



## Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:03 PM UTC

PDB ID : 6FF7 / pdb\_00006ff7  
EMDB ID : EMD-4240  
Title : human Bact spliceosome core structure  
Authors : Haselbach, D.; Komarov, I.; Agafonov, D.; Hartmuth, K.; Graf, B.; Kastner, B.; Luehrmann, R.; Stark, H.  
Deposited on : 2018-01-03  
Resolution : 4.50 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

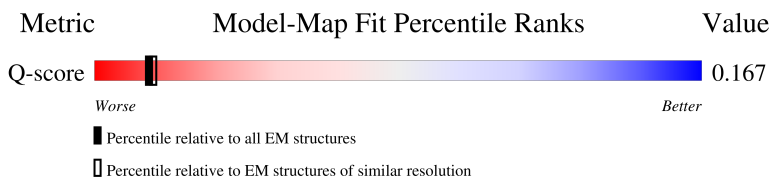
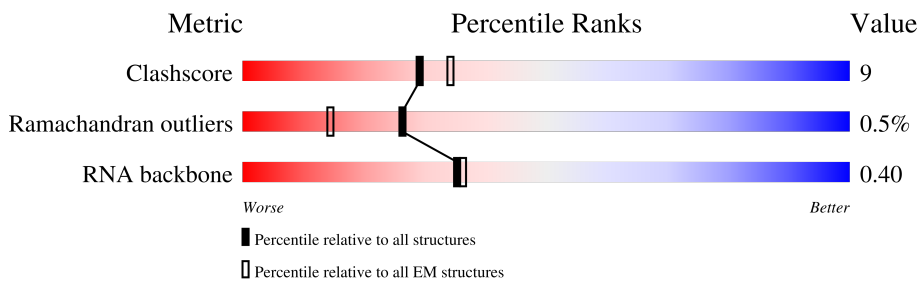
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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 4.50 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	-
RNA backbone	8273	3508	-
Q-score	-	25397	2937 ( 4.00 - 5.00 )

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  $\geq 3$ , 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	322	37% 62%
2	2	188	20% 12% 68%
3	3	619	19% 81%
4	5	116	32% 22% 6% 40%




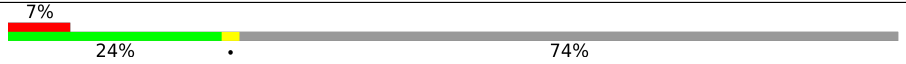
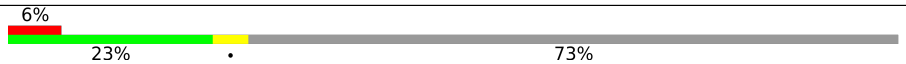
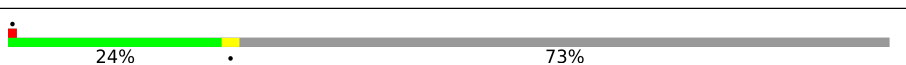

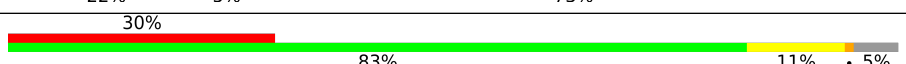
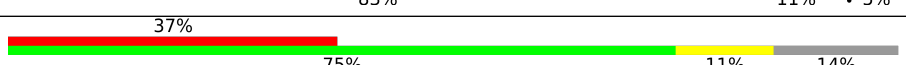

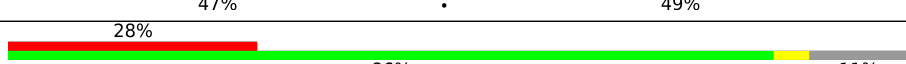

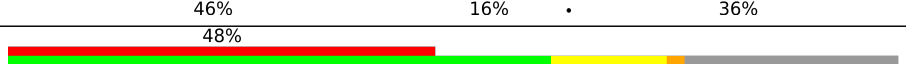
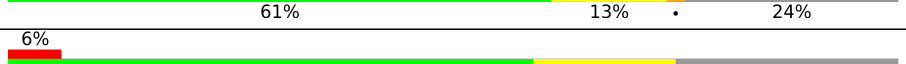





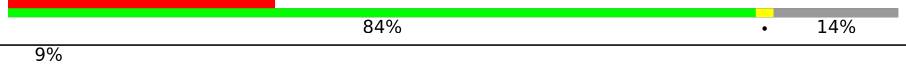
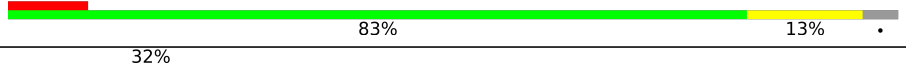
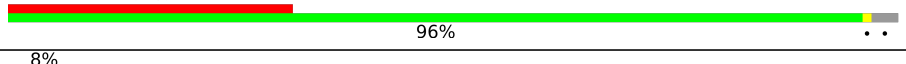

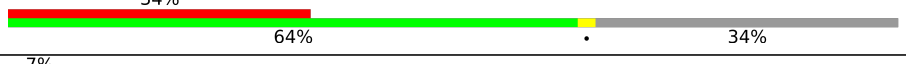

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Mol	Chain	Length	Quality of chain
5	6	107	60% 26% 11%
6	7	464	20% 80%
7	8	895	16% 84%
8	A	2335	94%
9	B	972	89% 7%
10	C	536	52% 47%
11	D	514	60% 38%
12	E	579	22% 78%
13	L	802	13% 87%
14	O	848	28% 70%
15	P	420	67% 32%
16	Q	144	94%
17	R	229	44% 55%
18	S	2752	99%
19	V	166	95%
20	Y	904	11% 89%
21	Z	369	7% 6% 87%
22	s	472	37% 63%
23	t	343	50% 50%
24	u	1304	66% 32%
25	v	1217	93% 5%
26	x	86	92% 8%
27	y	110	91% 9%
28	N	125	42% 38% 19%
28	z	125	47% 33% 19%

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Mol	Chain	Length	Quality of chain
29	0	396	
30	9	501	
31	F	357	
32	G	504	
32	H	504	
32	I	504	
32	J	504	
33	K	225	
34	M	855	
35	T	908	
36	U	1485	
37	W	255	
38	X	225	
39	a	118	
39	h	118	
40	b	86	
40	i	86	
41	c	92	
41	j	92	
42	d	76	
42	k	76	
43	e	126	
43	l	126	
44	f	240	
44	m	240	

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Mol	Chain	Length	Quality of chain
45	g	119	<p>66% 12% 22%</p>
45	n	119	<p>51% 59% 10% 31%</p>
46	o	301	<p>60% 67% 9% 24%</p>
47	p	793	<p>16% 20% 78%</p>
48	q	1041	<p>5% 57% 40%</p>
49	r	2136	<p>78% 19%</p>
50	w	285	<p>20% 16% 80%</p>

## 2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 88879 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 RNA-binding motif protein, X-linked 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	1	122	601	357	122	122	0	0

- Molecule 2 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	2	60	1262	565	207	430	60	0	0

- Molecule 3 is a protein called BUD13 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	3	118	584	348	118	118	0	0

- Molecule 4 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	5	70	1470	659	243	498	70	0	0

- Molecule 5 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	6	95	2035	910	377	653	95	0	0

- Molecule 6 is a protein called Splicing factor 3A subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	7	93	457	271	93	93	0	0

- Molecule 7 is a protein called Splicing factor 3B subunit 2.

Mol	Chain	Residues	Atoms			AltConf	Trace	
			Total	C	N			O
7	8	144	714	426	144	144	0	0

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

Mol	Chain	Residues	Atoms			AltConf	Trace	
			Total	C	N			O
8	A	2238	11093	6617	2238	2238	0	0

- Molecule 9 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms			AltConf	Trace	
			Total	C	N			O
9	B	902	4456	2652	902	902	0	0

- Molecule 10 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms			AltConf	Trace	
			Total	C	N			O
10	C	286	1418	846	286	286	0	0

- Molecule 11 is a protein called Pleiotropic regulator 1.

Mol	Chain	Residues	Atoms			AltConf	Trace	
			Total	C	N			O
11	D	320	1578	938	320	320	0	0

- Molecule 12 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms			AltConf	Trace	
			Total	C	N			O
12	E	130	642	382	130	130	0	0

- Molecule 13 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms			AltConf	Trace	
			Total	C	N			O
13	L	103	511	305	103	103	0	0

- Molecule 14 is a protein called Crooked neck-like protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	O	253	Total	C	N	O	0	0
			1260	754	253	253		

- Molecule 15 is a protein called Pre-mRNA-splicing factor RBM22.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	P	286	Total	C	N	O	0	0
			1413	841	286	286		

- Molecule 16 is a protein called Protein BUD31 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	Q	138	Total	C	N	O	0	0
			683	407	138	138		

- Molecule 17 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	R	102	Total	C	N	O	0	0
			507	303	102	102		

- Molecule 18 is a protein called Serine/arginine repetitive matrix protein 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	S	34	Total	C	N	O	0	0
			163	95	34	34		

- Molecule 19 is a protein called Peptidyl-prolyl cis-trans isomerase-like 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	V	159	Total	C	N	O	0	0
			775	457	159	159		

- Molecule 20 is a protein called Serine/arginine repetitive matrix protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	Y	95	Total	C	N	O	0	0
			470	280	95	95		

- Molecule 21 is a RNA chain called pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
21	Z	48	1013	454	173	338	48	0	0

- Molecule 22 is a protein called Peptidyl-prolyl cis-trans isomerase CWC27 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
22	s	175	859	509	175	175	0	0

- Molecule 23 is a protein called RING finger protein 113A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
23	t	172	849	505	172	172	0	0

- Molecule 24 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
24	u	881	4357	2595	881	881	0	0

- Molecule 25 is a protein called Splicing factor 3B subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
25	v	1189	5862	3484	1189	1189	0	0

- Molecule 26 is a protein called Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
26	x	79	391	233	79	79	0	0

- Molecule 27 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
27	y	100	490	290	100	100	0	0

- Molecule 28 is a protein called Splicing factor 3B subunit 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	z	101	Total	C	N	O	0	0
			500	298	101	101		
28	N	101	Total	C	N	O	0	0
			500	298	101	101		

- Molecule 29 is a protein called Smad nuclear-interacting protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	0	155	Total	C	N	O	0	0
			766	456	155	155		

