ND2	2.40	0.50
32:a:442:LYS:NZ	51:a:3001:IHP:O43	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:z:140:LEU:O	49:z:145:HIS:NE2	2.44	0.50
33:b:736:GLY:O	33:b:771:GLN:NE2	2.44	0.50
8:A:62:ILE:HA	8:A:82:SER:HA	1.92	0.50
30:Y:130:PRO:HA	30:Y:133:GLN:HB2	1.93	0.50
32:a:901:LEU:O	32:a:1242:ASN:ND2	2.45	0.50
35:d:1:G:O6	35:d:18:A:N6	2.45	0.50
21:O:308:ARG:NH1	32:a:684:GLU:OE2	2.45	0.50
32:a:1575:GLN:O	32:a:1578:ARG:NH1	2.41	0.50
33:b:701:GLU:OE2	33:b:785:ARG:NH1	2.42	0.50
33:b:841:ASP:OD1	33:b:841:ASP:N	2.45	0.50
39:o:133:VAL:HB	39:o:147:LEU:HB2	1.92	0.50
39:o:219:VAL:HB	39:o:229:TYR:HB3	1.93	0.50
49:z:289:VAL:HA	49:z:292:PHE:HB3	1.93	0.50
22:P:221:ALA:HB3	29:X:301:ARG:HD3	1.93	0.50
23:Q:209:ARG:NH2	33:b:66:TYR:O	2.45	0.50
26:U:39:GLU:OE2	35:d:25:C:N4	2.45	0.50
32:a:55:ASP:OD1	32:a:57:GLN:NE2	2.45	0.50
32:a:1093:ASP:OD1	32:a:1094:ARG:NH1	2.45	0.50
33:b:785:ARG:HD3	33:b:828:MET:HG2	1.92	0.50
20:N:232:ARG:NH2	27:V:315:PHE:O	2.44	0.50
28:W:498:ALA:HB1	28:W:543:LYS:HG2	1.93	0.50
32:a:1307:MET:HB3	32:a:1310:ARG:HB2	1.93	0.50
48:y:421:LEU:HA	48:y:424:MET:HE2	1.93	0.50
48:y:916:GLN:HG2	48:y:921:VAL:HB	1.93	0.50
18:M:7:ILE:HG23	18:v:90:PHE:HB2	1.93	0.50
20:N:937:ILE:HD12	20:N:940:ARG:HE	1.77	0.50
18:R:79:GLN:NE2	18:R:83:ASP:OD2	2.45	0.50
24:S:195:ILE:O	24:S:198:THR:OG1	2.29	0.50
30:Y:213:LYS:O	30:Y:216:LYS:NZ	2.43	0.50
32:a:1433:ASP:OD1	32:a:1439:ARG:NH1	2.45	0.50
33:b:137:HIS:O	33:b:142:LYS:NZ	2.44	0.50
33:b:888:ARG:O	33:b:893:GLY:N	2.45	0.50
36:e:46:U:O2	41:q:11:ARG:NH1	2.44	0.50
48:y:1266:GLN:O	48:y:1296:ARG:NH1	2.45	0.50
11:D:45:ILE:HG22	11:D:86:PRO:HD2	1.93	0.50
32:a:1108:ASP:OD2	32:a:1112:ARG:NH1	2.44	0.50
32:a:1158:LYS:NZ	32:a:1168:VAL:O	2.44	0.50
39:o:300:ILE:O	39:o:311:VAL:HA	2.12	0.50
46:w:145:ASP:HA	46:w:155:ARG:HA	1.94	0.50
10:C:893:ILE:HD13	10:C:896:ILE:HD11	1.93	0.50
21:O:427:LEU:O	21:O:438:LEU:HA	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:40:LEU:O	8:A:53:LEU:N	2.44	0.49
10:C:658:TRP:HA	10:C:661:ARG:HE	1.77	0.49
11:D:35:SER:OG	11:D:36:TYR:N	2.44	0.49
28:W:542:ASN:OD1	28:W:545:ARG:NH1	2.44	0.49
32:a:371:LEU:HD22	33:b:347:ILE:HD11	1.93	0.49
32:a:1410:ASP:OD1	32:a:1410:ASP:N	2.44	0.49
33:b:449:ILE:HD13	33:b:465:MET:HB3	1.93	0.49
37:f:166:G:OP2	37:f:166:G:N2	2.44	0.49
48:y:1330:LEU:HB3	48:y:1355:ILE:HB	1.94	0.49
26:U:64:ARG:NH1	26:U:161:ARG:O	2.44	0.49
27:V:97:VAL:HB	27:V:107:GLN:HG3	1.93	0.49
32:a:302:ILE:O	33:b:936:LYS:NZ	2.46	0.49
32:a:809:VAL:HG22	32:a:1051:LEU:HD21	1.93	0.49
32:a:944:ASP:OD2	32:a:1435:GLY:N	2.45	0.49
46:w:192:ILE:HA	46:w:198:CYS:HA	1.94	0.49
20:N:520:ASP:N	20:N:520:ASP:OD1	2.45	0.49
32:a:449:LYS:HB3	32:a:604:MET:HE1	1.94	0.49
48:y:827:THR:HA	48:y:1136:GLN:HA	1.93	0.49
48:y:852:VAL:HA	48:y:1037:MET:O	2.13	0.49
48:y:1139:ALA:O	48:y:1161:GLN:NE2	2.45	0.49
5:5:19:LEU:HA	5:5:65:ILE:HA	1.95	0.49
10:C:1030:LYS:O	10:C:1034:ASN:ND2	2.45	0.49
21:O:215:GLY:O	23:Q:57:ARG:NH2	2.44	0.49
32:a:439:GLN:O	32:a:444:ARG:NH1	2.46	0.49
32:a:1427:ARG:HA	32:a:1430:LEU:HB2	1.93	0.49
33:b:666:VAL:HG22	33:b:787:VAL:HG22	1.94	0.49
33:b:764:ASP:OD1	33:b:764:ASP:N	2.45	0.49
48:y:430:GLU:OE1	48:y:593:ARG:NH1	2.44	0.49
2:2:23:LEU:HA	2:2:69:VAL:HA	1.94	0.49
8:A:507:SER:O	8:A:518:GLN:HA	2.13	0.49
20:N:629:GLN:NE2	30:Y:409:GLN:OE1	2.46	0.49
32:a:1363:GLN:HB3	32:a:1365:ILE:HG12	1.94	0.49
33:b:829:GLU:N	33:b:905:GLN:O	2.44	0.49
7:9:6:PRO:HA	7:9:36:PRO:HA	1.94	0.49
12:E:574:ALA:HA	12:E:578:TRP:HB2	1.95	0.49
21:O:392:PRO:HG3	21:O:415:ILE:HA	1.94	0.49
25:T:134:CYS:SG	25:T:135:THR:N	2.84	0.49
26:U:29:GLY:O	30:Y:195:ARG:NH2	2.45	0.49
26:U:158:LYS:O	26:U:161:ARG:NH1	2.46	0.49
32:a:543:ALA:HB2	32:a:651:TRP:HE3	1.78	0.49
32:a:1213:VAL:HG22	32:a:1229:PHE:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:1278:VAL:HG13	32:a:1284:LEU:HD22	1.95	0.49
32:a:1641:ARG:NH1	32:a:1650:ASP:OD1	2.45	0.49
48:y:456:ASN:O	48:y:1125:ARG:NH1	2.42	0.49
48:y:879:LEU:HB2	48:y:1037:MET:HE1	1.93	0.49
48:y:1117:GLN:OE1	48:y:1125:ARG:NH1	2.45	0.49
10:C:918:VAL:HG13	10:C:925:VAL:HG21	1.94	0.49
20:N:602:ILE:O	20:N:668:ARG:NH1	2.45	0.49
22:P:67:GLU:OE1	22:P:91:ARG:NH2	2.46	0.49
26:U:26:THR:OG1	26:U:159:ARG:NH2	2.45	0.49
29:X:239:ARG:NH2	35:d:60:C:OP1	2.45	0.49
32:a:184:ASP:OD1	32:a:184:ASP:N	2.43	0.49
48:y:715:ASN:HA	48:y:746:PRO:HB3	1.94	0.49
11:D:58:CYS:O	11:D:87:LYS:NZ	2.40	0.49
26:U:56:ARG:HD2	26:U:67:LYS:HD3	1.94	0.49
32:a:1075:GLN:HB2	32:a:1079:THR:HG21	1.94	0.49
3:j:22:THR:HA	3:j:68:ILE:HA	1.94	0.49
39:o:81:LEU:O	39:o:92:LEU:HA	2.12	0.49
48:y:260:LEU:O	48:y:266:THR:OG1	2.31	0.49
48:y:442:GLU:HG3	48:y:1107:MET:H	1.77	0.49
8:A:92:TYR:HA	8:A:99:PHE:HA	1.93	0.49
10:C:1020:LEU:HD23	10:C:1023:ILE:HD12	1.94	0.49
20:N:580:ASP:OD1	20:N:580:ASP:N	2.45	0.49
21:O:438:LEU:HB2	21:O:448:GLN:HB3	1.94	0.49
33:b:452:THR:HG22	33:b:577:PHE:HB3	1.95	0.49
39:o:311:VAL:HB	39:o:321:TYR:HB2	1.94	0.49
48:y:1333:ILE:HG12	48:y:1352:VAL:HG22	1.95	0.49
25:T:120:ARG:NH1	25:T:142:CYS:O	2.46	0.49
33:b:360:ALA:HB1	33:b:365:SER:HB2	1.95	0.49
33:b:755:ASP:OD1	33:b:755:ASP:N	2.46	0.49
2:h:62:VAL:HA	4:l:110:LEU:HA	1.95	0.49
3:j:20:CYS:HA	3:j:71:LEU:HA	1.95	0.49
48:y:1157:LEU:HD12	48:y:1158:PRO:HD2	1.94	0.49
17:J:400:HIS:HB3	17:J:402:LEU:HG	1.94	0.48
18:K:29:LEU:HD11	18:R:86:MET:HE1	1.94	0.48
26:U:196:GLN:NE2	26:U:207:ASP:OD1	2.45	0.48
30:Y:425:GLY:HA2	32:a:1451:ASN:HA	1.95	0.48
32:a:857:ASN:ND2	32:a:860:GLN:OE1	2.45	0.48
33:b:261:ASP:OD1	33:b:261:ASP:N	2.46	0.48
8:A:237:THR:HA	8:A:248:VAL:HA	1.94	0.48
21:O:200:ILE:HG12	33:b:80:ILE:HD12	1.93	0.48
32:a:1660:TYR:OH	32:a:1717:ASN:O	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:b:459:SER:O	33:b:462:GLY:N	2.46	0.48
2:h:73:ARG:HA	1:i:77:ILE:HA	1.95	0.48
48:y:510:MET:SD	48:y:510:MET:N	2.77	0.48
13:F:40:VAL:N	13:F:60:GLU:O	2.46	0.48
18:K:95:GLN:HB3	18:R:100:ARG:HH22	1.78	0.48
30:Y:407:TYR:HB3	30:Y:411:LEU:HD11	1.95	0.48
32:a:414:ARG:NH1	33:b:408:LEU:O	2.41	0.48
32:a:1418:ARG:HE	32:a:1464:LEU:HD23	1.77	0.48
48:y:1138:ARG:O	48:y:1298:ARG:NE	2.46	0.48
48:y:1275:LEU:HD22	48:y:1284:LEU:HD21	1.95	0.48
20:N:344:ARG:NH2	32:a:1068:PRO:O	2.47	0.48
20:N:835:SER:OG	20:N:932:CYS:SG	2.69	0.48
33:b:671:SER:O	41:q:54:ASN:N	2.46	0.48
33:b:938:ARG:NE	33:b:943:LEU:O	2.41	0.48
10:C:1026:ASN:O	10:C:1032:GLN:NE2	2.46	0.48
20:N:455:ARG:NH2	20:N:482:ARG:O	2.43	0.48
20:N:577:PHE:HB3	20:N:731:ALA:HA	1.94	0.48
26:U:63:MET:HE1	26:U:160:ASN:HB3	1.95	0.48
29:X:295:ALA:HA	29:X:298:ILE:HD12	1.94	0.48
32:a:1084:PRO:HA	32:a:1086:ARG:HH21	1.78	0.48
32:a:1385:VAL:HG21	32:a:1414:ARG:HD3	1.96	0.48
37:f:153:A:N6	37:f:179:C:N3	2.62	0.48
48:y:547:ASP:OD1	48:y:547:ASP:N	2.46	0.48
10:C:1167:TYR:HB3	12:E:582:PRO:HD3	1.95	0.48
12:E:558:ARG:NH1	31:Z:207:GLU:O	2.46	0.48
17:J:411:CYS:CB	17:J:431:HIS:ND1	2.71	0.48
18:R:15:PRO:HB2	18:R:55:ILE:HD12	1.94	0.48
26:U:123:ARG:O	26:U:127:ASN:ND2	2.44	0.48
27:V:44:ASN:HB3	27:V:52:GLN:HB3	1.94	0.48
29:X:344:GLN:HE22	35:d:93:G:H21	1.62	0.48
32:a:1241:HIS:HB2	32:a:1287:LEU:HD21	1.95	0.48
18:M:15:PRO:HG2	18:M:55:ILE:HB	1.95	0.48
20:N:716:LYS:HZ1	20:N:744:GLN:HA	1.78	0.48
21:O:224:ALA:HA	21:O:248:THR:HG23	1.96	0.48
23:Q:54:VAL:HG13	23:Q:59:PHE:HZ	1.77	0.48
26:U:67:LYS:NZ	35:d:25:C:O2	2.47	0.48
26:U:78:LYS:HE2	26:U:94:ILE:HG12	1.94	0.48
32:a:939:TRP:HA	32:a:1071:PHE:HD1	1.79	0.48
32:a:1607:GLU:HG3	32:a:1634:SER:HA	1.96	0.48
28:W:609:GLN:HA	28:W:612:PHE:HB2	1.96	0.48
32:a:163:ARG:HG3	32:a:625:PRO:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:981:PHE:O	32:a:1166:THR:OG1	2.31	0.48
34:c:835:SER:O	34:c:839:GLY:N	2.46	0.48
10:C:897:LEU:HD11	10:C:932:ILE:HG12	1.96	0.48
10:C:1166:ILE:O	10:C:1170:THR:OG1	2.29	0.48
11:D:31:VAL:HG23	11:D:32:ILE:HG12	1.96	0.48
33:b:588:ILE:O	33:b:630:LEU:HA	2.14	0.48
2:h:64:ILE:HA	4:l:108:VAL:HA	1.96	0.48
20:N:897:TRP:O	20:N:901:ASN:ND2	2.40	0.48
20:N:951:THR:HA	20:N:985:LEU:HA	1.96	0.48
24:S:173:THR:O	24:S:177:LYS:NZ	2.45	0.48
26:U:83:THR:O	38:g:18:A:O2'	2.31	0.48
32:a:1034:LEU:HB2	32:a:1037:ALA:HB2	1.95	0.48
32:a:1057:ARG:NH1	32:a:1060:GLU:OE1	2.41	0.48
32:a:1631:LEU:HB2	32:a:1660:TYR:HB3	1.96	0.48
33:b:350:ASN:O	33:b:354:ARG:N	2.46	0.48
33:b:918:ILE:HD12	33:b:932:GLU:HB2	1.96	0.48
39:o:346:SER:OG	39:o:348:ASP:OD1	2.30	0.48
43:s:12:ASN:O	43:s:79:MET:HA	2.14	0.48
48:y:1145:ASN:O	48:y:1322:GLN:NE2	2.47	0.48
10:C:1223:SER:HB3	10:C:1226:VAL:HG12	1.95	0.47
20:N:500:MET:SD	20:N:500:MET:N	2.87	0.47
49:z:623:VAL:O	49:z:626:ALA:N	2.47	0.47
15:H:221:PRO:O	15:H:227:SER:N	2.47	0.47
23:Q:192:VAL:O	45:u:199:ASN:ND2	2.46	0.47
32:a:422:LEU:O	32:a:635:ARG:NE	2.44	0.47
32:a:1610:GLN:HB2	32:a:1630:LEU:HB3	1.96	0.47
33:b:221:ILE:O	33:b:495:ARG:NH1	2.46	0.47
33:b:458:ASP:OD1	33:b:458:ASP:N	2.44	0.47
46:w:60:ALA:H	46:w:69:GLU:HA	1.78	0.47
48:y:600:MET:HE2	48:y:625:PHE:HE1	1.80	0.47
10:C:1109:ARG:NH2	38:g:142:U:OP1	2.47	0.47
11:D:11:CYS:HB2	11:D:85:CYS:HB3	1.95	0.47
30:Y:215:ASN:HB3	32:a:664:HIS:HD2	1.79	0.47
32:a:1074:PHE:HD2	32:a:1080:GLU:HG2	1.79	0.47
32:a:2129:TYR:HA	32:a:2175:LEU:H	1.79	0.47
33:b:261:ASP:OD2	33:b:313:GLN:NE2	2.45	0.47
36:e:39:C:O2'	36:e:41:U:OP2	2.29	0.47
45:u:75:THR:HA	45:u:83:LEU:H	1.79	0.47
16:I:23:ASN:OD1	16:I:26:ARG:NH2	2.46	0.47
18:K:100:ARG:NH2	18:R:95:GLN:OE1	2.46	0.47
20:N:325:GLU:HA	20:N:328:ARG:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Q:195:LYS:NZ	45:u:197:LEU:O	2.43	0.47
32:a:164:MET:SD	32:a:164:MET:N	2.88	0.47
32:a:315:ALA:O	33:b:177:ARG:NH2	2.48	0.47
48:y:749:ILE:HG23	48:y:779:VAL:HG22	1.97	0.47
49:z:151:LEU:HD12	49:z:154:ARG:HE	1.80	0.47
20:N:430:THR:HG21	20:N:464:ARG:HE	1.79	0.47
21:O:471:ASP:N	21:O:471:ASP:OD1	2.44	0.47
21:O:493:ASP:OD1	21:O:493:ASP:N	2.43	0.47
22:P:49:ARG:HG3	22:P:54:LEU:HD13	1.97	0.47
32:a:452:LYS:NZ	36:e:48:A:OP1	2.42	0.47
35:d:30:A:N6	38:g:15:U:O2	2.48	0.47
48:y:682:VAL:HG12	48:y:1077:LEU:HD22	1.95	0.47
12:E:531:THR:HG22	12:E:570:LYS:HG2	1.97	0.47
20:N:273:LYS:HD3	20:N:273:LYS:HA	1.77	0.47
32:a:76:MET:HG2	32:a:506:LEU:HD21	1.97	0.47
32:a:597:LYS:NZ	36:e:29:A:OP1	2.48	0.47
33:b:684:LYS:O	33:b:795:VAL:N	2.47	0.47
12:E:560:LYS:NZ	35:d:43:A:N7	2.63	0.47
12:E:569:GLN:HA	12:E:572:HIS:HB3	1.96	0.47
20:N:716:LYS:NZ	20:N:743:TYR:O	2.48	0.47
22:P:50:TRP:HA	22:P:54:LEU:HB2	1.95	0.47
22:P:766:ARG:HH22	18:v:116:VAL:HG13	1.80	0.47
32:a:675:GLN:NE2	35:d:56:A:OP1	2.48	0.47
32:a:1163:ARG:NH1	33:b:61:GLU:OE1	2.48	0.47
32:a:1410:ASP:O	32:a:1414:ARG:NH1	2.46	0.47
2:h:27:MET:HA	2:h:50:TYR:O	2.15	0.47
48:y:543:LEU:HD12	48:y:623:ARG:HG3	1.96	0.47
48:y:934:TYR:HB3	49:z:104:VAL:HG13	1.96	0.47
20:N:423:GLU:HB3	20:N:574:GLY:HA3	1.96	0.47
21:O:305:THR:O	21:O:312:ALA:HA	2.15	0.47
21:O:399:LYS:NZ	21:O:400:PHE:O	2.48	0.47
32:a:723:ASN:ND2	45:u:253:THR:OG1	2.41	0.47
33:b:618:THR:HB	33:b:630:LEU:HB2	1.97	0.47
8:A:802:THR:HA	8:A:863:ALA:O	2.15	0.47
20:N:525:ARG:HD2	20:N:525:ARG:HA	1.77	0.47
30:Y:90:VAL:HG22	30:Y:96:ILE:H	1.80	0.47
32:a:390:ASP:OD1	32:a:390:ASP:N	2.44	0.47
33:b:514:TYR:HD2	33:b:521:ASP:HB2	1.78	0.47
1:i:45:GLY:HA3	1:i:61:ALA:HA	1.96	0.47
39:o:209:ILE:HG21	39:o:250:LEU:HD22	1.97	0.47
18:v:20:VAL:O	18:v:43:ASN:ND2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:y:177:GLY:HA2	48:y:220:ARG:HE	1.80	0.47
48:y:458:GLN:NE2	48:y:693:GLY:O	2.48	0.47
6:8:41:ILE:HA	6:8:71:LEU:HA	1.97	0.47
32:a:155:LYS:HE2	32:a:626:GLY:H	1.79	0.47
32:a:344:ASP:OD1	32:a:344:ASP:N	2.47	0.47
32:a:889:ARG:NH2	32:a:1004:ASN:O	2.48	0.47
32:a:1087:LEU:HB2	32:a:1098:PHE:HB3	1.96	0.47
39:o:133:VAL:HG21	39:o:169:THR:HG21	1.96	0.47
48:y:1200:ASN:HB3	48:y:1203:GLU:HB3	1.97	0.47
16:I:143:GLU:O	16:I:146:MET:N	2.48	0.46
49:z:114:LEU:HD23	49:z:151:LEU:HD22	1.97	0.46
8:A:20:GLY:O	8:A:28:GLN:HA	2.16	0.46
18:M:19:PRO:HG3	18:M:51:GLN:HB3	1.97	0.46
20:N:654:ASP:N	20:N:654:ASP:OD1	2.47	0.46
24:S:170:MET:HA	24:S:173:THR:HG22	1.97	0.46
25:T:112:ASN:OD1	32:a:480:LYS:NZ	2.43	0.46
28:W:526:GLU:HG3	28:W:560:LEU:HD22	1.95	0.46
45:u:368:MET:N	45:u:395:THR:O	2.46	0.46
1:I:86:LEU:HA	7:9:62:ILE:HA	1.98	0.46
10:C:1120:ALA:HA	10:C:1128:VAL:HG21	1.97	0.46
22:P:773:ASP:HA	22:P:776:ARG:HE	1.79	0.46
26:U:148:LEU:HD13	26:U:151:ALA:HB3	1.98	0.46
27:V:199:ASP:HA	30:Y:315:LYS:HE3	1.95	0.46
20:N:298:TYR:HB2	32:a:818:GLU:HA	1.98	0.46
20:N:716:LYS:N	20:N:748:GLU:O	2.48	0.46
21:O:226:ARG:NH1	21:O:245:HIS:O	2.45	0.46
22:P:20:LYS:HG3	22:P:54:LEU:HD23	1.98	0.46
26:U:182:ARG:NH1	26:U:184:GLU:OE2	2.47	0.46
48:y:266:THR:O	48:y:270:PHE:HB2	2.15	0.46
48:y:1059:ILE:HB	48:y:1091:TRP:HD1	1.80	0.46
23:Q:51:PRO:HA	23:Q:54:VAL:HB	1.98	0.46
25:T:109:ARG:NH1	32:a:56:ALA:O	2.48	0.46
32:a:199:GLU:O	32:a:240:ARG:NH2	2.49	0.46
32:a:983:LYS:HD2	32:a:987:LYS:HE2	1.96	0.46
32:a:1109:LEU:HD11	32:a:1156:ASP:HB2	1.97	0.46
48:y:700:ALA:HB1	48:y:818:LEU:HB3	1.98	0.46
48:y:852:VAL:HB	48:y:1061:MET:HG3	1.98	0.46
21:O:237:LYS:HA	33:b:82:GLN:HG2	1.98	0.46
21:O:353:THR:HA	21:O:368:LEU:O	2.15	0.46
39:o:181:ILE:HG13	39:o:182:ARG:HD3	1.97	0.46
49:z:49:PRO:HG2	49:z:53:LEU:HD13	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:z:361:HIS:HA	49:z:364:VAL:HG22	1.97	0.46
32:a:313:LYS:O	32:a:321:ASN:ND2	2.49	0.46
33:b:645:ARG:NH2	33:b:653:ILE:O	2.48	0.46
37:f:152:G:N2	37:f:153:A:N7	2.63	0.46
6:n:34:PHE:HA	6:n:40:LEU:HA	1.98	0.46
46:w:148:ILE:HA	46:w:292:VAL:HA	1.97	0.46