- Molecule 30 is a protein called Splicing factor 3A subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	9	432	Total	C	N	O	0	0
			2139	1275	432	432		

- Molecule 31 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	F	299	Total	C	N	O	0	0
			1471	873	299	299		

- Molecule 32 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	G	132	Total	C	N	O	0	0
			659	395	132	132		
32	H	135	Total	C	N	O	0	0
			674	404	135	135		
32	I	134	Total	C	N	O	0	0
			669	401	134	134		
32	J	135	Total	C	N	O	0	0
			674	404	135	135		

- Molecule 33 is a protein called Pre-mRNA-splicing factor SPF27.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	K	213	Total	C	N	O	0	0
			1059	633	213	213		

- Molecule 34 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
34	M	738	3665	2189	738	738	0	0

- Molecule 35 is a protein called Pre-mRNA-splicing factor CWC22 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
35	T	462	2292	1368	462	462	0	0

- Molecule 36 is a protein called Intron-binding protein aquarius.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
36	U	1329	6588	3930	1329	1329	0	0

- Molecule 37 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
37	W	162	804	480	162	162	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	89	ASP	CYS	conflict	UNP P09661
W	119	CYS	SER	conflict	UNP P09661

- Molecule 38 is a protein called U2 small nuclear ribonucleoprotein B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
38	X	171	844	502	171	171	0	0

- Molecule 39 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
39	a	89	440	262	89	89	0	0
39	h	98	485	289	98	98	0	0

- Molecule 40 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	b	73	Total	C	N	O	0	0
			356	210	73	73		
40	i	74	Total	C	N	O	0	0
			361	213	74	74		

- Molecule 41 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	c	78	Total	C	N	O	0	0
			386	230	78	78		
41	j	79	Total	C	N	O	0	0
			391	233	79	79		

- Molecule 42 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	d	73	Total	C	N	O	0	0
			358	212	73	73		
42	k	74	Total	C	N	O	0	0
			363	215	74	74		

- Molecule 43 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	e	88	Total	C	N	O	0	0
			434	258	88	88		
43	l	83	Total	C	N	O	0	0
			409	243	83	83		

- Molecule 44 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	f	89	Total	C	N	O	0	0
			439	261	89	89		
44	m	71	Total	C	N	O	0	0
			349	207	71	71		

- Molecule 45 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	g	93	Total	C	N	O	0	0
			461	275	93	93		

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
45	n	82	406	242	82	82	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
46	o	229	1119	661	229	229	0	0

- Molecule 47 is a protein called Splicing factor 3A subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
47	p	175	870	520	175	175	0	0

- Molecule 48 is a protein called Putative pre-mRNA-splicing factor ATP-dependent RNA helicase DHX16.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
48	q	625	3091	1841	625	625	0	0

- Molecule 49 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
49	r	1722	8530	5086	1722	1722	0	0

- Molecule 50 is a protein called Pre-mRNA-splicing factor ISY1 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
50	w	56	276	164	56	56	0	0

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

Mol	Chain	Residues	Atoms		AltConf
51	2	1	Total	Zn	0
			1	1	
51	P	3	Total	Zn	0
			3	3	

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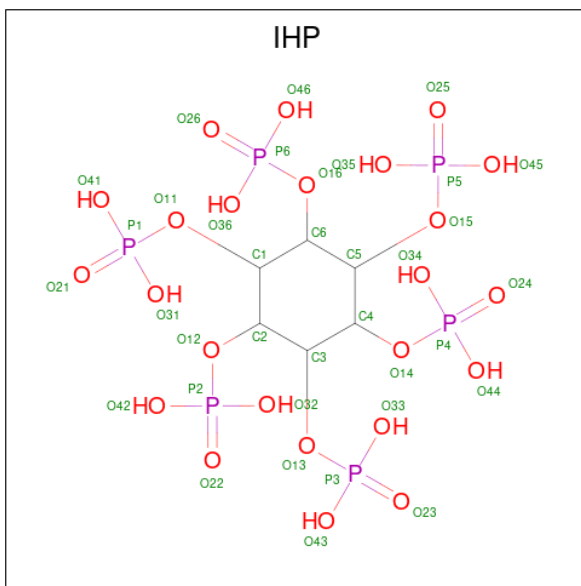
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Mol	Chain	Residues	Atoms		AltConf
51	Q	3	Total	Zn	0
			3	3	
51	Z	1	Total	Zn	0
			1	1	
51	y	3	Total	Zn	0
			3	3	

- Molecule 52 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

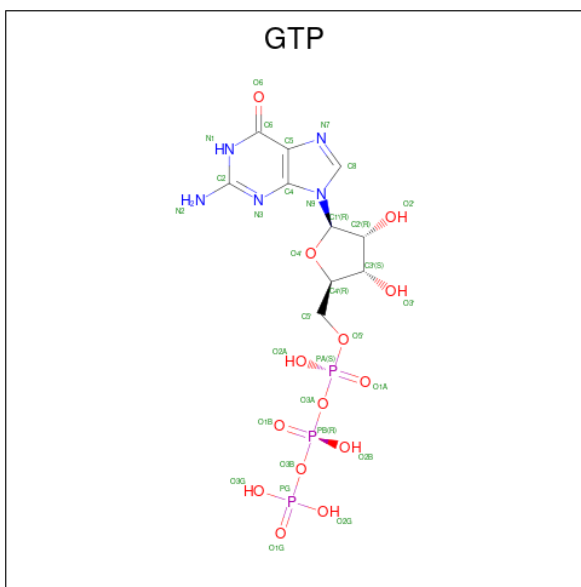
Mol	Chain	Residues	Atoms		AltConf
52	6	4	Total	Mg	0
			4	4	
52	r	1	Total	Mg	0
			1	1	

- Molecule 53 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: C<sub>6</sub>H<sub>18</sub>O<sub>24</sub>P<sub>6</sub>).



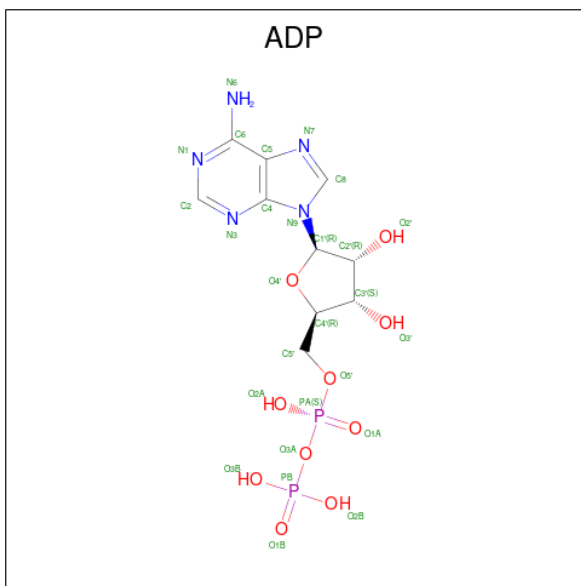
Mol	Chain	Residues	Atoms				AltConf
53	A	1	Total	C	O	P	0
			36	6	24	6	

- Molecule 54 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>).



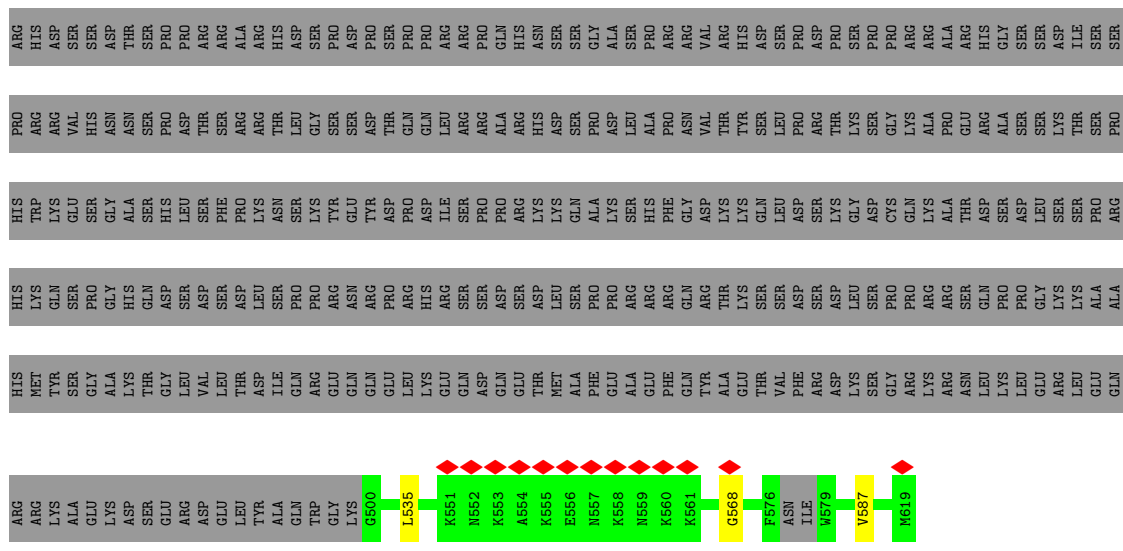
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
54	B	1	32	10	5	14	3	0

- Molecule 55 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).