48:y:370:GLY:O	48:y:400:LYS:NZ	2.46	0.46
20:N:329:TRP:HZ3	32:a:1422:LEU:HA	1.79	0.46
21:O:332:ALA:O	21:O:350:HIS:ND1	2.48	0.46
22:P:211:ASN:ND2	29:X:221:ASN:O	2.49	0.46
30:Y:101:ILE:O	30:Y:104:GLN:NE2	2.49	0.46
32:a:1318:THR:O	32:a:1326:GLY:N	2.48	0.46
20:N:408:LEU:HD21	20:N:432:ILE:HG12	1.98	0.46
32:a:759:GLU:OE2	32:a:763:ARG:NH1	2.49	0.46
32:a:1231:ARG:NH1	32:a:1280:ASN:O	2.49	0.46
39:o:69:VAL:HA	39:o:85:GLY:HA3	1.97	0.46
45:u:118:ALA:HA	45:u:125:VAL:HA	1.97	0.46
48:y:787:ARG:O	48:y:793:ASN:ND2	2.49	0.46
10:C:1224:PRO:HA	10:C:1227:ILE:HG22	1.98	0.46
20:N:782:ASP:N	20:N:782:ASP:OD1	2.46	0.46
32:a:823:SER:OG	32:a:933:ARG:NH1	2.49	0.46
33:b:703:GLU:O	33:b:706:GLN:NE2	2.49	0.46
2:h:48:GLU:HA	2:h:58:HIS:HA	1.98	0.46
45:u:246:VAL:HG21	45:u:261:HIS:HA	1.98	0.46
46:w:143:TYR:HA	46:w:157:GLN:HA	1.97	0.46
8:A:325:ILE:H	8:A:375:SER:H	1.63	0.45
23:Q:213:ASP:OD2	23:Q:216:ARG:NH1	2.48	0.45
25:T:58:ARG:NH2	25:T:98:GLU:O	2.39	0.45
32:a:195:LEU:HB2	32:a:204:LEU:HD12	1.99	0.45
32:a:1012:LYS:HG2	32:a:1036:PHE:HZ	1.81	0.45
32:a:1016:VAL:HA	32:a:1025:THR:HA	1.97	0.45
32:a:1083:HIS:O	32:a:1086:ARG:NE	2.49	0.45
32:a:1424:GLN:H	32:a:1427:ARG:HD3	1.79	0.45
35:d:55:C:OP2	35:d:74:U:O2'	2.31	0.45
48:y:809:ALA:HB1	48:y:821:VAL:HG22	1.98	0.45
49:z:150:PRO:HA	49:z:153:LEU:HG	1.98	0.45
12:E:682:LEU:HA	12:E:687:PHE:HA	1.96	0.45
22:P:31:TRP:HB3	22:P:43:ALA:HB1	1.99	0.45
32:a:136:ILE:HG22	32:a:138:PRO:HD2	1.98	0.45
32:a:513:LEU:HB3	32:a:516:LEU:HD13	1.97	0.45
32:a:1195:ARG:HB3	32:a:1229:PHE:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:1614:ILE:HD12	32:a:1618:LYS:HB3	1.99	0.45
33:b:106:GLU:HB2	33:b:537:TYR:HB3	1.98	0.45
33:b:225:VAL:HB	33:b:253:VAL:HG22	1.97	0.45
39:o:208:ILE:O	39:o:219:VAL:HA	2.16	0.45
48:y:432:ILE:HB	48:y:438:ILE:HD11	1.97	0.45
8:A:670:GLN:HA	8:A:698:PRO:HA	1.97	0.45
20:N:273:LYS:HA	20:N:276:VAL:HG12	1.98	0.45
20:N:674:THR:OG1	38:g:153:C:O2'	2.30	0.45
20:N:981:PRO:HG2	20:N:984:LEU:HB3	1.98	0.45
21:O:303:LEU:O	21:O:314:ILE:HA	2.17	0.45
26:U:97:ARG:HH11	26:U:101:LEU:HD12	1.81	0.45
27:V:224:LEU:HD13	27:V:230:LEU:HD12	1.97	0.45
32:a:428:LYS:O	32:a:432:ARG:HB2	2.16	0.45
32:a:974:ASN:HB2	32:a:1178:TYR:HB3	1.98	0.45
32:a:2130:GLY:HA3	32:a:2142:ILE:HA	1.98	0.45
37:f:19:G:OP1	37:f:19:G:N2	2.48	0.45
39:o:231:MET:HE1	39:o:250:LEU:HD21	1.98	0.45
48:y:1169:ALA:HB2	48:y:1344:ASN:HA	1.99	0.45
45:u:283:ARG:HA	45:u:292:ASN:HA	1.97	0.45
10:C:1212:LEU:HA	10:C:1215:VAL:HB	1.98	0.45
20:N:827:MET:HE1	20:N:943:ILE:HA	1.98	0.45
26:U:46:LYS:HB2	26:U:70:VAL:HG12	1.98	0.45
26:U:48:CYS:SG	26:U:50:ARG:NH1	2.89	0.45
29:X:365:ILE:HG12	29:X:368:ARG:HH21	1.81	0.45
30:Y:302:ALA:HB1	32:a:814:VAL:HG11	1.98	0.45
32:a:522:PHE:HB2	32:a:552:ARG:HB2	1.99	0.45
32:a:1633:ALA:O	32:a:1658:GLN:NE2	2.45	0.45
7:m:21:LEU:HA	7:m:67:ILE:HA	1.98	0.45
21:O:194:TRP:NE1	21:O:491:GLU:OE2	2.49	0.45
23:Q:195:LYS:NZ	45:u:194:SER:O	2.50	0.45
32:a:101:LYS:HE2	32:a:473:PHE:HE2	1.82	0.45
2:h:33:LEU:HA	2:h:44:LEU:HA	1.99	0.45
8:A:144:LEU:HA	8:A:154:ILE:HA	1.98	0.45
20:N:796:LEU:HB3	20:N:802:LEU:HG	1.98	0.45
22:P:713:MET:HE3	24:S:124:LEU:HD12	1.98	0.45
24:S:126:LEU:O	24:S:130:HIS:ND1	2.50	0.45
30:Y:91:ASP:OD1	30:Y:91:ASP:N	2.46	0.45
32:a:791:GLN:HE22	32:a:1028:TYR:HB3	1.80	0.45
32:a:998:ARG:NH2	32:a:1007:ASP:OD1	2.48	0.45
32:a:1618:LYS:HG2	32:a:1621:LYS:HE2	1.97	0.45
48:y:71:GLN:HG3	48:y:1314:PHE:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:99:MET:HA	5:5:69:ILE:HA	1.99	0.45
8:A:345:GLY:HA2	8:A:361:ILE:H	1.81	0.45
8:A:613:THR:HA	8:A:632:ALA:HA	1.98	0.45
10:C:978:LEU:HA	10:C:981:TYR:HB2	1.97	0.45
20:N:606:GLN:HA	20:N:607:PRO:HD3	1.83	0.45
31:Z:206:LYS:HG2	31:Z:223:ARG:HA	1.98	0.45
32:a:1640:SER:O	32:a:1717:ASN:ND2	2.46	0.45
33:b:471:ASP:OD1	33:b:471:ASP:N	2.44	0.45
48:y:514:ILE:HA	48:y:541:ILE:HG22	1.98	0.45
18:K:90:PHE:HD2	24:S:111:MET:HE2	1.81	0.45
35:d:73:A:OP1	35:d:75:G:O2'	2.34	0.45
37:f:55:U:O2'	37:f:57:A:N7	2.48	0.45
39:o:169:THR:OG1	39:o:179:TRP:NE1	2.47	0.45
47:x:536:ASP:O	47:x:540:THR:N	2.49	0.45
8:A:41:LEU:HA	8:A:53:LEU:H	1.80	0.45
10:C:1130:PRO:HG3	12:E:528:ILE:HG12	1.99	0.45
11:D:39:PRO:HA	11:D:72:CYS:HA	1.98	0.45
21:O:214:PRO:HG2	21:O:256:THR:HA	1.99	0.45
21:O:402:ASP:O	30:Y:113:TYR:OH	2.34	0.45
32:a:593:ARG:HH22	32:a:1551:PHE:HB3	1.81	0.45
2:2:62:VAL:HA	4:4:110:LEU:HA	1.99	0.44
8:A:84:SER:HA	8:A:110:SER:HA	1.99	0.44
20:N:426:SER:OG	20:N:428:LYS:NZ	2.43	0.44
22:P:781:GLU:HA	22:P:784:LEU:HB2	1.99	0.44
27:V:20:GLU:HB3	27:V:83:VAL:HG21	1.98	0.44
32:a:1318:THR:O	32:a:1325:LEU:N	2.50	0.44
33:b:473:PRO:O	33:b:498:SER:OG	2.29	0.44
3:j:63:ILE:HA	7:m:69:MET:HA	1.98	0.44
48:y:182:ARG:HH22	48:y:275:ASP:HB3	1.80	0.44
48:y:517:PHE:HB2	48:y:539:VAL:HG23	1.98	0.44
22:P:749:LEU:HD11	24:S:156:LEU:HD22	2.00	0.44
26:U:20:PHE:O	26:U:72:GLN:NE2	2.51	0.44
32:a:796:LYS:HE2	32:a:796:LYS:HB3	1.80	0.44
32:a:1640:SER:HB3	32:a:1652:MET:HA	1.98	0.44
2:h:63:LEU:N	4:l:109:VAL:O	2.43	0.44
39:o:161:ARG:HG2	39:o:162:ARG:HG3	1.99	0.44
41:q:7:LEU:HD12	41:q:8:PRO:HD2	1.99	0.44
46:w:156:ILE:HA	46:w:271:GLY:HA3	1.98	0.44
48:y:495:TRP:NE1	48:y:575:THR:O	2.48	0.44
8:A:428:GLY:HA3	8:A:433:SER:HA	1.99	0.44
8:A:642:ILE:HA	8:A:665:LEU:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:808:THR:HA	8:A:863:ALA:HB2	1.99	0.44
16:I:59:CYS:SG	16:I:72:HIS:HE1	2.32	0.44
20:N:561:SER:HA	20:N:567:ALA:HB3	1.98	0.44
21:O:428:VAL:HG11	21:O:477:LEU:HD21	2.00	0.44
26:U:169:VAL:HG22	26:U:186:PRO:HD3	1.98	0.44
28:W:554:LEU:HD22	28:W:560:LEU:HG	1.99	0.44
32:a:1502:PHE:HB3	32:a:1754:TYR:HD2	1.81	0.44
33:b:735:PHE:HA	33:b:743:ASN:O	2.18	0.44
40:p:99:ALA:HA	40:p:128:ILE:HA	1.99	0.44
13:F:14:THR:HA	13:F:60:GLU:HA	1.99	0.44
20:N:1005:SER:HA	20:N:1008:LEU:HB3	2.00	0.44
28:W:621:PRO:HB2	28:W:625:ARG:HH21	1.82	0.44
32:a:570:ASP:HB3	32:a:573:GLN:HG3	1.99	0.44
35:d:58:G:O6	35:d:76:A:N6	2.49	0.44
48:y:350:ASP:OD1	48:y:350:ASP:N	2.45	0.44
48:y:474:ARG:O	48:y:478:THR:OG1	2.30	0.44
48:y:964:VAL:O	48:y:968:PHE:HB2	2.17	0.44
11:D:25:LYS:NZ	38:g:147:C:OP1	2.45	0.44
20:N:480:SER:HA	20:N:485:ASP:HA	1.98	0.44
20:N:691:ASP:OD2	20:N:736:ARG:NH1	2.49	0.44
20:N:826:LYS:HA	20:N:829:LEU:HB2	1.98	0.44
25:T:80:LYS:HA	25:T:80:LYS:HD3	1.79	0.44
26:U:11:ASN:HB3	30:Y:218:ILE:HG13	2.00	0.44
29:X:263:SER:OG	29:X:267:ARG:NH1	2.51	0.44
32:a:761:ILE:O	32:a:1245:ARG:NH2	2.50	0.44
32:a:1310:ARG:HH22	32:a:1563:HIS:HB2	1.82	0.44
39:o:202:ASN:ND2	39:o:204:THR:OG1	2.51	0.44
48:y:72:TYR:HE2	48:y:93:SER:HB3	1.82	0.44
8:A:337:ALA:N	8:A:350:ALA:O	2.50	0.44
10:C:1053:ARG:HA	10:C:1056:MET:HE2	1.99	0.44
22:P:65:ARG:HE	22:P:69:GLU:HG3	1.83	0.44
28:W:616:LEU:HG	28:W:643:LEU:HD11	2.00	0.44
32:a:136:ILE:HG12	32:a:418:THR:HG22	2.00	0.44
32:a:1275:ARG:NH1	32:a:1378:GLU:OE2	2.50	0.44
32:a:2152:GLY:HA2	32:a:2157:VAL:HA	2.00	0.44
33:b:384:VAL:HG11	33:b:416:LEU:HD12	2.00	0.44
36:e:105:U:H1'	36:e:109:G:H22	1.83	0.44
2:h:35:SER:O	2:h:43:GLN:N	2.50	0.44
39:o:94:ASN:HB3	39:o:99:CYS:HA	1.99	0.44
48:y:810:ILE:HG12	48:y:836:ILE:HG13	2.00	0.44
8:A:784:THR:O	8:A:802:THR:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:595:GLU:O	10:C:599:ASN:ND2	2.47	0.44
25:T:13:ASP:OD1	25:T:13:ASP:N	2.47	0.44
32:a:720:TRP:HD1	45:u:251:THR:HA	1.83	0.44
44:t:159:TYR:HA	49:z:171:ARG:HG2	1.99	0.44
47:x:421:VAL:HA	47:x:437:SER:HA	1.99	0.44
20:N:725:ARG:HH11	20:N:728:ARG:HH22	1.64	0.44
26:U:11:ASN:OD1	26:U:119:GLN:NE2	2.48	0.44
32:a:1442:PHE:HA	32:a:1445:TYR:HD2	1.83	0.44
39:o:171:SER:OG	39:o:175:THR:OG1	2.36	0.44
39:o:213:ILE:HA	39:o:237:SER:HA	1.99	0.44
48:y:114:LYS:HE3	48:y:114:LYS:HB2	1.83	0.44
49:z:123:GLN:OE1	49:z:125:ARG:NH1	2.51	0.44
18:K:2:SER:O	18:K:2:SER:OG	2.35	0.44
18:M:99:THR:HA	18:M:102:GLU:HB2	1.99	0.44
21:O:455:GLN:N	21:O:483:ASP:OD2	2.51	0.44
22:P:65:ARG:HH21	22:P:69:GLU:HG3	1.82	0.44
26:U:156:TYR:CZ	26:U:158:LYS:HB2	2.53	0.44
32:a:353:ASP:HB3	32:a:356:ILE:HG13	2.00	0.44
32:a:1169:GLN:OE1	32:a:1172:ASN:ND2	2.51	0.44
32:a:1434:LYS:O	32:a:1439:ARG:NH1	2.51	0.44
32:a:1436:TRP:HA	32:a:1439:ARG:HB2	1.99	0.44
32:a:1820:LYS:HA	32:a:1914:MET:HA	2.00	0.44
33:b:594:PRO:HB3	33:b:603:MET:HG2	2.00	0.44
4:l:44:ILE:HA	4:l:109:VAL:HA	1.99	0.44
48:y:347:GLU:HG3	48:y:372:LEU:HD12	2.00	0.44
48:y:472:LEU:HD13	48:y:1115:MET:HB3	1.99	0.44
20:N:519:VAL:HB	20:N:550:VAL:HA	1.99	0.43
22:P:50:TRP:O	22:P:55:ASP:N	2.51	0.43
33:b:264:ILE:HG21	33:b:381:LEU:HD12	2.00	0.43
33:b:854:ARG:NH1	33:b:879:ASP:OD2	2.51	0.43
36:e:12:U:H3	36:e:65:G:H1	1.65	0.43
48:y:1134:ASP:O	48:y:1155:GLY:N	2.52	0.43
11:D:15:ALA:HB1	11:D:44:ARG:HB2	2.00	0.43
32:a:1094:ARG:HB3	32:a:1096:HIS:CE1	2.53	0.43
33:b:886:ASP:O	33:b:890:HIS:ND1	2.42	0.43
4:l:56:VAL:HA	4:l:67:LEU:HA	1.99	0.43
39:o:301:ALA:HB1	39:o:333:VAL:HG12	2.00	0.43
20:N:611:ILE:HA	20:N:688:TYR:O	2.18	0.43
27:V:199:ASP:OD1	27:V:199:ASP:N	2.50	0.43
32:a:1362:ASP:N	32:a:1362:ASP:OD1	2.46	0.43
32:a:2180:THR:HA	32:a:2216:CYS:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:b:736:GLY:HA2	33:b:743:ASN:HB2	2.01	0.43
33:b:836:VAL:HB	33:b:871:ILE:HB	1.99	0.43
3:j:47:THR:HA	3:j:56:ALA:O	2.19	0.43
45:u:105:VAL:HA	45:u:143:ASP:HA	2.00	0.43
10:C:1110:VAL:HG11	38:g:144:A:H5''	1.99	0.43
20:N:396:ARG:NH2	20:N:468:GLU:O	2.51	0.43
20:N:541:ARG:HA	20:N:541:ARG:HD3	1.79	0.43
20:N:653:SER:OG	30:Y:389:SER:OG	2.32	0.43
33:b:678:THR:OG1	33:b:680:ASN:O	2.33	0.43
35:d:69:A:O2'	36:e:42:U:O3'	2.36	0.43
32:a:246:LEU:HD22	32:a:408:PRO:HG2	2.00	0.43
32:a:758:ARG:HA	32:a:758:ARG:HD2	1.83	0.43
32:a:929:GLU:OE1	32:a:933:ARG:NE	2.51	0.43
34:c:1404:LYS:O	34:c:1423:ASN:N	2.51	0.43
8:A:213:LEU:HA	8:A:220:VAL:HA	2.00	0.43
20:N:613:VAL:HG22	20:N:690:LEU:HB2	2.01	0.43
21:O:187:LYS:HA	21:O:187:LYS:HD3	1.86	0.43
22:P:700:ARG:NH2	24:S:89:LEU:O	2.52	0.43
29:X:275:ASN:OD1	29:X:278:LEU:N	2.51	0.43
34:c:1563:VAL:O	34:c:1648:ARG:N	2.51	0.43
39:o:173:ASP:OD1	39:o:173:ASP:N	2.51	0.43
18:v:91:THR:HA	18:v:94:GLN:HG2	2.01	0.43
48:y:824:PRO:HG2	48:y:1154:LEU:HD13	2.01	0.43
8:A:886:GLU:HA	8:A:910:ALA:O	2.18	0.43
11:D:59:VAL:HG12	11:D:87:LYS:HD2	2.00	0.43
12:E:461:THR:HG23	12:E:464:GLU:H	1.83	0.43
26:U:123:ARG:HH22	30:Y:222:PRO:HD2	1.84	0.43
32:a:414:ARG:HH22	33:b:409:LYS:HA	1.83	0.43
32:a:1645:LEU:HB2	32:a:1714:ALA:HB3	2.00	0.43
33:b:103:THR:OG1	33:b:104:LEU:N	2.50	0.43
33:b:493:PHE:HB2	33:b:551:LEU:HD23	2.01	0.43
34:c:1201:GLU:HA	34:c:1253:THR:HA	2.00	0.43
40:p:99:ALA:HA	40:p:129:PHE:H	1.84	0.43
44:t:170:ILE:HG22	49:z:163:GLU:HB3	2.01	0.43
48:y:850:LEU:HD23	48:y:1059:ILE:HG23	2.01	0.43
2:2:45:ALA:HA	2:2:61:GLU:HA	1.99	0.43
21:O:223:SER:OG	21:O:224:ALA:N	2.50	0.43
22:P:78:MET:HA	22:P:79:PRO:HD3	1.83	0.43
33:b:480:LYS:HA	33:b:480:LYS:HD2	1.80	0.43
43:s:156:ASN:HA	43:s:189:ILE:HA	2.01	0.43
16:I:56:CYS:O	16:I:60:LEU:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:O:337:ARG:HA	21:O:337:ARG:HD3	1.80	0.43
26:U:159:ARG:HD2	38:g:19:G:H5''	2.00	0.43
33:b:346:ASP:HA	33:b:367:ARG:HG2	2.01	0.43
39:o:150:HIS:NE2	39:o:169:THR:OG1	2.38	0.43
48:y:520:VAL:HG21	48:y:626:ARG:HH21	1.83	0.43
18:M:100:ARG:HD2	18:M:100:ARG:HA	1.90	0.43
20:N:708:SER:HB2	20:N:991:LEU:HD23	2.00	0.43
21:O:337:ARG:HB2	21:O:346:ILE:HB	2.01	0.43
28:W:494:LEU:HD12	28:W:547:VAL:HG22	2.01	0.43
32:a:641:MET:HA	32:a:644:ILE:HG22	2.00	0.43
32:a:641:MET:O	32:a:645:THR:OG1	2.32	0.43
32:a:1485:LEU:HD22	32:a:1490:PHE:HB2	2.01	0.43
33:b:836:VAL:O	33:b:870:THR:HA	2.18	0.43
37:f:167:U:O2'	37:f:169:C:OP2	2.36	0.43
48:y:50:TYR:OH	48:y:142:GLU:OE1	2.35	0.43
48:y:167:GLN:O	48:y:171:SER:HB3	2.19	0.43
27:V:235:ILE:HG22	38:g:164:A:H61	1.84	0.42
32:a:105:ASN:OD1	32:a:114:ARG:NH1	2.52	0.42
33:b:177:ARG:HA	33:b:177:ARG:HD3	1.88	0.42
33:b:631:GLY:HA3	33:b:637:LEU:HD21	2.00	0.42
36:e:97:G:O2'	1:i:36:TYR:O	2.29	0.42
38:g:1:G:N2	38:g:2:U:O2	2.50	0.42
48:y:48:ASP:HA	48:y:51:GLU:HG2	2.00	0.42
49:z:49:PRO:HD2	49:z:53:LEU:HD22	2.00	0.42
25:T:36:PRO:O	25:T:40:LYS:NZ	2.43	0.42
32:a:1536:LEU:HD21	32:a:1576:ILE:HD11	2.00	0.42
39:o:262:TRP:HE3	39:o:272:ARG:HB2	1.85	0.42
46:w:57:ALA:HB1	49:z:109:MET:HE1	2.01	0.42
5:5:29:ILE:HA	5:5:40:LEU:HA	2.01	0.42
10:C:1071:LYS:HA	10:C:1074:ARG:HE	1.84	0.42
14:G:180:GLY:O	20:N:756:GLN:NE2	2.46	0.42
18:K:121:THR:HA	18:K:124:VAL:HB	2.02	0.42
18:M:17:VAL:HG23	18:M:55:ILE:HD11	2.01	0.42
20:N:451:THR:O	20:N:452:GLN:NE2	2.52	0.42
21:O:395:ILE:HB	21:O:409:LEU:HB2	2.01	0.42
25:T:15:TRP:NE1	25:T:19:GLU:OE1	2.52	0.42
32:a:945:THR:OG1	32:a:946:GLU:OE1	2.35	0.42
39:o:261:VAL:HB	39:o:275:LYS:HB2	2.01	0.42
44:t:185:LEU:HD23	44:t:188:LYS:HD3	2.01	0.42
48:y:464:ASP:OD2	48:y:468:ARG:NH2	2.46	0.42
48:y:602:ASP:HB2	48:y:606:ARG:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:723:TYR:O	8:A:729:PHE:HA	2.19	0.42
10:C:1227:ILE:HD12	10:C:1227:ILE:HA	1.95	0.42
12:E:567:ASP:OD1	12:E:567:ASP:N	2.52	0.42
18:K:10:GLU:OE1	18:v:70:SER:N	2.52	0.42
32:a:224:THR:HG23	36:e:12:U:H5''	2.01	0.42
32:a:610:HIS:NE2	51:a:3001:IHP:O24	2.43	0.42
32:a:1328:LEU:HD23	32:a:1368:LEU:HD22	2.01	0.42
44:t:175:GLN:OE1	44:t:179:LYS:NZ	2.46	0.42
20:N:940:ARG:HG2	20:N:1001:LEU:HD11	2.01	0.42
22:P:76:LYS:O	30:Y:296:TYR:OH	2.36	0.42
23:Q:182:PHE:HB3	23:Q:183:LYS:H	1.69	0.42
23:Q:218:GLU:HA	23:Q:221:LYS:HD2	2.01	0.42
28:W:606:GLU:HA	28:W:609:GLN:HG2	2.00	0.42
32:a:599:MET:HA	32:a:602:ILE:HB	2.00	0.42