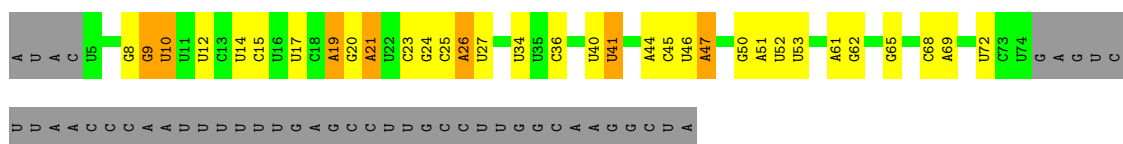
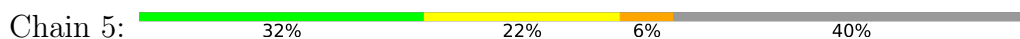


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
55	r	1	27	10	5	10	2	0
55	r	1	27	10	5	10	2	0

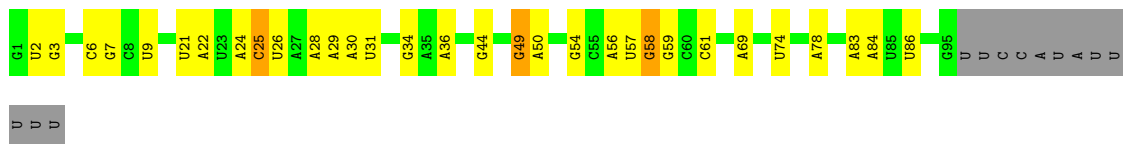




• Molecule 4: U5 snRNA



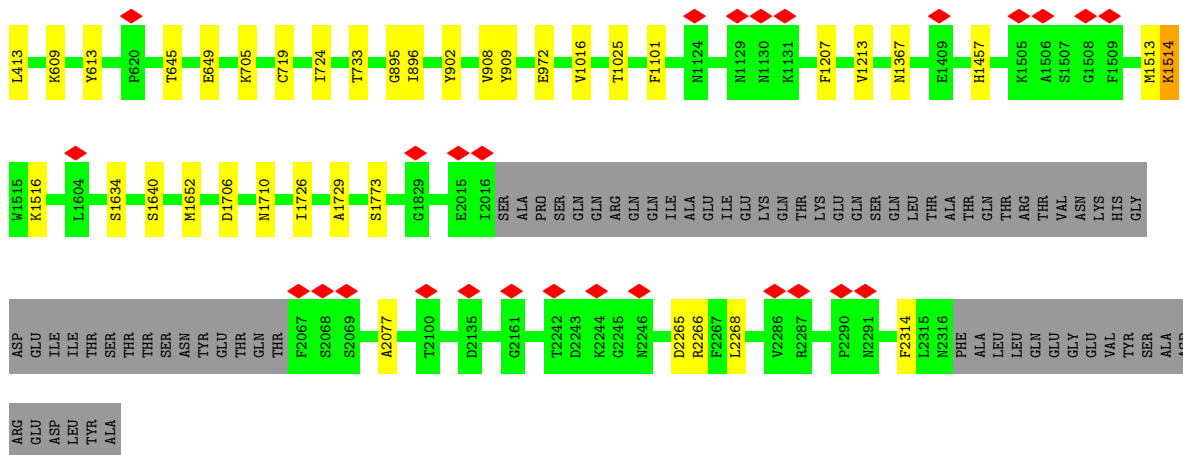
• Molecule 5: U6 snRNA



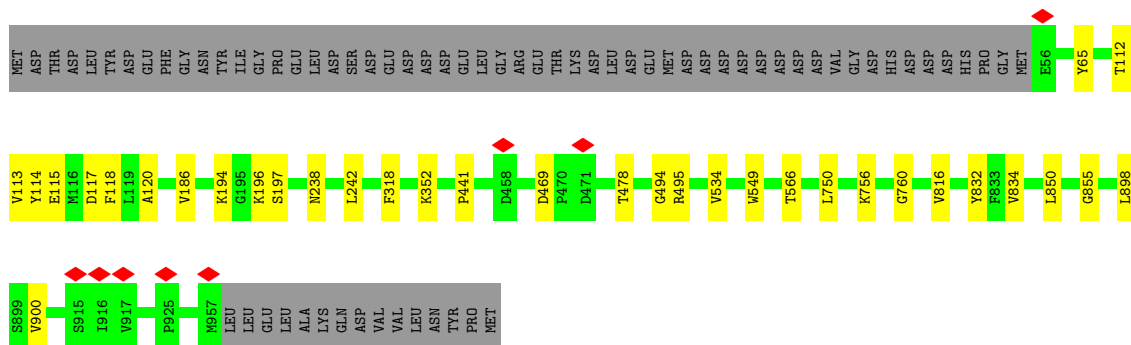
• Molecule 6: Splicing factor 3A subunit 2



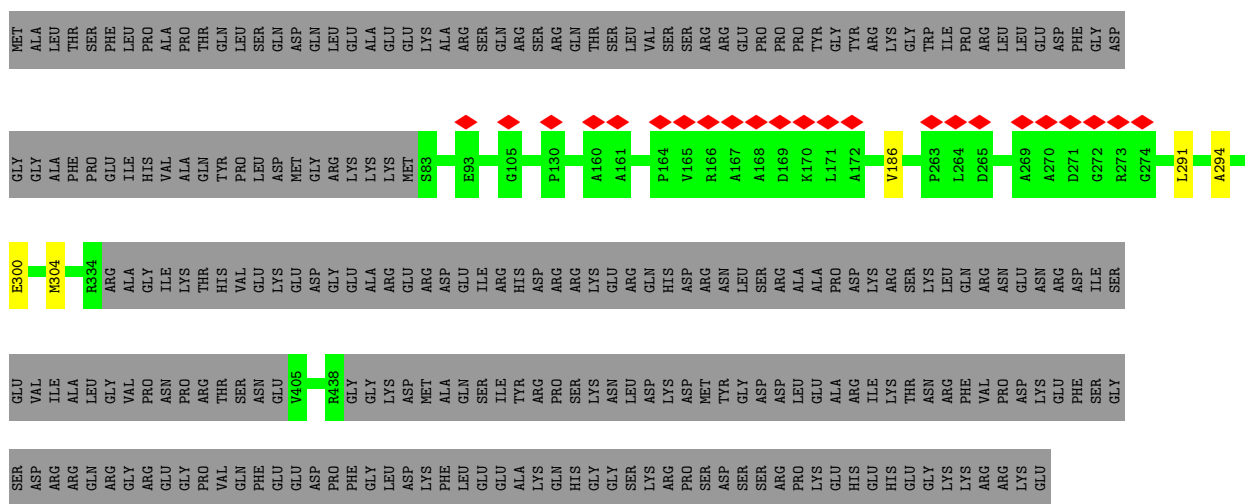




- Molecule 9: 116 kDa U5 small nuclear ribonucleoprotein component



- Molecule 10: SNW domain-containing protein 1



- Molecule 11: Pleiotropic regulator 1





LYS  
GLU  
LYS  
GLU  
ARG  
VAL  
SER  
ASP  
ALA  
LEU  
GLY  
LEU  
MET

GLU  
LYS  
GLU  
ASP  
ALA  
GLY  
HIS  
PRO  
ASP  
GLU  
VAL  
ASP  
SER  
SER

• Molecule 15: Pre-mRNA-splicing factor RBM22



MET  
ALA  
THR  
SER  
LEU  
GLY  
SER  
ASN  
THR  
TYR  
ASN  
ARG  
GLY  
ASN  
W15  
R64  
D105  
S128  
V134  
F167  
E172  
P192  
LEU  
ALA  
ASP  
GLN  
ASN  
ILE  
LYS  
PRO  
ASP  
R201  
L223  
D224  
P225  
P226  
E227  
D228  
R229  
D241  
T242  
Q254  
T276  
A280  
A283  
I292  
Y293

M294  
G295  
A308  
GLY  
LYS  
GLU  
LYS  
PRO  
ASP  
THR  
THR  
ASP  
SER  
PRO  
MET  
ILE  
PHE  
HIS  
LEU  
GLU  
VAL  
PRO  
GLY  
PRO  
LEU  
PRO  
MET  
ALA  
LEU  
PRO  
GLY  
PRO  
PRO  
ILE  
HIS  
TYR  
PRO  
GLU  
SER  
GLN  
ALA  
SER  
ALA  
GLN  
ARG  
MET  
PHE  
ALA  
PRO  
GLY  
HIS  
PRO  
SER  
SER  
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ALA

LEU  
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ALA  
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GLY  
PHE  
GLY  
GLY  
HIS  
MET  
PHE  
HIS  
PRO  
MET  
GLY  
VAL  
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PRO  
PRO  
PRO  
PHE  
MET  
ARG  
ALA  
PRO  
GLY  
PRO  
PRO  
ILE  
HIS  
TYR  
PRO  
GLU  
SER  
GLN  
ASP  
PRO  
GLN  
ARG  
MET  
GLY  
ALA  
HIS  
ALA  
PRO  
GLY  
HIS  
SER  
SER  
PRO  
PRO

• Molecule 16: Protein BUD31 homolog



MET  
PRO  
K3  
D13  
G14  
I106  
R140  
GLY  
CYS  
SER  
GLY

• Molecule 17: Spliceosome-associated protein CWC15 homolog



MET  
THR  
THR  
ALA  
ALA  
ARG  
PRO  
THR  
PHE  
GLU  
ASP  
PRO  
ALA  
ALA  
GLY  
GLY  
ARG  
GLY  
K18  
T47  
W75  
ARG  
ASP  
ARG  
PRO  
THR  
ARG  
GLU  
HIS  
THR  
SER  
SER  
SER  
SER  
VAL  
SER  
SER  
LYS  
LYS  
PRO  
ARG  
LEU  
ASP  
GLN  
ILE  
PRO  
ALA  
ALA  
ASN  
LEU  
ASP  
ALA  
ASP  
PRO  
PRO  
THR  
LEU  
THR  
ASP  
GLU

ASP  
GLU  
PHE  
GLU  
GLU  
SER  
ASP  
ASP  
ASP  
THR  
ALA  
ALA  
LEU  
LEU  
ALA  
ALA  
K18  
T47  
W75  
ARG  
ASP  
ARG  
PRO  
THR  
ARG  
GLU  
HIS  
THR  
SER  
SER  
SER  
SER  
VAL  
SER  
SER  
LYS  
LYS  
PRO  
ARG  
LEU  
ASP  
GLN  
ILE  
PRO  
ALA  
ALA  
ASN  
LEU  
ASP  
ALA  
ASP  
PRO  
PRO  
THR  
LEU  
THR  
ASP  
GLU

GLY  
PRO  
SER  
GLN  
PRO  
GLN  
ALA  
ASN  
PHE  
LYS  
VAL  
LYS  
R186  
R187  
V201  
K229

• Molecule 18: Serine/arginine repetitive matrix protein 2



M1  
Y2  
N3  
G4  
I5  
G6  
L7  
P8  
S13  
R27  
G28  
P34  
ASP  
TYR  
LEU  
GLU  
GLY  
GLY  
GLU  
GLU  
LEU  
ARG  
ARG  
LEU  
GLU  
ALA  
ALA  
LEU  
VAL  
LYS  
ARG  
PRO  
PRO  
ALA  
VAL  
THR  
THR  
GLU  
THR  
HIS  
GLN  
LEU  
ALA  
ARG  
LYS  
ARG  
VAL  
GLU  
LEU  
LYS  
LYS  
ASN  
GLY  
ARG  
LEU  
ARG  
GLU  
GLU  
LEU  
ALA  
ALA  
MET  
MET  
GLU  
GLU