33:b:481:MET:HG2	33:b:492:ALA:HA	2.00	0.42
33:b:508:LYS:HD2	33:b:522:SER:HB2	2.02	0.42
40:p:56:ILE:N	40:p:151:ASP:O	2.49	0.42
49:z:187:LEU:HD22	49:z:192:ARG:HB3	2.02	0.42
20:N:688:TYR:HA	20:N:733:LYS:HB2	2.02	0.42
20:N:784:PRO:HG2	20:N:789:LEU:HD11	2.01	0.42
22:P:752:PHE:HA	22:P:755:LEU:HB2	2.02	0.42
22:P:764:PRO:HA	22:P:767:LEU:HB2	2.01	0.42
23:Q:38:HIS:ND1	36:e:52:U:O2'	2.51	0.42
23:Q:224:MET:O	23:Q:228:ILE:HB	2.19	0.42
27:V:88:HIS:HA	27:V:93:THR:HG21	2.00	0.42
27:V:236:LYS:HA	27:V:236:LYS:HD3	1.80	0.42
33:b:924:GLN:HB3	33:b:928:HIS:HB2	2.01	0.42
39:o:127:ALA:HB2	39:o:157:CYS:HB3	2.01	0.42
4:4:66:VAL:HA	4:4:100:PHE:HA	2.01	0.42
8:A:678:VAL:H	8:A:684:GLY:HA3	1.85	0.42
18:M:121:THR:HA	18:M:124:VAL:HG22	2.00	0.42
20:N:539:VAL:HG13	20:N:543:ARG:HD3	2.01	0.42
21:O:270:VAL:HG21	21:O:305:THR:HG21	2.02	0.42
22:P:33:ARG:O	22:P:36:SER:OG	2.37	0.42
24:S:209:ILE:HA	24:S:212:GLN:HB2	2.00	0.42
32:a:600:ARG:NH1	36:e:29:A:OP1	2.52	0.42
32:a:674:LYS:HB3	32:a:674:LYS:HE2	1.82	0.42
48:y:496:GLN:OE1	48:y:502:VAL:N	2.53	0.42
48:y:938:TYR:HB2	49:z:104:VAL:HG21	2.02	0.42
48:y:1056:TYR:HE2	48:y:1078:LEU:HB2	1.84	0.42
2:2:33:LEU:HA	2:2:44:LEU:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:638:GLU:N	8:A:668:GLY:O	2.45	0.42
10:C:1020:LEU:HA	10:C:1023:ILE:HD12	2.01	0.42
17:J:449:VAL:HG22	17:J:451:GLN:H	1.84	0.42
32:a:824:PRO:O	32:a:933:ARG:NH1	2.53	0.42
32:a:1483:GLY:O	32:a:1487:HIS:ND1	2.45	0.42
32:a:1655:THR:OG1	32:a:1656:THR:N	2.53	0.42
33:b:122:LEU:HG	33:b:199:LEU:HB2	2.01	0.42
33:b:243:ILE:HG22	33:b:292:TYR:HD2	1.85	0.42
33:b:675:PHE:HA	33:b:685:ILE:O	2.20	0.42
35:d:29:A:N7	38:g:16:G:O2'	2.47	0.42
45:u:54:CYS:N	45:u:89:ILE:O	2.53	0.42
48:y:521:GLU:OE1	48:y:536:ARG:NE	2.52	0.42
21:O:473:SER:HB2	23:Q:60:ARG:HG2	2.01	0.42
32:a:437:ALA:O	32:a:439:GLN:NE2	2.51	0.42
32:a:1618:LYS:HA	32:a:1621:LYS:HG2	2.01	0.42
12:E:510:TYR:HE1	12:E:592:TYR:HA	1.85	0.42
20:N:808:LEU:O	20:N:813:ARG:NH1	2.53	0.42
23:Q:188:TRP:O	32:a:1083:HIS:NE2	2.42	0.42
25:T:134:CYS:SG	25:T:136:HIS:N	2.86	0.42
32:a:461:HIS:O	32:a:462:ARG:NH1	2.45	0.42
33:b:122:LEU:HD23	33:b:189:VAL:HG22	2.01	0.42
33:b:196:LYS:NZ	5:k:9:LYS:O	2.53	0.42
33:b:263:LEU:HB3	33:b:269:LEU:HD12	2.01	0.42
33:b:858:THR:H	33:b:873:ALA:HA	1.85	0.42
8:A:438:LEU:HA	8:A:775:ASN:O	2.19	0.41
11:D:49:CYS:HB3	11:D:87:LYS:HD3	2.02	0.41
12:E:524:LEU:O	12:E:529:LYS:NZ	2.45	0.41
13:F:16:TYR:HA	13:F:58:PHE:HA	2.02	0.41
21:O:355:ARG:HH11	21:O:364:THR:HG21	1.85	0.41
23:Q:192:VAL:HG11	32:a:1160:ARG:HG2	2.02	0.41
26:U:165:CYS:SG	26:U:173:CYS:HB2	2.60	0.41
33:b:486:ASP:N	33:b:486:ASP:OD1	2.50	0.41
33:b:641:MET:HE3	33:b:645:ARG:HG3	2.02	0.41
46:w:231:PRO:HA	46:w:252:CYS:HA	2.02	0.41
48:y:532:PRO:HD2	48:y:635:GLN:HB2	2.02	0.41
21:O:260:TYR:HE2	23:Q:41:ILE:HG23	1.85	0.41
32:a:974:ASN:OD1	32:a:1100:ARG:NH1	2.46	0.41
32:a:1334:LEU:HA	32:a:1354:ARG:O	2.20	0.41
33:b:213:ASP:OD1	33:b:213:ASP:N	2.50	0.41
45:u:76:ASN:N	45:u:81:GLU:O	2.48	0.41
10:C:1250:CYS:HB3	10:C:1269:TYR:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:N:419:ILE:HB	20:N:569:VAL:HG22	2.02	0.41
20:N:601:GLN:HA	20:N:604:VAL:HG22	2.02	0.41
18:R:3:LEU:HD12	18:R:24:VAL:HG21	2.02	0.41
24:S:184:ASN:O	24:S:188:LEU:HB2	2.19	0.41
32:a:168:PRO:HB2	32:a:559:ASP:HB3	2.02	0.41
37:f:164:C:O2	37:f:165:A:N6	2.53	0.41
2:h:36:VAL:HA	2:h:42:MET:HA	2.02	0.41
40:p:23:ILE:HA	40:p:135:GLY:HA3	2.03	0.41
48:y:541:ILE:HG21	48:y:656:ILE:HG21	2.02	0.41
48:y:913:LYS:NZ	48:y:925:ALA:O	2.44	0.41
10:C:1186:GLN:HB2	10:C:1226:VAL:HG23	2.01	0.41
20:N:497:THR:H	20:N:500:MET:HE2	1.84	0.41
20:N:611:ILE:O	20:N:670:VAL:HA	2.20	0.41
31:Z:203:LYS:NZ	38:g:3:A:OP2	2.47	0.41
32:a:119:LEU:HD21	32:a:476:PHE:HB2	2.02	0.41
32:a:663:ARG:NH1	35:d:64:U:OP2	2.42	0.41
32:a:1111:GLN:O	32:a:1115:THR:OG1	2.30	0.41
33:b:68:THR:HG23	33:b:71:GLU:H	1.86	0.41
33:b:669:THR:HG22	33:b:690:GLU:HB2	2.03	0.41
39:o:214:ASP:OD1	39:o:214:ASP:N	2.44	0.41
44:t:164:ASP:OD1	44:t:164:ASP:N	2.50	0.41
48:y:467:LEU:HD12	48:y:467:LEU:HA	1.92	0.41
8:A:1012:VAL:HA	8:A:1023:ILE:HA	2.02	0.41
20:N:415:HIS:CG	20:N:568:PRO:HG3	2.56	0.41
20:N:476:GLU:HA	20:N:491:THR:HA	2.03	0.41
22:P:55:ASP:HB3	22:P:58:ILE:HG13	2.02	0.41
22:P:226:ASP:H	29:X:293:ASN:HB3	1.85	0.41
22:P:796:GLU:HA	22:P:799:LYS:HD2	2.01	0.41
26:U:66:LYS:NZ	38:g:19:G:OP1	2.44	0.41
30:Y:213:LYS:HA	32:a:661:GLU:HA	2.01	0.41
33:b:368:SER:O	33:b:372:PHE:HB2	2.19	0.41
41:q:1:MET:N	41:q:5:ILE:O	2.48	0.41
48:y:1110:GLN:HB2	48:y:1116:GLU:HB3	2.03	0.41
48:y:1307:VAL:HG21	48:y:1328:LEU:HG	2.02	0.41
8:A:5:ASN:HA	8:A:1111:LEU:HA	2.03	0.41
10:C:1053:ARG:HD3	12:E:559:PRO:HG2	2.01	0.41
18:M:7:ILE:HG22	18:v:86:MET:HG2	2.01	0.41
20:N:293:GLU:HA	20:N:296:ASN:HB2	2.03	0.41
21:O:196:LEU:HB2	21:O:489:TYR:CZ	2.56	0.41
33:b:132:VAL:HG22	33:b:438:ILE:HG21	2.03	0.41
33:b:185:PRO:HA	33:b:202:ILE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:g:-10:C:H5''	38:g:-9:C:H5	1.84	0.41
39:o:128:SER:OG	39:o:129:THR:N	2.53	0.41
39:o:336:HIS:HB2	39:o:341:ILE:HB	2.01	0.41
48:y:916:GLN:NE2	48:y:923:GLY:O	2.50	0.41
8:A:689:THR:HA	31:Z:308:ASN:HA	2.03	0.41
17:J:432:ALA:HA	17:J:435:MET:HE2	2.01	0.41
22:P:210:TYR:O	29:X:260:ARG:NH1	2.44	0.41
26:U:83:THR:OG1	26:U:84:CYS:N	2.53	0.41
32:a:103:LEU:HB3	32:a:638:LEU:HD21	2.02	0.41
32:a:152:ARG:NH1	32:a:616:PHE:O	2.54	0.41
32:a:300:ASN:HB3	33:b:939:ARG:HD3	2.03	0.41
32:a:714:SER:HB3	32:a:718:ARG:HH22	1.85	0.41
32:a:807:VAL:HG12	45:u:204:THR:HG23	2.03	0.41
32:a:1355:SER:OG	41:q:16:ASN:OD1	2.38	0.41
33:b:769:GLY:HA3	33:b:812:ALA:HB3	2.02	0.41
39:o:348:ASP:OD2	39:o:350:ARG:NH2	2.54	0.41
48:y:1223:LYS:HA	48:y:1223:LYS:HD3	1.92	0.41
10:C:1057:ARG:NH1	12:E:557:VAL:O	2.47	0.41
10:C:1132:LEU:HG	10:C:1147:VAL:HG13	2.02	0.41
18:M:74:ILE:HG23	18:R:74:ILE:HG23	2.03	0.41
22:P:219:LYS:HD3	22:P:219:LYS:HA	1.90	0.41
23:Q:218:GLU:OE2	23:Q:221:LYS:NZ	2.46	0.41
28:W:477:LEU:HD11	28:W:517:LEU:HD13	2.02	0.41
30:Y:298:ALA:HB2	45:u:207:THR:HG21	2.03	0.41
32:a:1013:ASN:O	32:a:1026:ASN:ND2	2.44	0.41
32:a:1459:ARG:HA	32:a:1459:ARG:HD3	1.95	0.41
10:C:936:VAL:HG13	10:C:951:ALA:HB1	2.01	0.41
10:C:1011:PRO:HA	10:C:1012:PRO:HD3	1.97	0.41
10:C:1177:LEU:HD13	10:C:1214:TYR:HB2	2.02	0.41
12:E:537:ARG:HH21	12:E:564:ILE:HD11	1.85	0.41
16:I:118:LYS:HA	16:I:223:LEU:HA	2.03	0.41
18:M:40:ASP:N	18:M:45:GLN:O	2.53	0.41
20:N:708:SER:HA	20:N:991:LEU:HB3	2.02	0.41
32:a:82:ARG:HH22	38:g:14:A:H3'	1.85	0.41
32:a:109:PRO:HD3	32:a:630:TRP:HZ2	1.85	0.41
32:a:303:ILE:HG12	33:b:936:LYS:HG3	2.02	0.41
32:a:635:ARG:NH2	36:e:26:A:O3'	2.52	0.41
32:a:1491:LYS:HA	32:a:1491:LYS:HD3	1.91	0.41
35:d:67:G:H22	36:e:43:U:H4'	1.85	0.41
37:f:32:U:H2'	37:f:33:G:H8	1.86	0.41
48:y:659:ARG:NH2	48:y:663:GLU:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:y:1176:ASP:OD1	48:y:1176:ASP:N	2.52	0.41
8:A:460:TRP:O	8:A:475:ILE:N	2.48	0.41
20:N:337:ALA:HB2	32:a:1417:PRO:HG2	2.03	0.41
20:N:596:VAL:HA	20:N:599:VAL:HG12	2.03	0.41
21:O:471:ASP:OD2	21:O:473:SER:OG	2.37	0.41
23:Q:53:GLU:O	23:Q:57:ARG:HB2	2.20	0.41
25:T:58:ARG:HA	25:T:58:ARG:HD3	1.84	0.41
26:U:157:TYR:HA	26:U:160:ASN:HD22	1.86	0.41
32:a:591:MET:HB3	32:a:598:LEU:HD22	2.02	0.41
32:a:1582:TRP:HB3	32:a:1620:TYR:HE1	1.86	0.41
3:j:43:MET:O	3:j:61:VAL:N	2.47	0.41
40:p:96:GLY:O	40:p:132:VAL:N	2.47	0.41
48:y:965:SER:O	48:y:971:HIS:NE2	2.54	0.41
49:z:267:ILE:HD13	49:z:267:ILE:HA	1.96	0.41
18:M:96:LEU:HD23	18:M:96:LEU:HA	1.93	0.40
20:N:502:LEU:HD21	20:N:766:LEU:HD13	2.03	0.40
22:P:77:LEU:O	30:Y:296:TYR:OH	2.39	0.40
32:a:179:ALA:HA	32:a:183:LEU:HB3	2.02	0.40
32:a:1654:SER:OG	32:a:1655:THR:N	2.54	0.40
33:b:154:HIS:HA	33:b:155:PRO:HD3	1.96	0.40
33:b:310:SER:HA	33:b:316:ILE:O	2.21	0.40
34:c:997:THR:HA	34:c:1022:SER:H	1.86	0.40
48:y:470:PHE:HB2	48:y:673:ILE:HG21	2.03	0.40
49:z:283:ILE:HG21	49:z:344:LEU:HD13	2.03	0.40
49:z:444:LEU:HG	49:z:448:ASN:HA	2.02	0.40
10:C:1213:ASN:OD1	12:E:586:ILE:O	2.40	0.40
20:N:511:LEU:O	20:N:543:ARG:NH1	2.53	0.40
25:T:99:ASN:OD1	35:d:1:G:O2'	2.36	0.40
26:U:129:ASP:OD1	26:U:129:ASP:N	2.43	0.40
27:V:41:LEU:HD23	27:V:41:LEU:HA	1.93	0.40
32:a:167:PRO:HA	32:a:168:PRO:HD3	1.96	0.40
32:a:899:MET:HE3	32:a:1448:LEU:HD12	2.02	0.40
32:a:1020:LYS:NZ	37:f:26:A:OP1	2.47	0.40
32:a:1109:LEU:HG	32:a:1152:ALA:HB1	2.03	0.40
32:a:1279:VAL:O	32:a:1282:GLN:NE2	2.48	0.40
32:a:1456:THR:OG1	32:a:1457:HIS:N	2.55	0.40
33:b:104:LEU:HD13	33:b:536:ARG:HH12	1.86	0.40
34:c:668:ASP:O	34:c:672:GLY:CA	2.69	0.40
39:o:239:THR:N	39:o:253:ASN:O	2.55	0.40
45:u:237:ASN:HA	45:u:266:ILE:HG22	2.02	0.40
8:A:33:SER:HA	8:A:38:LEU:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:311:PHE:HA	8:A:329:TYR:HA	2.03	0.40
8:A:477:SER:HA	8:A:482:THR:HA	2.02	0.40
11:D:81:ASP:OD1	11:D:81:ASP:N	2.55	0.40
20:N:866:ASN:HD22	32:a:836:THR:HG22	1.86	0.40
24:S:183:SER:HA	24:S:186:VAL:HG22	2.03	0.40
26:U:64:ARG:HD2	26:U:163:HIS:CD2	2.56	0.40
28:W:571:SER:OG	28:W:574:THR:OG1	2.36	0.40
31:Z:191:ALA:O	32:a:1617:ARG:NH2	2.54	0.40
32:a:252:ASP:OD1	32:a:252:ASP:N	2.49	0.40
32:a:293:TRP:HB2	32:a:1136:ARG:HH22	1.87	0.40
32:a:820:ARG:HA	32:a:820:ARG:HD2	1.80	0.40
32:a:1260:VAL:HG21	32:a:1325:LEU:HB3	2.02	0.40
32:a:1595:GLN:HA	32:a:1598:ASP:HB2	2.04	0.40
4:l:52:LEU:HA	4:l:72:GLU:HA	2.03	0.40
18:v:5:CYS:SG	18:v:6:SER:N	2.93	0.40
48:y:323:GLU:HA	48:y:326:MET:HE2	2.03	0.40
10:C:1217:PRO:HG2	12:E:591:TYR:H	1.87	0.40
20:N:877:ASP:OD1	20:N:877:ASP:N	2.49	0.40
25:T:111:THR:OG1	25:T:115:THR:N	2.49	0.40
26:U:216:ARG:O	26:U:219:THR:OG1	2.30	0.40
30:Y:109:ASP:OD1	30:Y:109:ASP:N	2.55	0.40
32:a:237:THR:HG23	32:a:240:ARG:HH21	1.86	0.40
32:a:268:ALA:HA	32:a:282:LEU:HD13	2.03	0.40
32:a:297:ASN:HA	32:a:1341:ARG:HH21	1.87	0.40
32:a:465:LYS:O	36:e:23:C:N4	2.54	0.40
32:a:521:ASN:HB2	32:a:523:ASN:HD21	1.86	0.40
33:b:183:SER:O	33:b:482:TYR:OH	2.38	0.40
33:b:529:ARG:NH1	33:b:540:GLU:OE2	2.54	0.40
33:b:863:ILE:HB	33:b:866:SER:HB2	2.04	0.40
40:p:25:LEU:HA	40:p:132:VAL:HA	2.03	0.40
45:u:331:GLN:HA	45:u:381:PHE:HA	2.03	0.40
48:y:567:VAL:HG12	48:y:589:LEU:HA	2.04	0.40
21:O:250:ARG:HA	21:O:250:ARG:HD2	1.88	0.40
25:T:25:LEU:HD23	25:T:28:LYS:HD2	2.03	0.40
32:a:150:MET:HB3	32:a:572:PHE:HZ	1.86	0.40
32:a:1086:ARG:HA	32:a:1086:ARG:HD3	1.92	0.40
33:b:160:ARG:HB2	33:b:163:GLN:HE21	1.87	0.40
33:b:829:GLU:HB2	33:b:907:VAL:HG22	2.04	0.40
34:c:498:ASN:HA	34:c:648:LEU:H	1.86	0.40
48:y:225:LEU:HG	48:y:253:PHE:HE1	1.86	0.40
48:y:597:ILE:HD13	48:y:627:VAL:HG12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:y:1173:LEU:HD21	48:y:1214:MET:HE1	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	77/92 (84%)	77 (100%)	0	0	100	100
1	i	66/92 (72%)	64 (97%)	2 (3%)	0	100	100
2	2	72/86 (84%)	72 (100%)	0	0	100	100
2	h	62/86 (72%)	58 (94%)	4 (6%)	0	100	100
3	3	74/126 (59%)	72 (97%)	2 (3%)	0	100	100
3	j	66/126 (52%)	63 (96%)	3 (4%)	0	100	100
4	4	81/118 (69%)	79 (98%)	2 (2%)	0	100	100
4	l	64/118 (54%)	61 (95%)	3 (5%)	0	100	100
5	5	80/119 (67%)	78 (98%)	2 (2%)	0	100	100
5	k	74/119 (62%)	68 (92%)	6 (8%)	0	100	100
6	8	84/240 (35%)	81 (96%)	3 (4%)	0	100	100
6	n	60/240 (25%)	60 (100%)	0	0	100	100
7	9	64/76 (84%)	64 (100%)	0	0	100	100
7	m	57/76 (75%)	55 (96%)	2 (4%)	0	100	100
8	A	1142/1217 (94%)	1069 (94%)	73 (6%)	0	100	100
9	B	68/86 (79%)	65 (96%)	2 (3%)	1 (2%)	8	39
10	C	813/1304 (62%)	779 (96%)	34 (4%)	0	100	100
11	D	87/110 (79%)	75 (86%)	11 (13%)	1 (1%)	11	46
12	E	190/895 (21%)	177 (93%)	13 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	F	76/424 (18%)	68 (90%)	8 (10%)	0	100	100
14	G	63/476 (13%)	60 (95%)	3 (5%)	0	100	100
15	H	94/793 (12%)	94 (100%)	0	0	100	100
16	I	173/464 (37%)	161 (93%)	10 (6%)	2 (1%)	10	43
17	J	394/501 (79%)	369 (94%)	25 (6%)	0	100	100
18	K	114/504 (23%)	113 (99%)	1 (1%)	0	100	100
18	M	121/504 (24%)	120 (99%)	1 (1%)	0	100	100
18	R	114/504 (23%)	111 (97%)	3 (3%)	0	100	100
18	v	121/504 (24%)	121 (100%)	0	0	100	100
19	L	26/619 (4%)	24 (92%)	2 (8%)	0	100	100
20	N	779/1041 (75%)	723 (93%)	53 (7%)	3 (0%)	30	67
21	O	318/514 (62%)	304 (96%)	14 (4%)	0	100	100
22	P	316/802 (39%)	308 (98%)	8 (2%)	0	100	100
23	Q	96/229 (42%)	89 (93%)	7 (7%)	0	100	100
24	S	153/225 (68%)	142 (93%)	11 (7%)	0	100	100
25	T	140/144 (97%)	130 (93%)	10 (7%)	0	100	100
26	U	293/420 (70%)	270 (92%)	20 (7%)	3 (1%)	12	48
27	V	279/492 (57%)	257 (92%)	21 (8%)	1 (0%)	30	67
28	W	455/908 (50%)	439 (96%)	16 (4%)	0	100	100
29	X	237/848 (28%)	232 (98%)	5 (2%)	0	100	100
30	Y	294/536 (55%)	270 (92%)	22 (8%)	2 (1%)	18	56
31	Z	91/343 (26%)	83 (91%)	7 (8%)	1 (1%)	11	46
32	a	2171/2335 (93%)	2070 (95%)	95 (4%)	6 (0%)	36	72
33	b	896/972 (92%)	849 (95%)	42 (5%)	5 (1%)	21	59
34	c	1720/2136 (80%)	1668 (97%)	51 (3%)	1 (0%)	48	83
39	o	297/357 (83%)	278 (94%)	19 (6%)	0	100	100
40	p	157/166 (95%)	145 (92%)	12 (8%)	0	100	100
41	q	70/2752 (2%)	65 (93%)	5 (7%)	0	100	100
42	r	160/255 (63%)	154 (96%)	6 (4%)	0	100	100
43	s	159/225 (71%)	153 (96%)	6 (4%)	0	100	100
44	t	46/285 (16%)	45 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	u	359/520 (69%)	339 (94%)	19 (5%)	1 (0%)	36	72
46	w	213/301 (71%)	207 (97%)	6 (3%)	0	100	100
47	x	358/579 (62%)	332 (93%)	23 (6%)	3 (1%)	16	54
48	y	1319/1485 (89%)	1272 (96%)	47 (4%)	0	100	100
49	z	684/855 (80%)	636 (93%)	44 (6%)	4 (1%)	21	59
All	All	16637/30344 (55%)	15818 (95%)	785 (5%)	34 (0%)	44	77