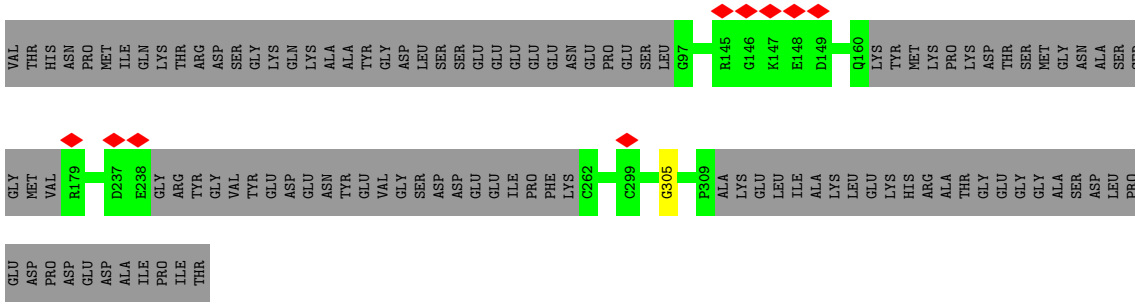
GLN  
GLY  
TYR  
GLU  
GLU  
GLN  
GLN  
ILE  
GLN  
LYS  
VAL  
ALA  
THR  
PHE  
ARG  
LEU  
MET  
LEU  
LEU  
GLU  
LYS  
VAL  
ASN  
PRO  
GLY  
GLY  
LYS  
GLU  
GLU  
THR  
THR  
GLY  
THR  
HIS  
GLN  
LEU  
ALA  
ARG  
LYS  
ARG  
VAL  
GLU  
LEU  
LYS  
LYS  
ASN  
GLY  
ARG  
LEU  
ARG  
ALA  
ALA  
MET  
MET  
PHE



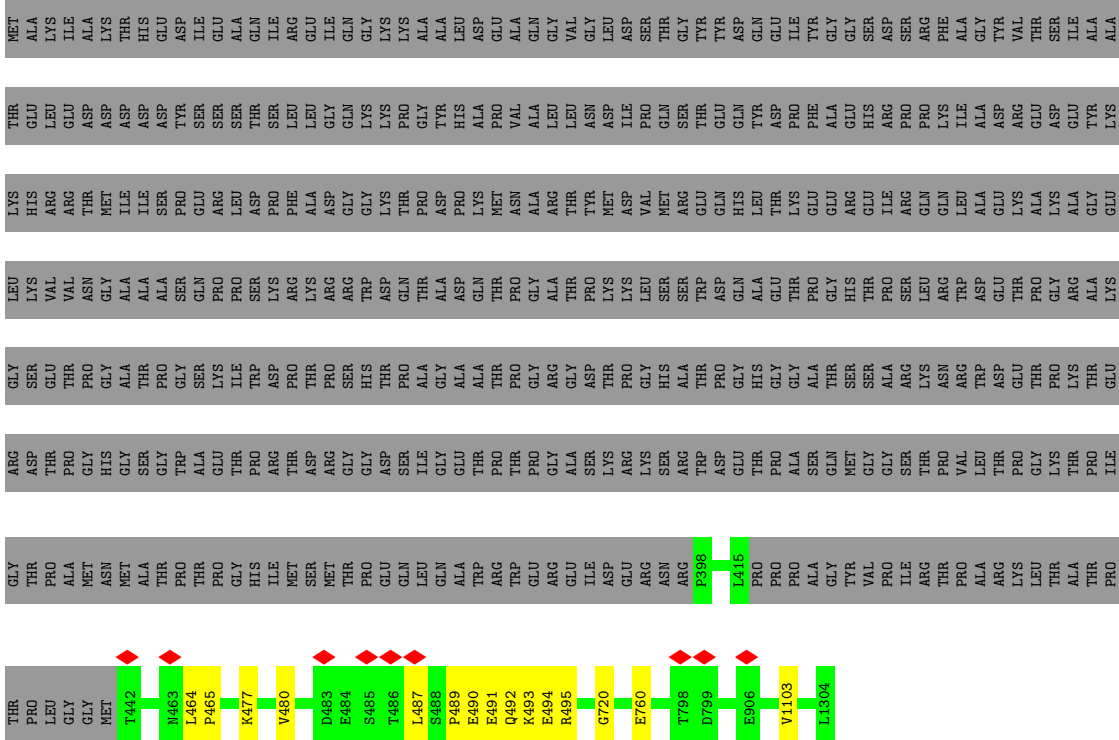




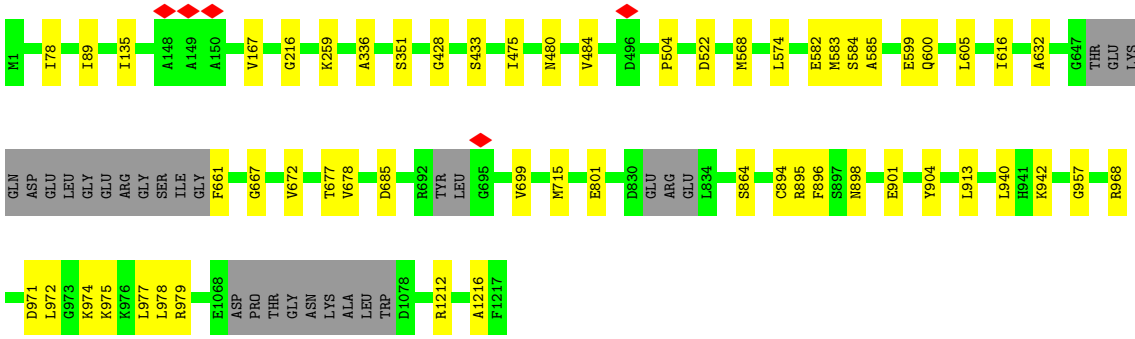
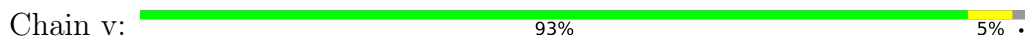




• Molecule 24: Splicing factor 3B subunit 1

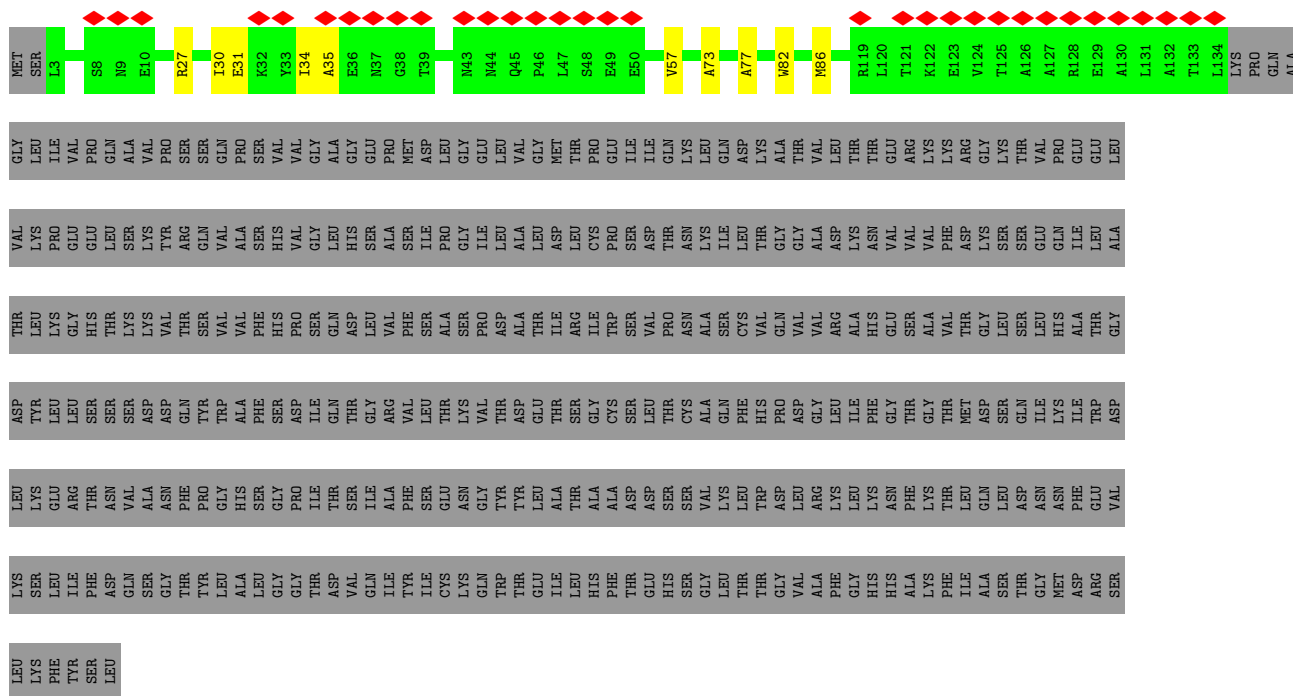


• Molecule 25: Splicing factor 3B subunit 3

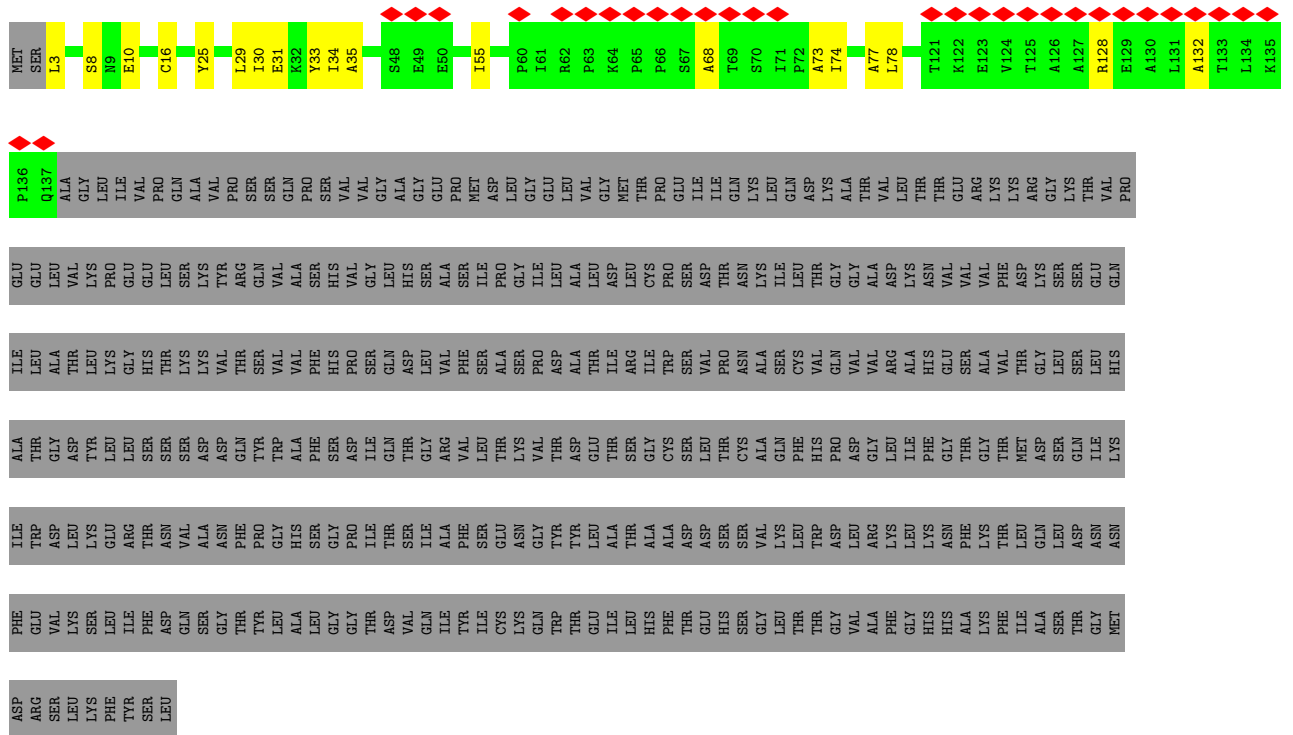






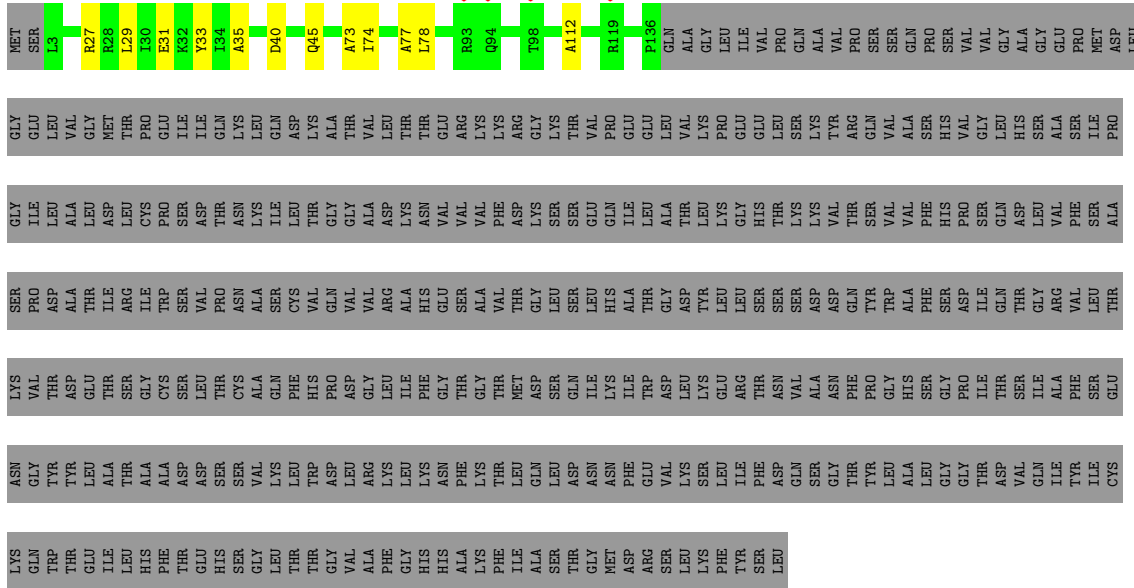


- Molecule 32: Pre-mRNA-processing factor 19

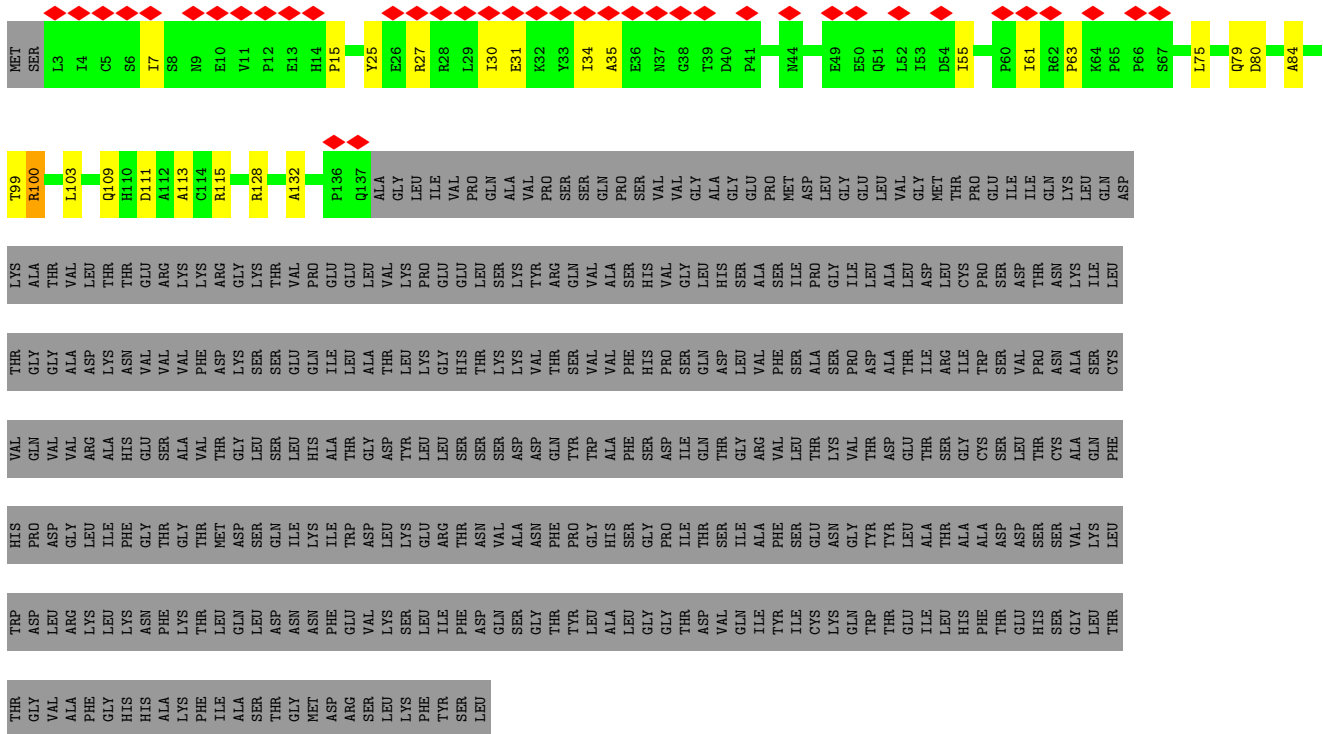


- Molecule 32: Pre-mRNA-processing factor 19

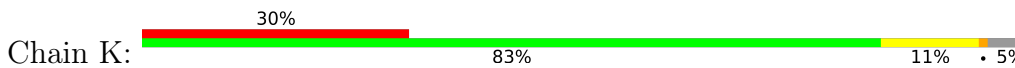