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	I	139	PRO
16	I	218	PRO
26	U	225	PRO
26	U	226	PRO
33	b	57	VAL
47	x	243	VAL
49	z	720	ILE
20	N	860	LYS
26	U	134	VAL
31	Z	208	THR
32	a	520	TYR
32	a	1092	ILE
47	x	263	VAL
49	z	550	TRP
11	D	61	CYS
32	a	1275	ARG
33	b	801	LEU
45	u	235	LYS
30	Y	96	ILE
32	a	982	GLU
33	b	94	ILE
20	N	639	ILE
20	N	854	PHE
32	a	701	ILE
27	V	235	ILE
30	Y	92	SER
33	b	84	GLU
47	x	299	LEU
33	b	113	VAL
49	z	141	PRO

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Mol	Chain	Res	Type
9	B	78	PRO
49	z	587	CYS
34	c	531	ILE
32	a	1419	ILE

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	
5	k	1/101 (1%)	1 (100%)	0	100	100
9	B	2/77 (3%)	2 (100%)	0	100	100
10	C	342/1104 (31%)	342 (100%)	0	100	100
11	D	69/95 (73%)	69 (100%)	0	100	100
12	E	102/776 (13%)	102 (100%)	0	100	100
14	G	10/397 (2%)	10 (100%)	0	100	100
16	I	33/382 (9%)	33 (100%)	0	100	100
17	J	42/446 (9%)	42 (100%)	0	100	100
18	K	106/435 (24%)	106 (100%)	0	100	100
18	M	111/435 (26%)	111 (100%)	0	100	100
18	R	106/435 (24%)	106 (100%)	0	100	100
18	v	111/435 (26%)	111 (100%)	0	100	100
19	L	11/545 (2%)	11 (100%)	0	100	100
20	N	624/897 (70%)	624 (100%)	0	100	100
21	O	274/441 (62%)	274 (100%)	0	100	100
22	P	208/709 (29%)	208 (100%)	0	100	100
23	Q	83/203 (41%)	83 (100%)	0	100	100
24	S	144/196 (74%)	144 (100%)	0	100	100
25	T	129/130 (99%)	129 (100%)	0	100	100
26	U	181/361 (50%)	181 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	V	180/451 (40%)	180 (100%)	0	100	100
28	W	180/838 (22%)	177 (98%)	3 (2%)	53	68
29	X	85/751 (11%)	85 (100%)	0	100	100
30	Y	209/459 (46%)	209 (100%)	0	100	100
31	Z	35/294 (12%)	35 (100%)	0	100	100
32	a	1496/2108 (71%)	1496 (100%)	0	100	100
33	b	784/866 (90%)	784 (100%)	0	100	100
39	o	256/300 (85%)	256 (100%)	0	100	100
41	q	30/2432 (1%)	30 (100%)	0	100	100
44	t	41/240 (17%)	41 (100%)	0	100	100
45	u	45/456 (10%)	45 (100%)	0	100	100
48	y	1200/1336 (90%)	1200 (100%)	0	100	100
49	z	290/749 (39%)	290 (100%)	0	100	100
All	All	7520/19880 (38%)	7517 (100%)	3 (0%)	100	100