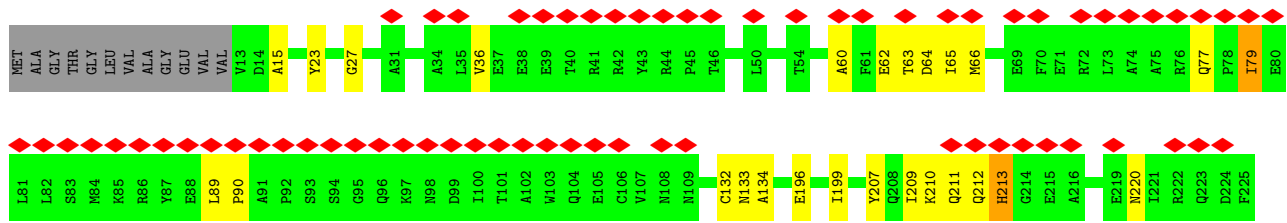


• Molecule 32: Pre-mRNA-processing factor 19

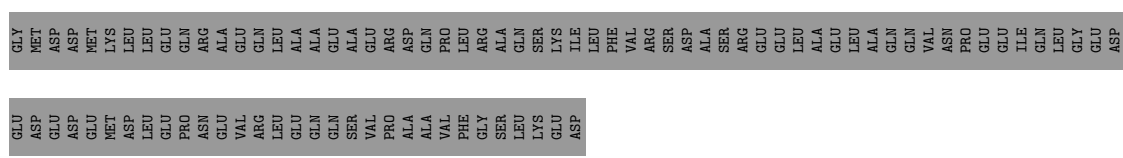
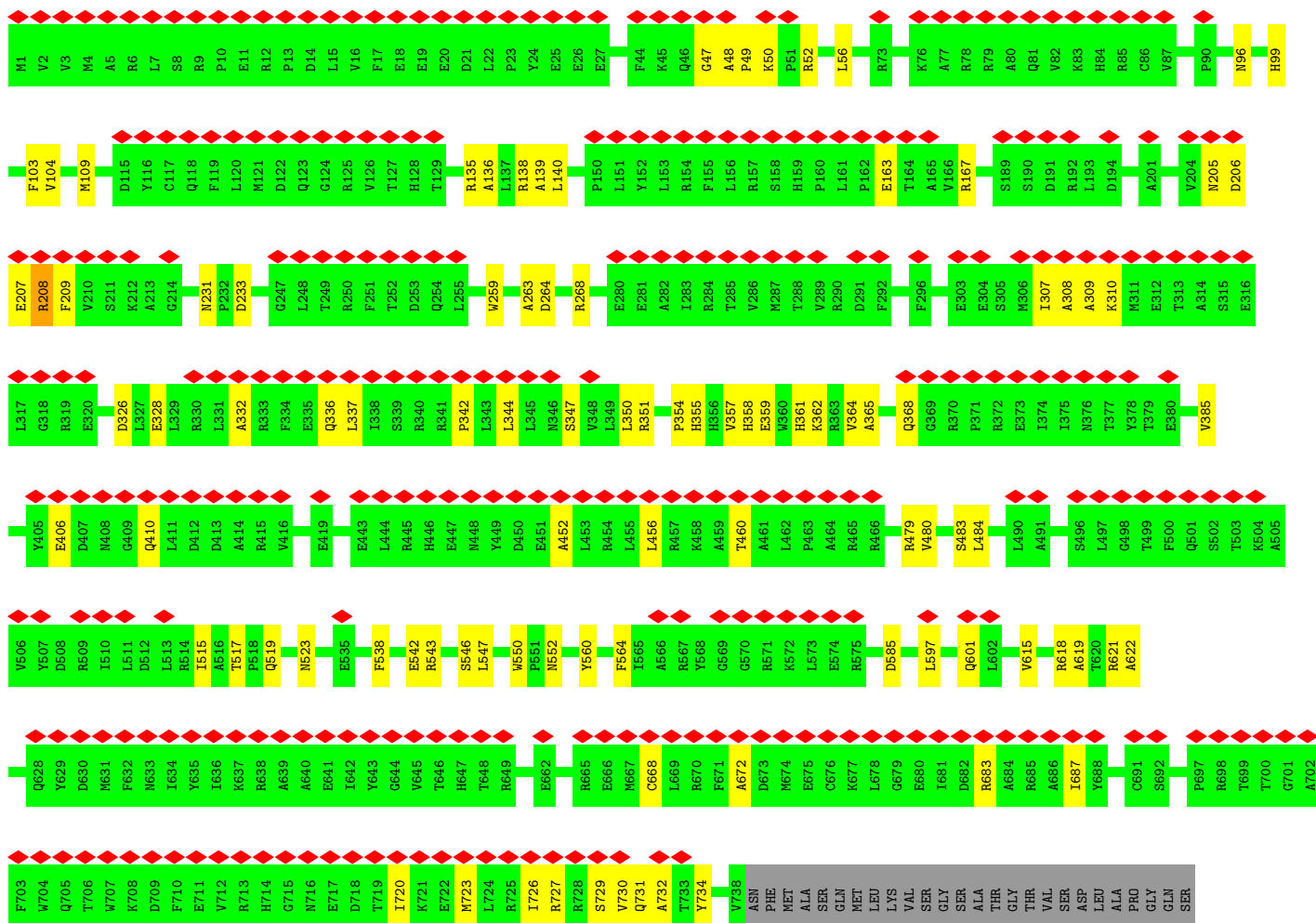
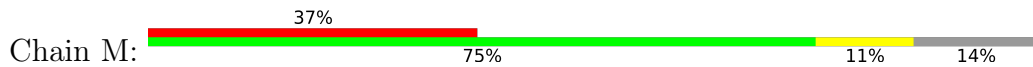


• Molecule 33: Pre-mRNA-splicing factor SPF27



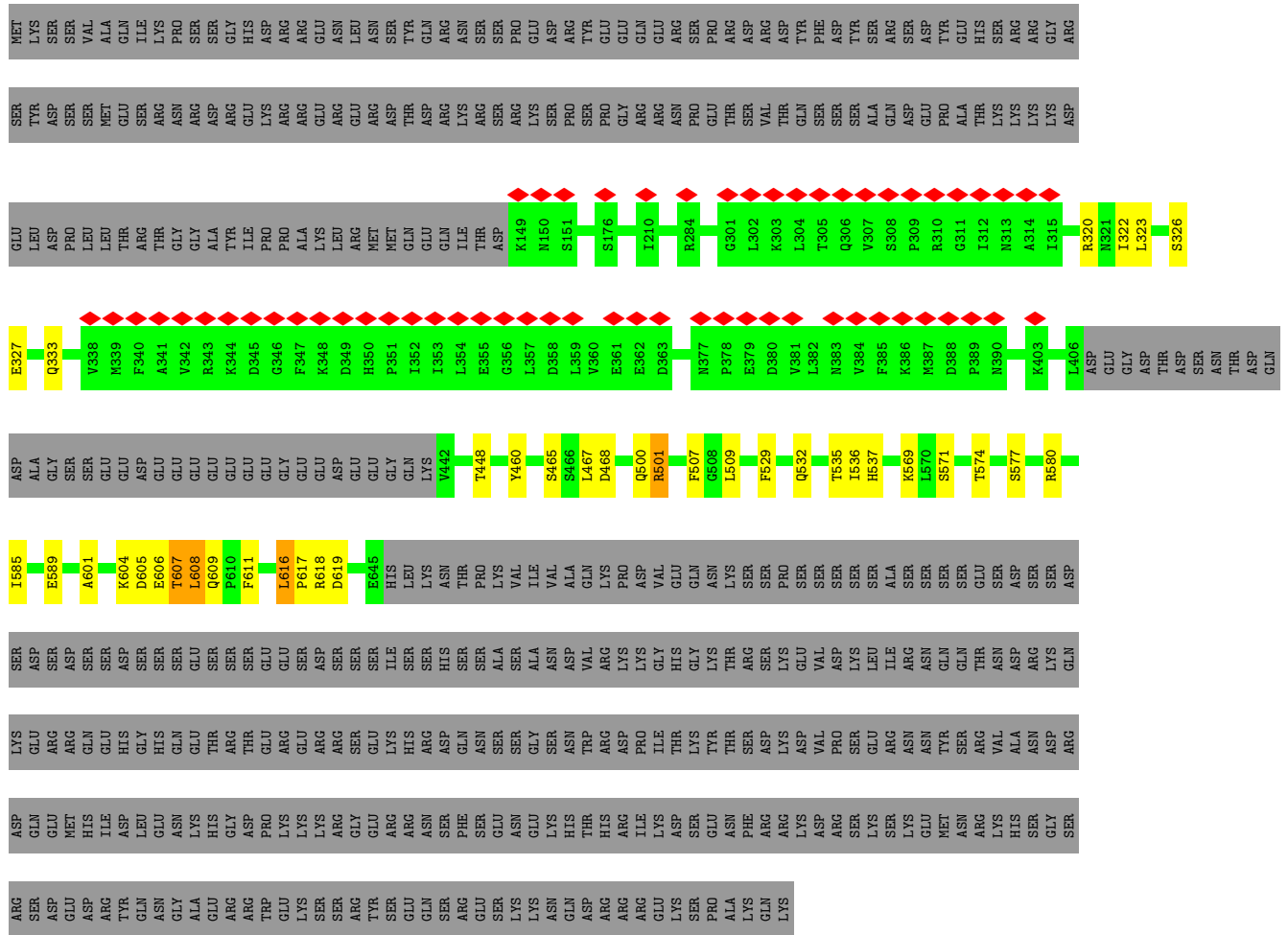


• Molecule 34: Pre-mRNA-splicing factor SYF1

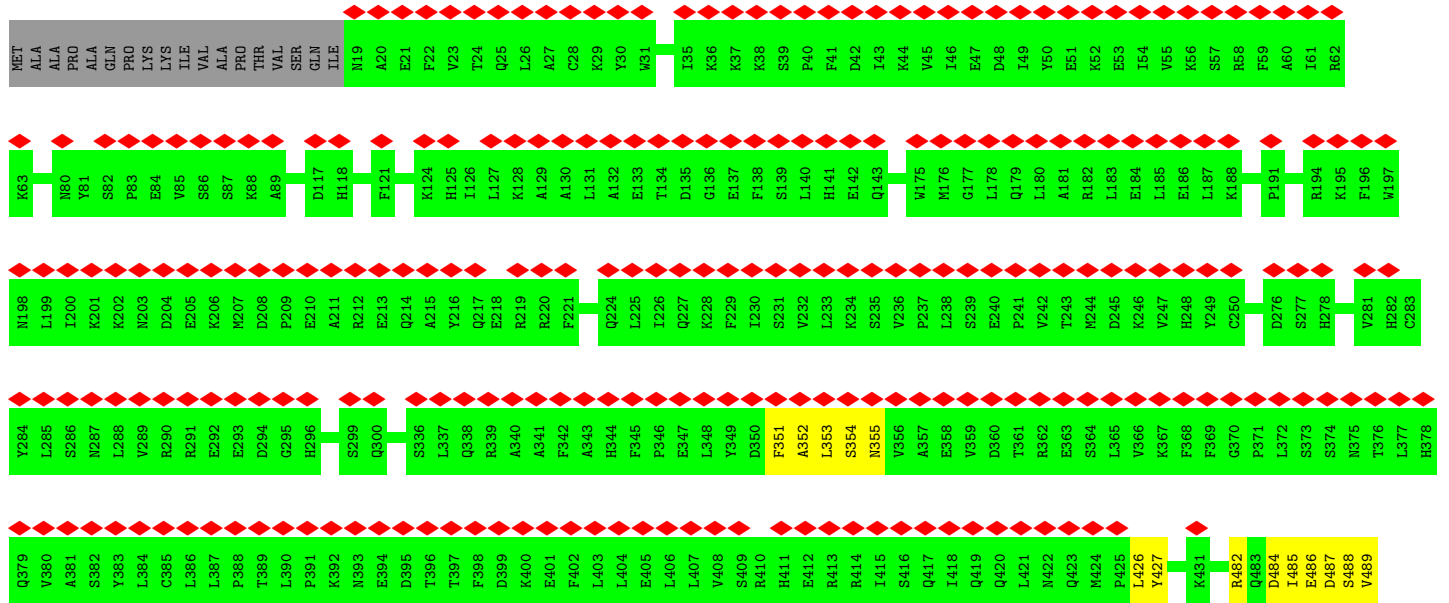
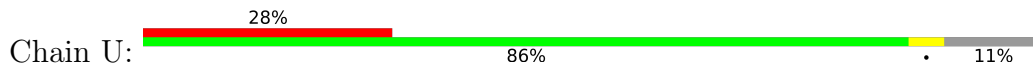