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
28	W	458	THR
28	W	557	THR
28	W	575	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
10	C	1091	HIS
12	E	458	ASN
12	E	496	ASN
12	E	534	GLN
12	E	579	GLN
17	J	431	HIS
18	K	45	GLN
18	K	105	HIS
18	M	22	ASN
18	M	79	GLN
18	M	94	GLN

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Mol	Chain	Res	Type
20	N	415	HIS
20	N	629	GLN
20	N	773	HIS
21	O	283	HIS
21	O	408	ASN
22	P	81	GLN
22	P	736	ASN
23	Q	56	ASN
18	R	79	GLN
18	R	101	GLN
24	S	68	ASN
24	S	169	ASN
24	S	171	GLN
25	T	95	GLN
26	U	31	ASN
26	U	183	HIS
26	U	206	ASN
29	X	340	GLN
29	X	344	GLN
30	Y	104	GLN
30	Y	133	GLN
32	a	65	HIS
32	a	160	HIS
32	a	294	ASN
32	a	321	ASN
32	a	357	ASN
32	a	691	HIS
32	a	775	ASN
32	a	963	GLN
32	a	1013	ASN
32	a	1014	ASN
32	a	1023	ASN
32	a	1056	HIS
32	a	1172	ASN
32	a	1188	ASN
32	a	1373	GLN
32	a	1466	ASN
32	a	1665	GLN
33	b	87	GLN
33	b	137	HIS
33	b	210	ASN
33	b	245	HIS

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Mol	Chain	Res	Type
33	b	335	ASN
33	b	366	GLN
33	b	402	HIS
33	b	548	ASN
33	b	575	GLN
33	b	771	GLN
33	b	856	HIS
33	b	894	GLN
39	o	101	ASN
39	o	188	GLN
39	o	215	ASN
39	o	253	ASN
39	o	257	ASN
18	v	22	ASN
48	y	141	HIS
48	y	167	GLN
48	y	224	GLN
48	y	316	GLN
48	y	330	HIS
48	y	338	GLN
48	y	344	HIS
48	y	458	GLN
48	y	586	GLN
48	y	857	GLN
48	y	1066	GLN
48	y	1178	GLN
48	y	1231	ASN
48	y	1266	GLN
49	z	118	GLN
49	z	239	ASN
49	z	254	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
35	d	91/106 (85%)	34 (37%)	0
36	e	95/117 (81%)	31 (32%)	0
37	f	131/188 (69%)	32 (24%)	0
38	g	74/319 (23%)	35 (47%)	0
All	All	391/730 (53%)	132 (33%)	0

All (132) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
35	d	6	C
35	d	7	G
35	d	8	C
35	d	9	U
35	d	10	U
35	d	12	G
35	d	21	U
35	d	25	C
35	d	26	U
35	d	27	A
35	d	28	A
35	d	29	A
35	d	35	A
35	d	36	A
35	d	37	C
35	d	44	G
35	d	49	G
35	d	51	U
35	d	52	U
35	d	54	G
35	d	55	C
35	d	56	A
35	d	59	G
35	d	60	C
35	d	61	C
35	d	62	C
35	d	66	C
35	d	68	C
35	d	74	U
35	d	79	C
35	d	80	G
35	d	81	C
35	d	87	C
35	d	90	G
36	e	9	G
36	e	19	A
36	e	20	G
36	e	21	A
36	e	22	U
36	e	23	C
36	e	24	G
36	e	25	C
36	e	28	A

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Mol	Chain	Res	Type
36	e	34	U
36	e	36	C
36	e	40	U
36	e	43	U
36	e	45	C
36	e	53	U
36	e	57	G
36	e	59	G
36	e	70	A
36	e	75	G
36	e	90	U
36	e	91	U
36	e	92	U
36	e	93	U
36	e	94	U
36	e	95	G
36	e	96	A
36	e	100	C
36	e	106	U
36	e	107	U
36	e	115	C
36	e	116	U
37	f	12	G
37	f	13	C
37	f	14	C
37	f	23	A
37	f	24	A
37	f	25	G
37	f	29	A
37	f	30	A
37	f	31	G
37	f	32	U
37	f	35	A
37	f	36	G
37	f	40	C
37	f	44	U
37	f	45	C
37	f	47	U
37	f	48	A
37	f	49	U
37	f	62	U
37	f	84	C

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Mol	Chain	Res	Type
37	f	101	U
37	f	102	U
37	f	103	U
37	f	147	G
37	f	153	A
37	f	157	G
37	f	163	G
37	f	164	C
37	f	169	C
37	f	171	U
37	f	178	A
37	f	179	C
38	g	-13	C
38	g	-12	G
38	g	-11	G
38	g	-9	C
38	g	-6	C
38	g	1	G
38	g	2	U
38	g	3	A
38	g	9	C
38	g	14	A
38	g	16	G
38	g	17	U
38	g	18	A
38	g	20	A
38	g	21	A
38	g	22	C
38	g	23	U
38	g	25	G
38	g	27	U
38	g	135	G
38	g	136	U
38	g	137	C
38	g	143	U
38	g	144	A
38	g	145	U
38	g	148	U
38	g	149	G
38	g	152	C
38	g	154	U
38	g	158	U

Continued on next page...

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Mol	Chain	Res	Type
38	g	160	U
38	g	161	U
38	g	162	C
38	g	163	C
38	g	164	A

There are no RNA pucker outliers to report.