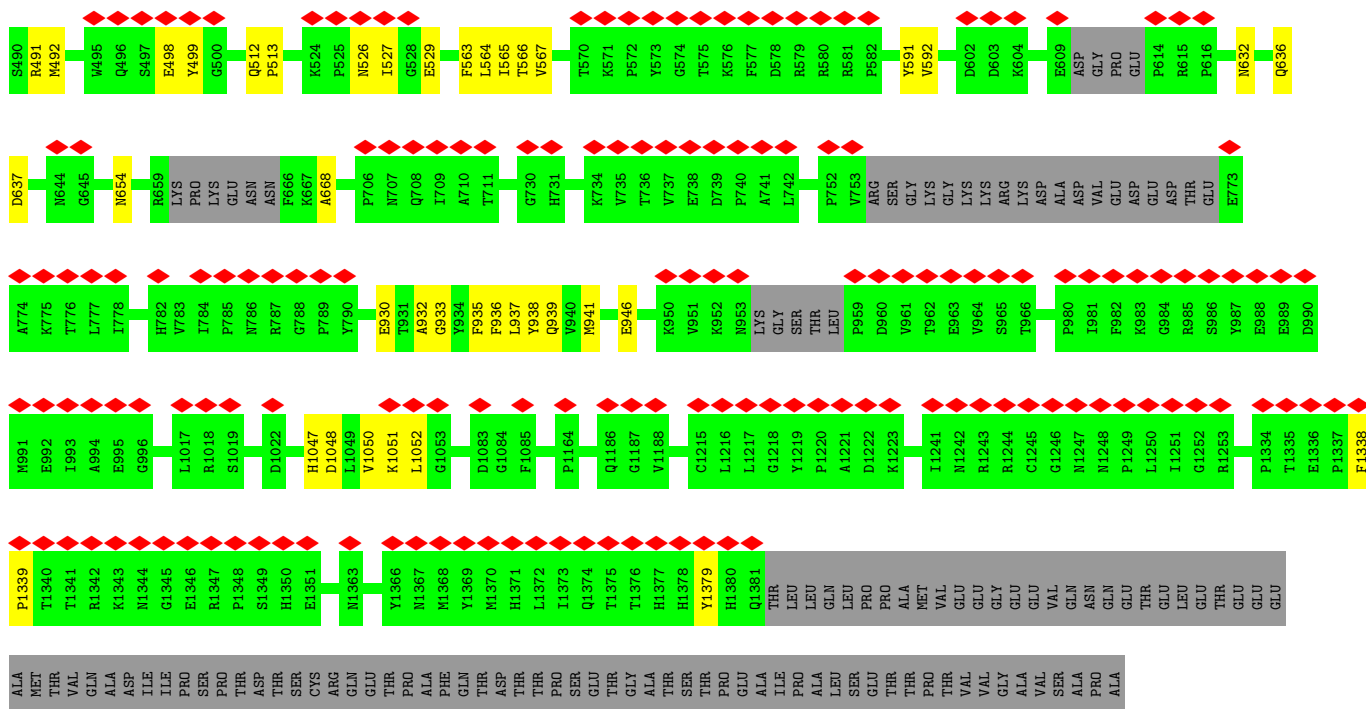
• Molecule 35: Pre-mRNA-splicing factor CWC22 homolog



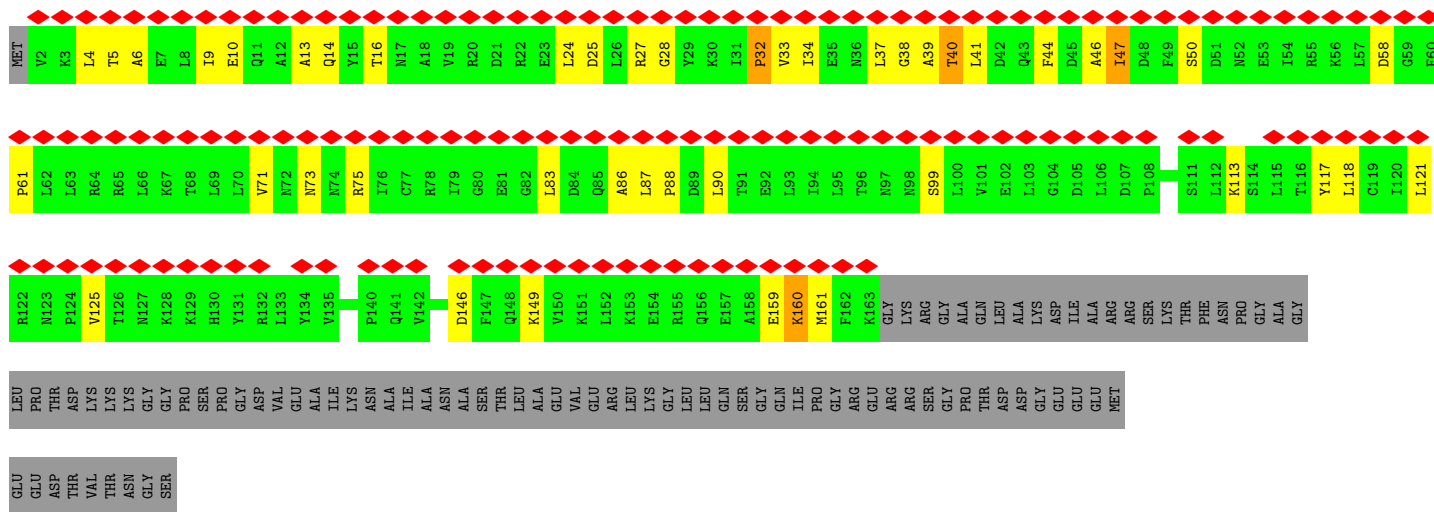


• Molecule 36: Intron-binding protein aquarius

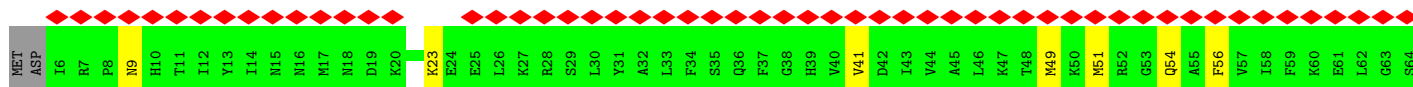


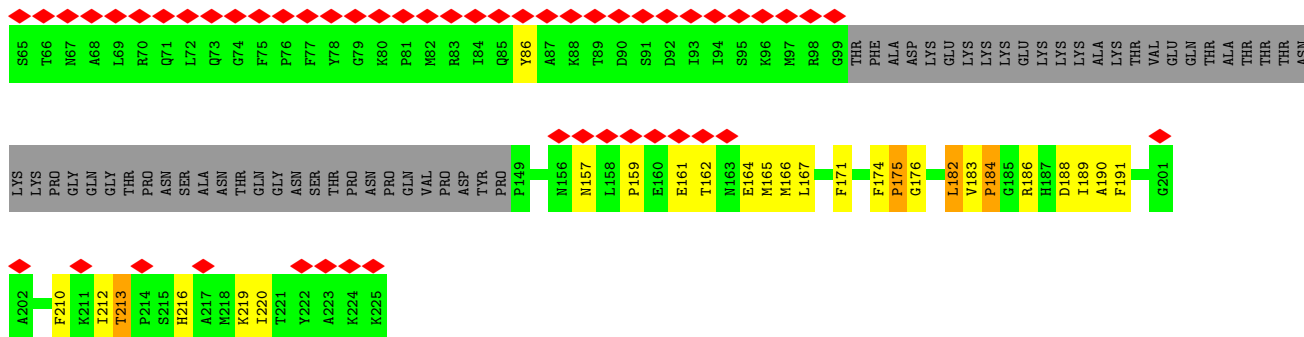


• Molecule 37: U2 small nuclear ribonucleoprotein A'

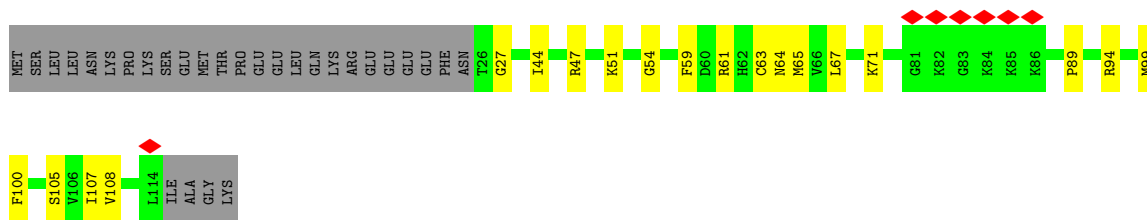


• Molecule 38: U2 small nuclear ribonucleoprotein B''

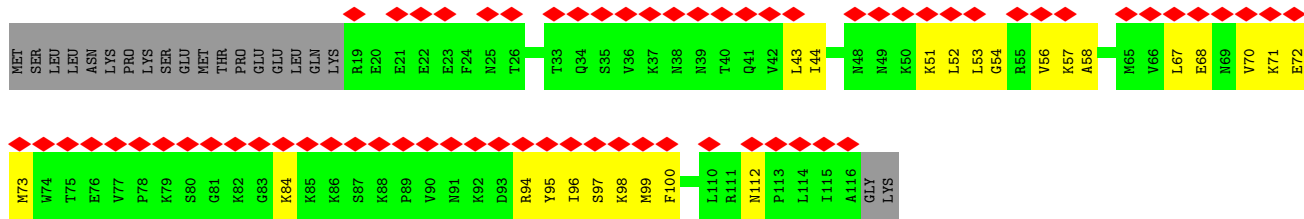




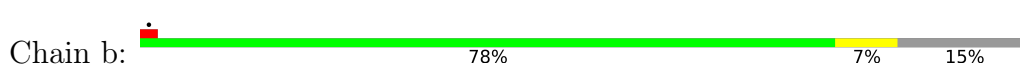
● Molecule 39: Small nuclear ribonucleoprotein Sm D2



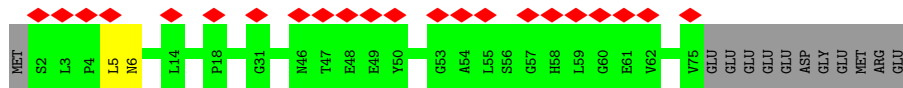
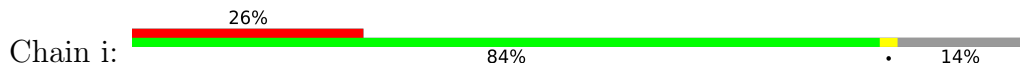
● Molecule 39: Small nuclear ribonucleoprotein Sm D2