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 21 ligands modelled in this entry, 19 are monoatomic - leaving 2 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$
52	GTP	b	1500	53	33,34,34	0.90	1 (3%)	50,54,54	1.57	8 (16%)
51	IHP	a	3001	-	36,36,36	1.59	6 (16%)	60,60,60	1.36	6 (10%)

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	GTP	b	1500	53	-	5/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	IHP	a	3001	-	-	4/30/54/54	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	a	3001	IHP	P3-O13	3.82	1.66	1.59
51	a	3001	IHP	P4-O14	3.70	1.66	1.59
51	a	3001	IHP	P2-O12	3.25	1.65	1.59
51	a	3001	IHP	P6-O16	3.19	1.65	1.59
51	a	3001	IHP	P5-O15	3.15	1.65	1.59
51	a	3001	IHP	P1-O11	3.04	1.64	1.59
52	b	1500	GTP	C2-N3	2.00	1.38	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	b	1500	GTP	C5-C4-N3	-4.57	121.12	128.39
52	b	1500	GTP	C2-N3-C4	4.49	120.04	112.30
51	a	3001	IHP	C6-C5-C4	3.85	118.86	110.43
51	a	3001	IHP	O13-C3-C2	3.76	116.77	108.76
51	a	3001	IHP	C5-C6-C1	3.75	118.66	110.43
51	a	3001	IHP	O14-C4-C5	2.98	115.10	108.76
52	b	1500	GTP	N9-C8-N7	-2.81	108.19	113.40
52	b	1500	GTP	N9-C4-N3	2.81	131.56	125.95
52	b	1500	GTP	C2-N1-C6	-2.75	120.12	125.11
51	a	3001	IHP	C6-C1-C2	2.69	116.32	110.43
52	b	1500	GTP	C8-N7-C5	2.51	108.73	104.26
52	b	1500	GTP	C5-C6-N1	2.47	119.54	113.25
52	b	1500	GTP	O6-C6-C5	-2.41	120.17	126.53
51	a	3001	IHP	C5-C4-C3	2.10	115.03	110.43

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
51	a	3001	IHP	C2-C3-O13-P3
51	a	3001	IHP	C5-C4-O14-P4
52	b	1500	GTP	C5'-O5'-PA-O3A
51	a	3001	IHP	C1-O11-P1-O21
52	b	1500	GTP	C5'-O5'-PA-O1A
51	a	3001	IHP	C5-O15-P5-O45

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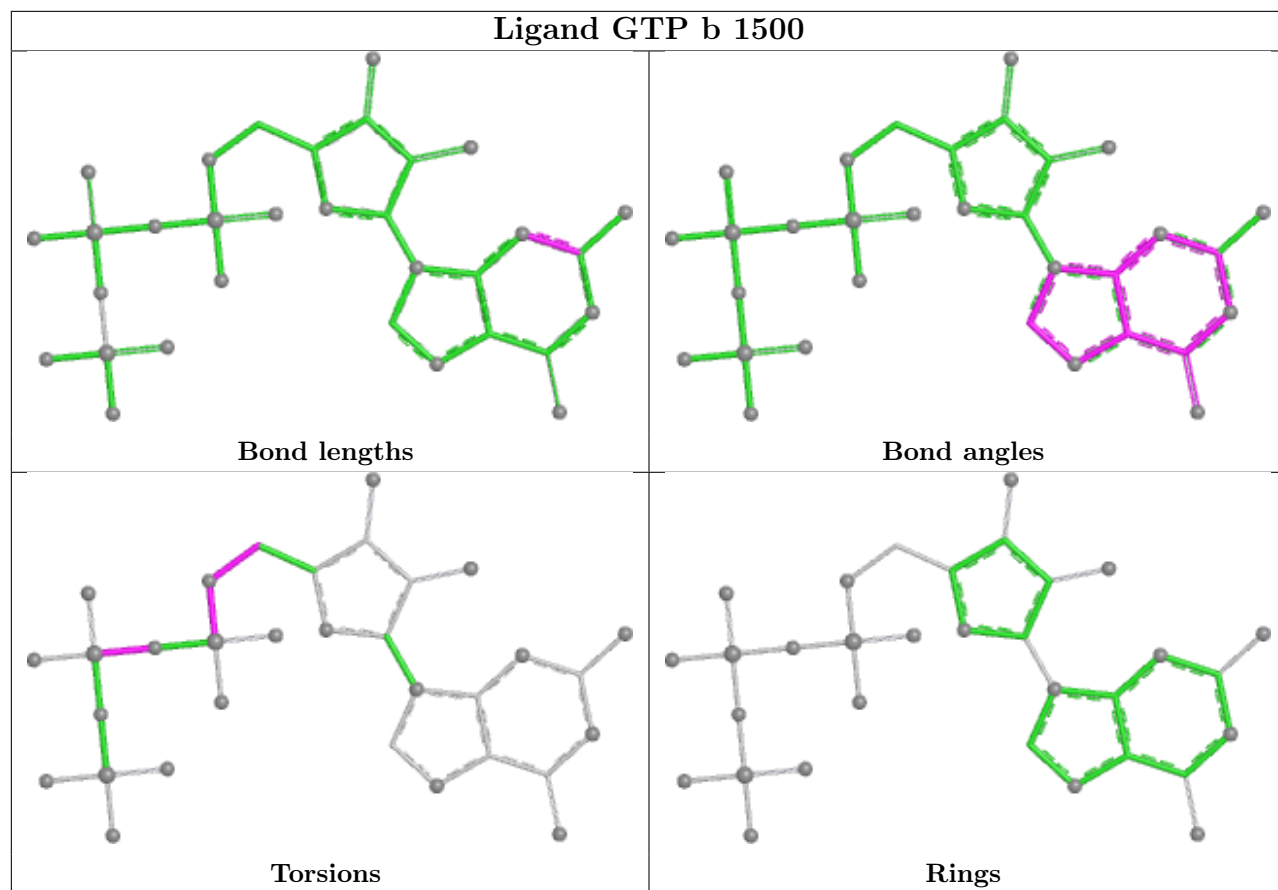
Mol	Chain	Res	Type	Atoms
52	b	1500	GTP	C4'-C5'-O5'-PA
52	b	1500	GTP	PA-O3A-PB-O1B
52	b	1500	GTP	PA-O3A-PB-O2B

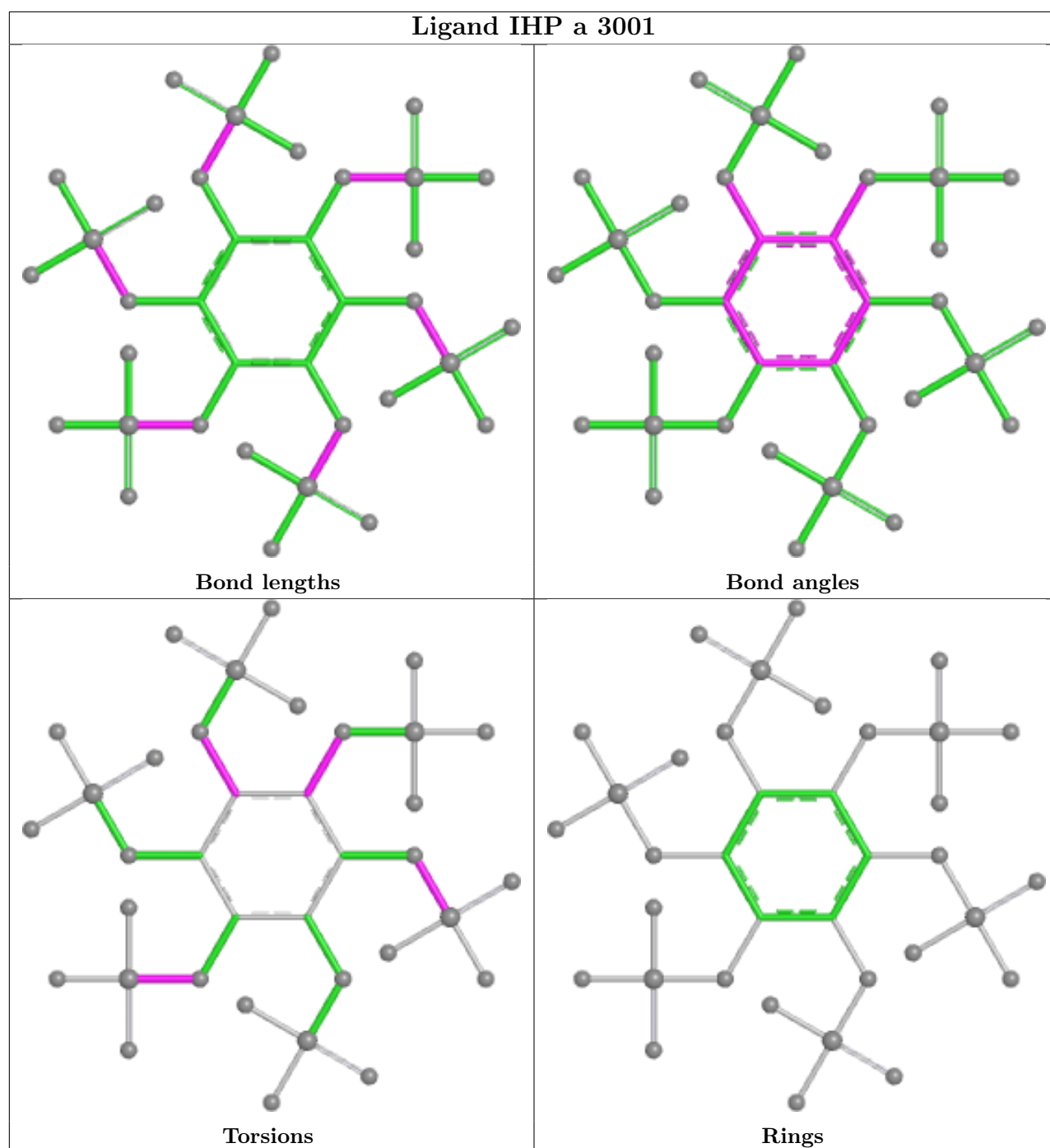
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
51	a	3001	IHP	2	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

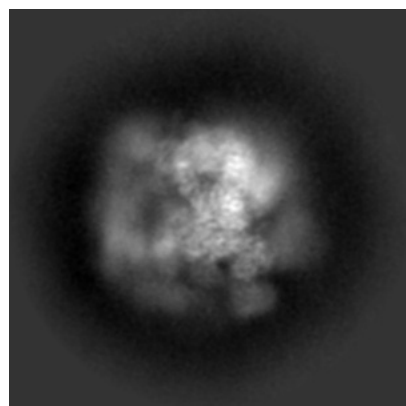
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16658. These allow visual inspection of the internal detail of the map and identification of artifacts.

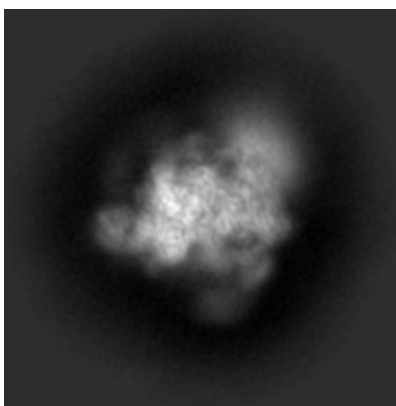
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

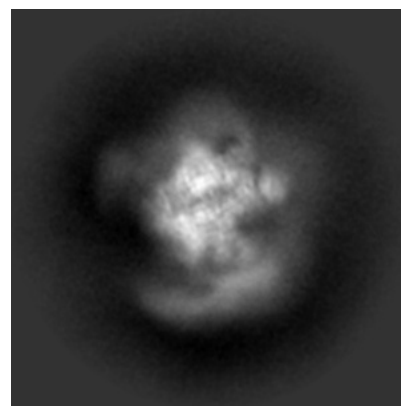
6.1.1 Primary map



X

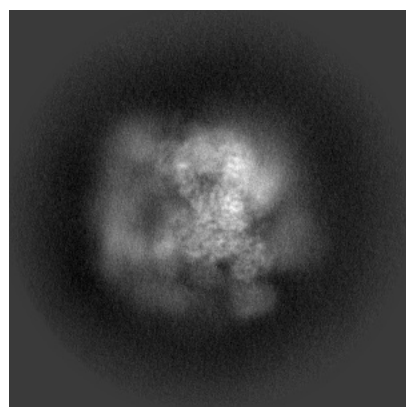


Y

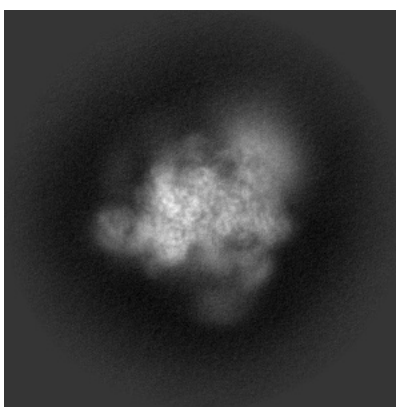


Z

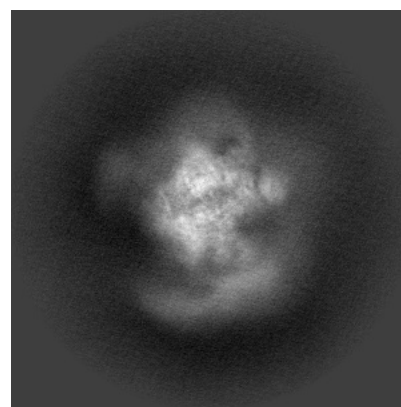
6.1.2 Raw map



X



Y

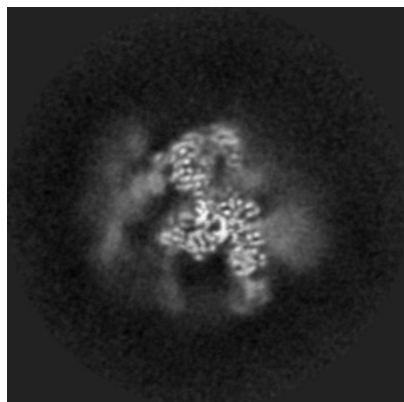


Z

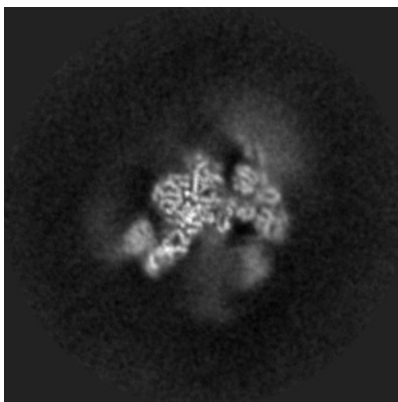
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

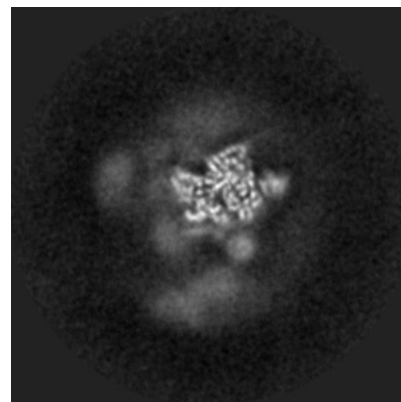
6.2.1 Primary map



X Index: 260

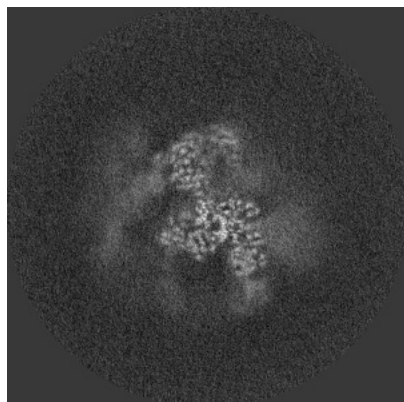


Y Index: 260

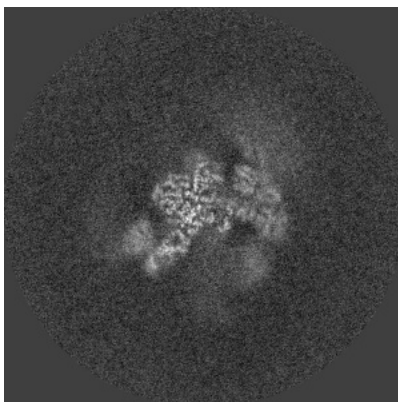


Z Index: 260

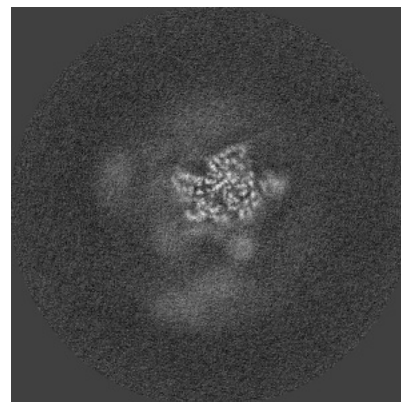
6.2.2 Raw map



X Index: 260



Y Index: 260

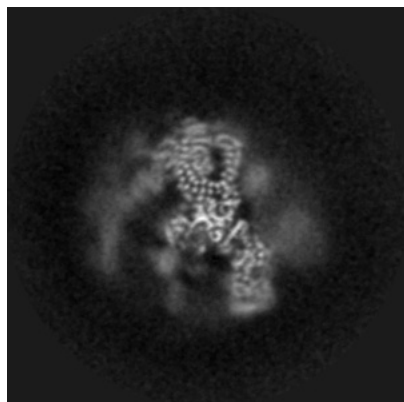


Z Index: 260

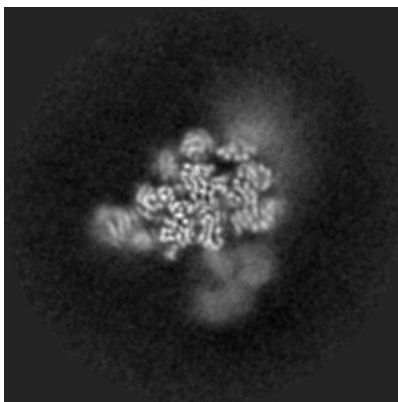
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

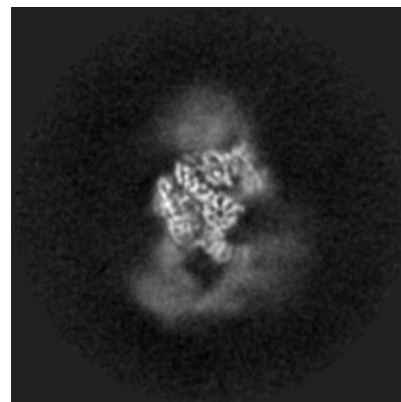
6.3.1 Primary map



X Index: 248

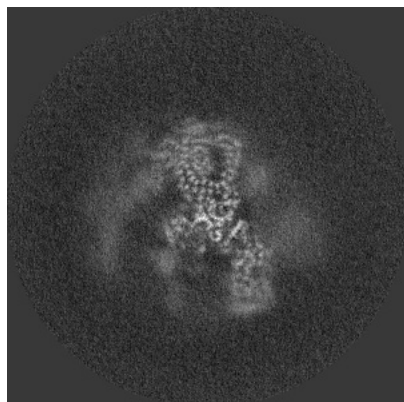


Y Index: 295

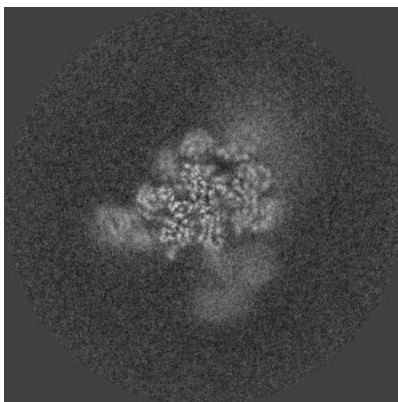


Z Index: 216

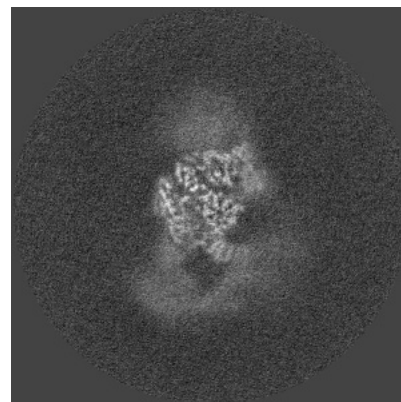
6.3.2 Raw map



X Index: 248



Y Index: 295

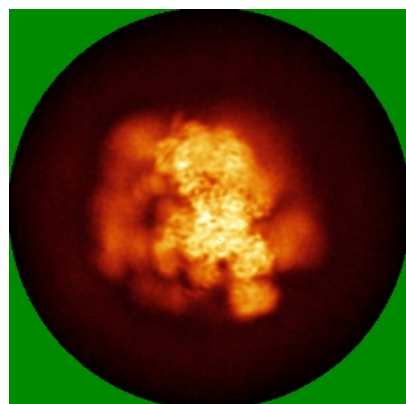


Z Index: 215

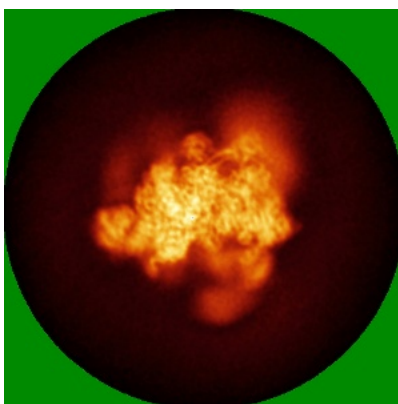
The images above show the largest variance slices of the map in three orthogonal directions.

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

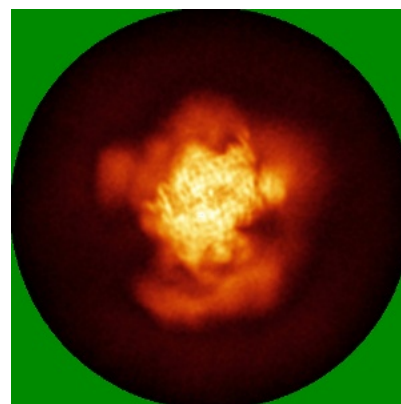
6.4.1 Primary map



X

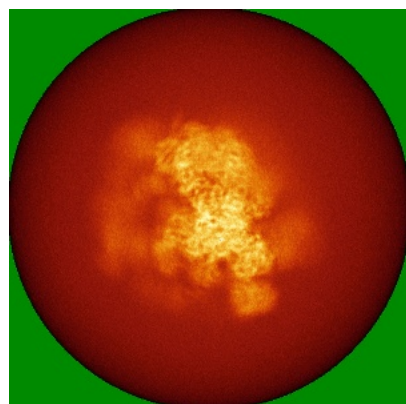


Y

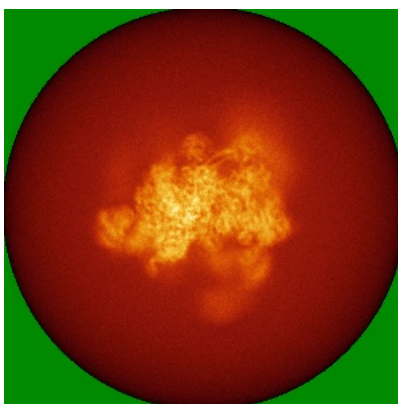


Z

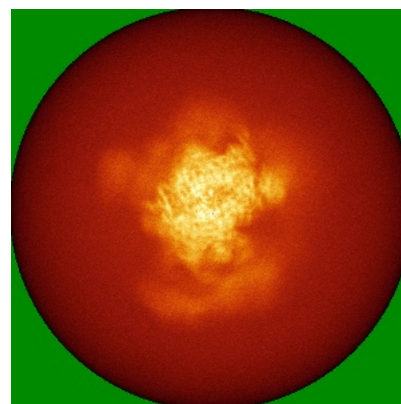
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

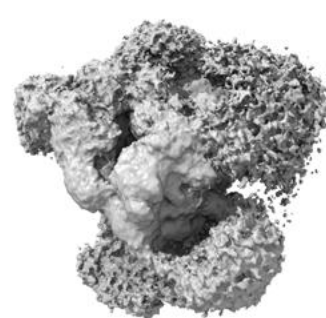
6.5.1 Primary map



X



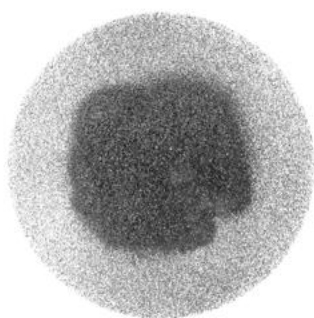
Y



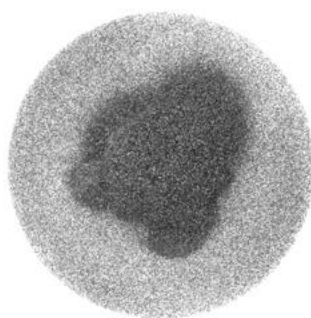
Z

The images above show the 3D surface view of the map at the recommended contour level 0.008. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

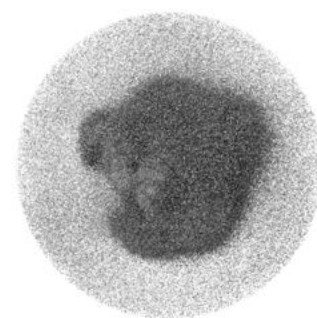
6.5.2 Raw map



X



Y



Z

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

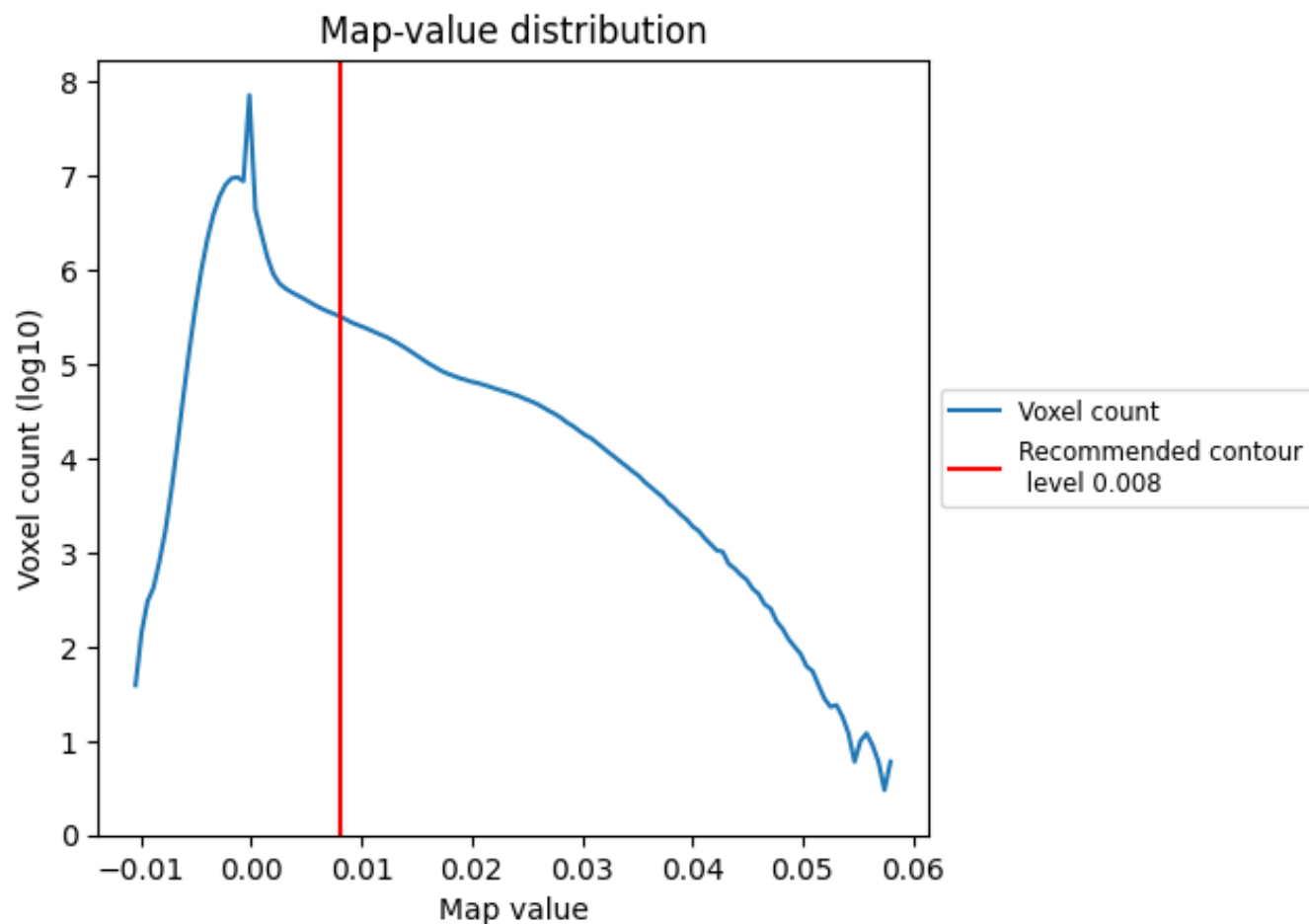
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

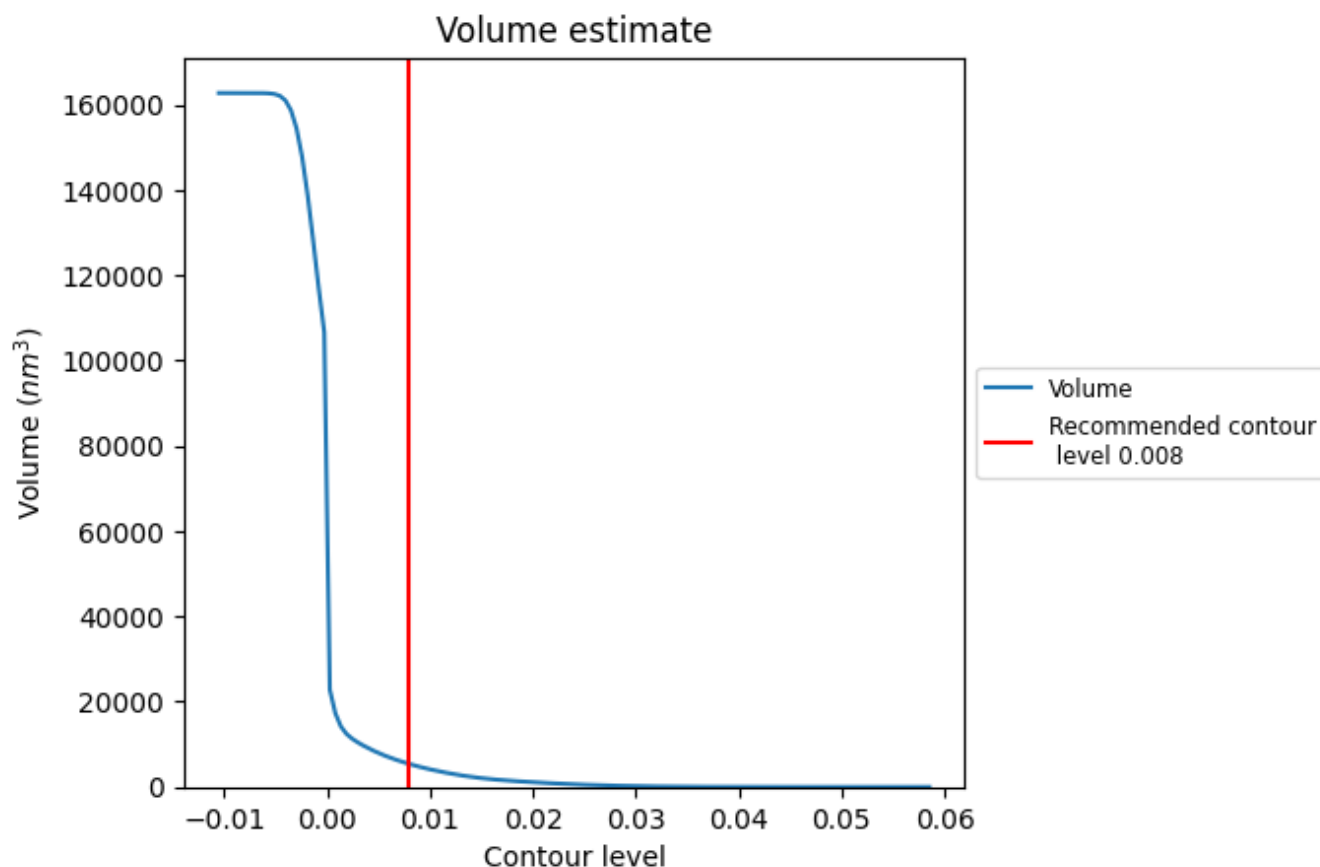
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

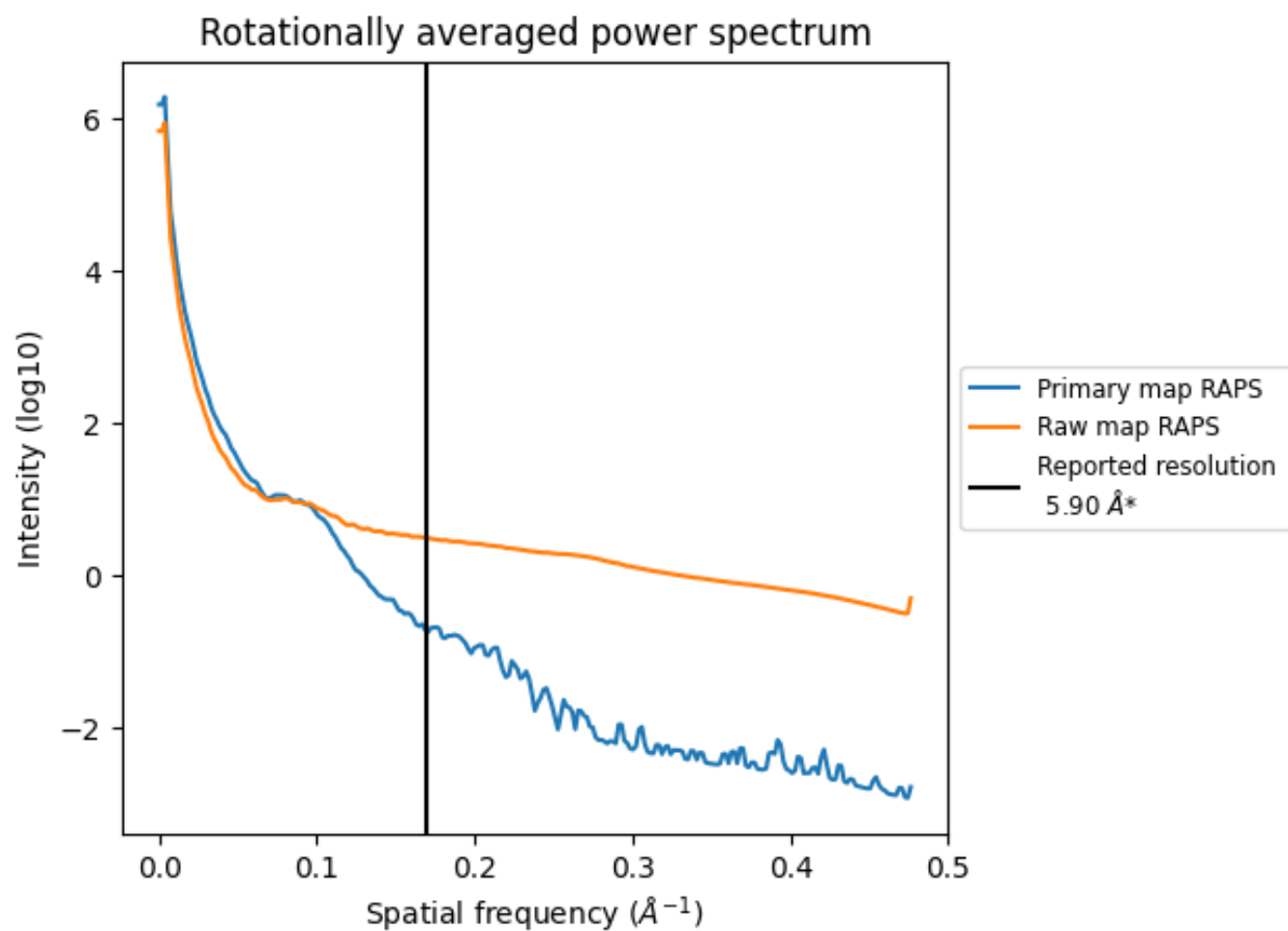
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5401 nm³; this corresponds to an approximate mass of 4879 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 ⓘ

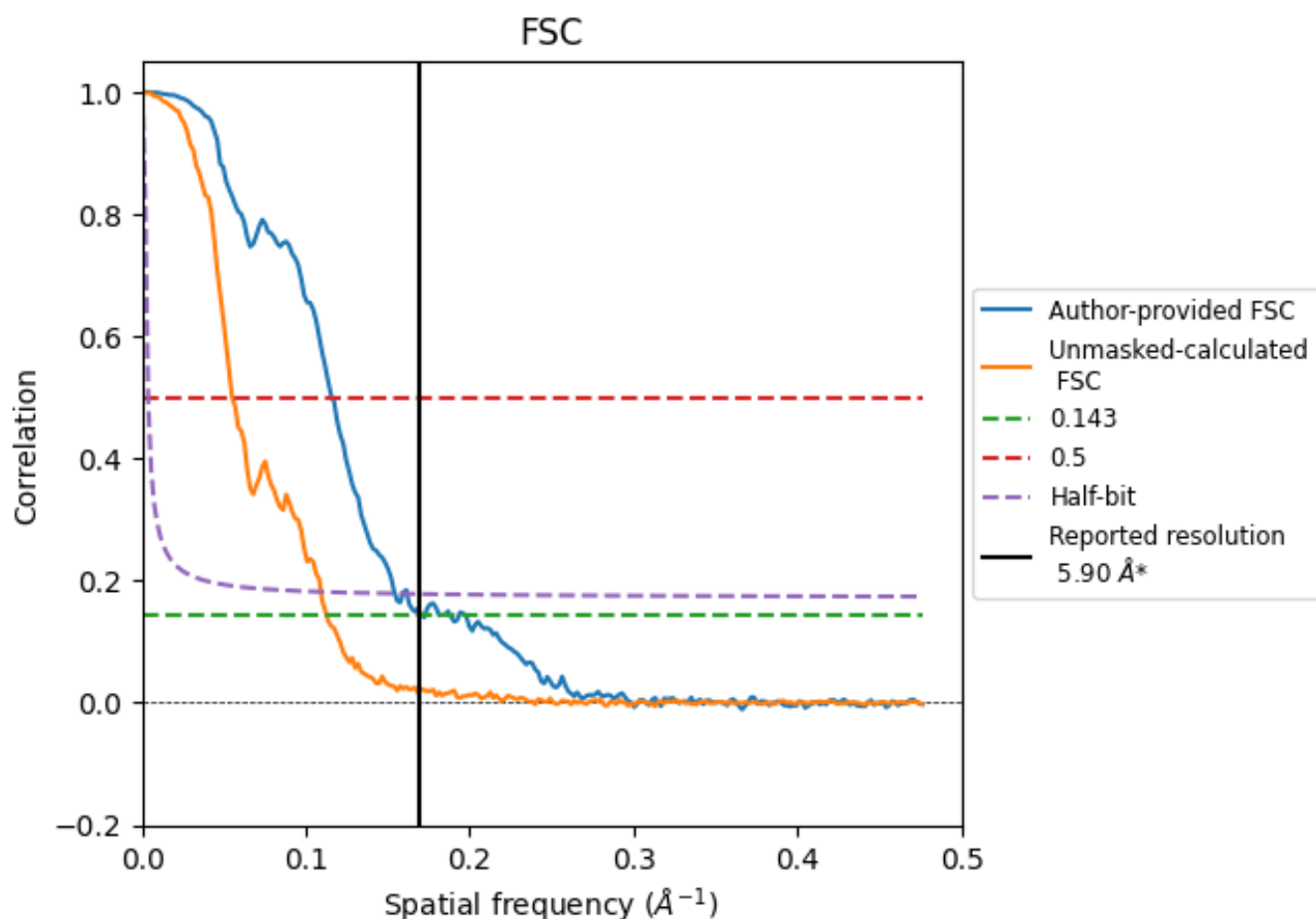


*Reported resolution corresponds to spatial frequency of 0.169 Å⁻¹

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 0.169 Å⁻¹

8.2 Resolution estimates [i](#)

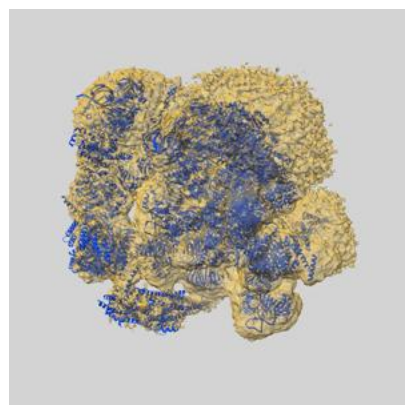
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.90	-	-
Author-provided FSC curve	5.85	8.63	6.48
Unmasked-calculated*	8.88	18.21	9.17

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.88 differs from the reported value 5.9 by more than 10 %

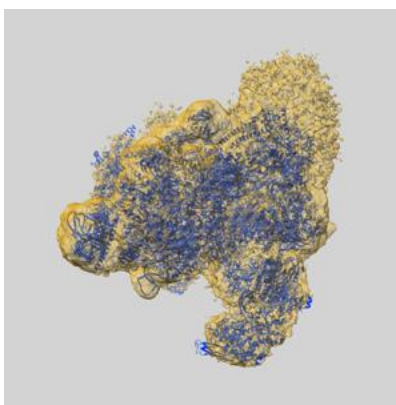
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-16658 and PDB model 8CH6. Per-residue inclusion information can be found in section [3](#) on page [16](#).

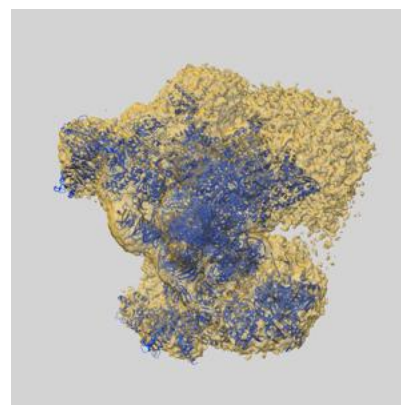
9.1 Map-model overlay [i](#)



X



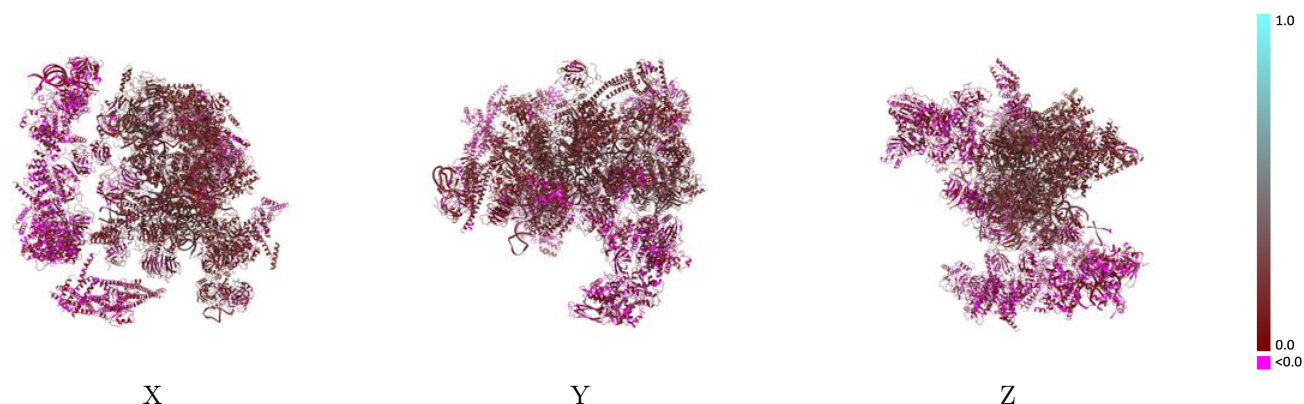
Y



Z

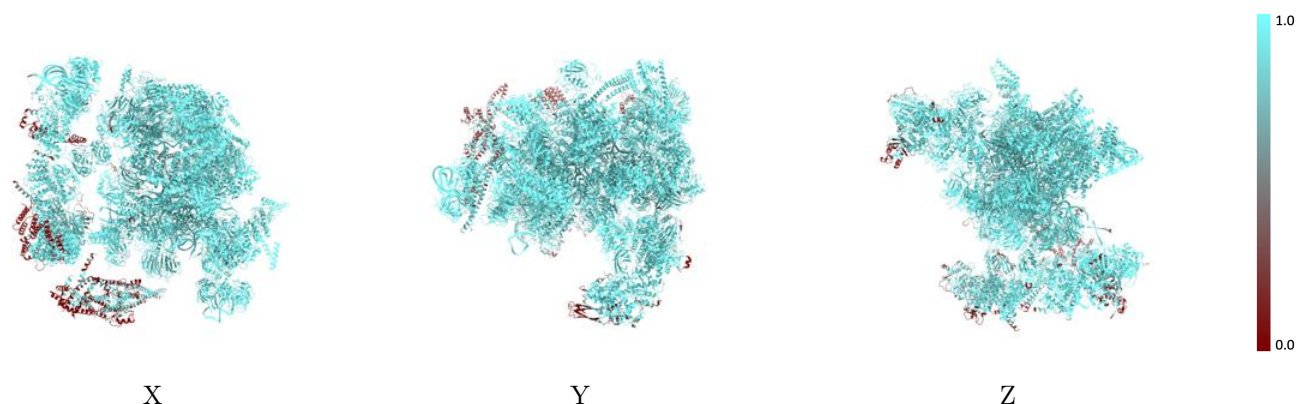
The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



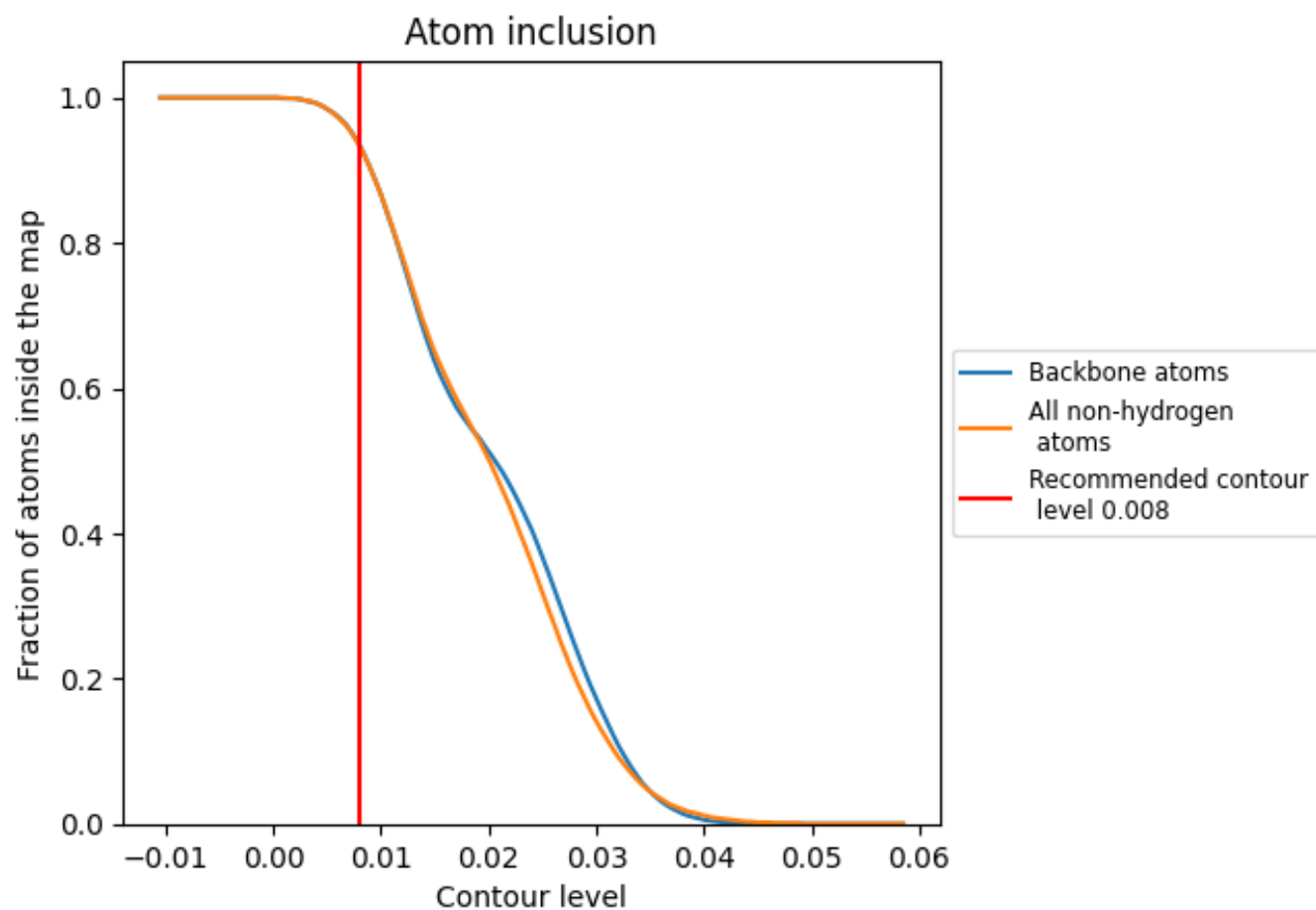
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.008).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9340	 0.1540
1	 1.0000	 0.0660
2	 0.9970	 0.0750
3	 1.0000	 0.0880
4	 0.9760	 0.0500
5	 1.0000	 0.0540
8	 1.0000	 0.0560
9	 1.0000	 0.1280
A	 1.0000	 0.2080
B	 1.0000	 0.2630
C	 1.0000	 0.2250
D	 1.0000	 0.1730
E	 1.0000	 0.2060
F	 0.9240	 0.1030
G	 1.0000	 0.2420
H	 0.9060	 0.0660
I	 0.9500	 0.1610
J	 0.7820	 0.0980
K	 0.4960	 0.0470
L	 1.0000	 0.2100
M	 0.5760	 0.0740
N	 1.0000	 0.1800
O	 1.0000	 0.2300
P	 0.7290	 0.1480
Q	 1.0000	 0.2160
R	 0.4040	 0.0800
S	 0.4540	 0.0980
T	 1.0000	 0.1910
U	 1.0000	 0.1740
V	 1.0000	 0.1690
W	 1.0000	 0.1580
X	 1.0000	 0.2050
Y	 1.0000	 0.2280
Z	 0.9970	 0.1790
a	 1.0000	 0.2030



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Chain	Atom inclusion	Q-score
b	 1.0000	 0.2060
c	 0.9060	 0.0830
d	 1.0000	 0.2540
e	 1.0000	 0.2500
f	 0.9650	 0.1380
g	 1.0000	 0.2490
h	 1.0000	 0.2580
i	 1.0000	 0.1840
j	 1.0000	 0.1550
k	 1.0000	 0.2230
l	 1.0000	 0.2280
m	 1.0000	 0.1410
n	 1.0000	 0.1570
o	 0.9970	 0.1020
p	 1.0000	 0.1470
q	 1.0000	 0.2510
r	 0.9690	 0.0720
s	 0.9130	 0.0600
t	 0.7880	 0.0750
u	 0.9840	 0.1530
v	 0.3870	 0.0640
w	 0.9930	 0.0850
x	 0.9730	 0.0850
y	 0.8370	 0.0520
z	 0.8100	 0.0550