● Molecule 40: Small nuclear ribonucleoprotein F



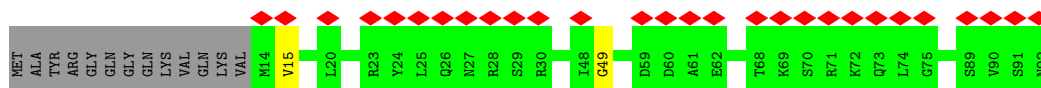
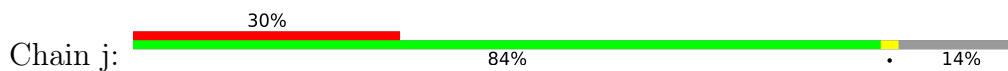
● Molecule 40: Small nuclear ribonucleoprotein F



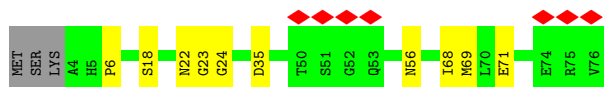
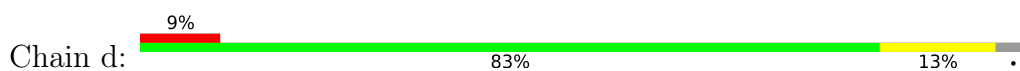
● Molecule 41: Small nuclear ribonucleoprotein E



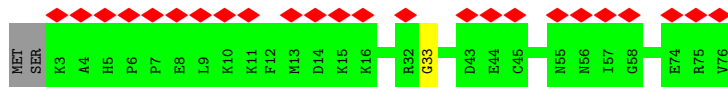
• Molecule 41: Small nuclear ribonucleoprotein E



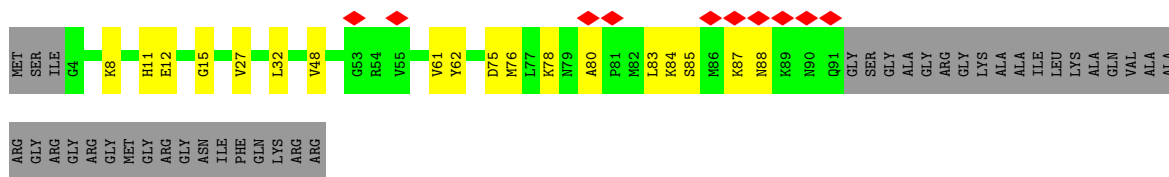
• Molecule 42: Small nuclear ribonucleoprotein G



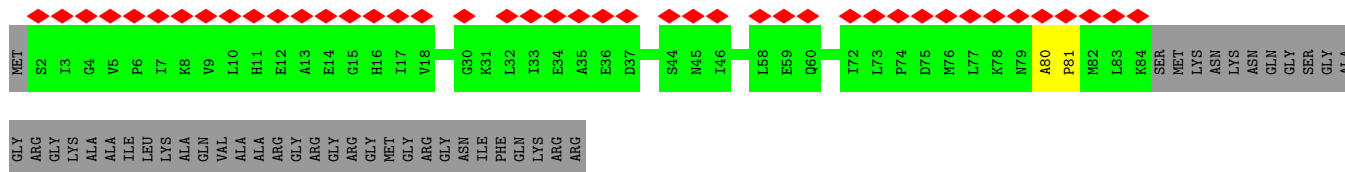
• Molecule 42: Small nuclear ribonucleoprotein G



• Molecule 43: Small nuclear ribonucleoprotein Sm D3



• Molecule 43: Small nuclear ribonucleoprotein Sm D3

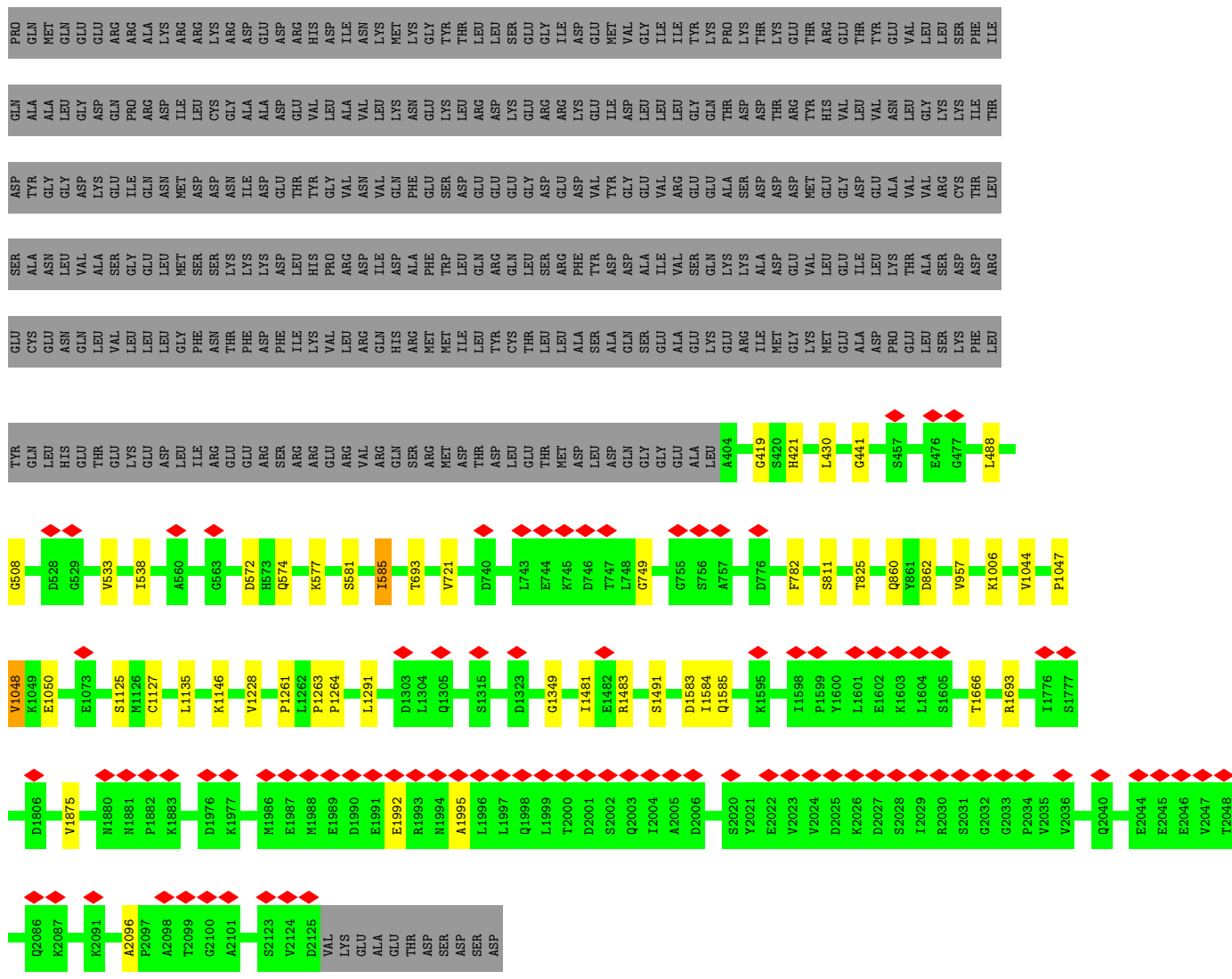


• Molecule 44: Small nuclear ribonucleoprotein-associated proteins B and B'

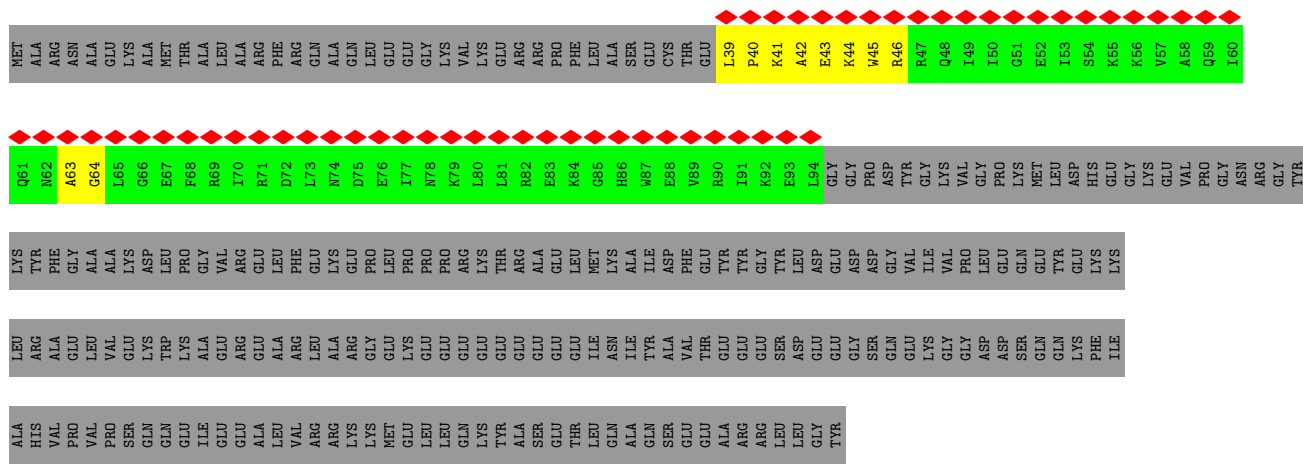








• Molecule 50: Pre-mRNA-splicing factor ISY1 homolog



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	165853	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.062	Depositor
Minimum map value	-0.014	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.013	Depositor
Map size ( $\text{\AA}$ )	487.19998, 487.19998, 487.19998	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.16, 1.16, 1.16	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: ADP, GTP, MG, ZN, IHP

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	0.23	0/600	0.60	0/833
2	2	0.11	0/1404	0.25	0/2177
3	3	0.30	0/583	0.75	1/811 (0.1%)
4	5	0.15	0/1638	0.33	0/2545
5	6	0.13	0/2279	0.28	0/3551
6	7	0.21	0/456	0.59	0/632
7	8	0.23	0/713	0.62	0/993
8	A	0.27	1/11090 (0.0%)	0.70	13/15463 (0.1%)
9	B	0.31	1/4455 (0.0%)	0.74	2/6203 (0.0%)
10	C	0.30	0/1416	0.81	1/1972 (0.1%)
11	D	0.28	0/1577	0.75	0/2193
12	E	0.24	0/640	0.67	2/888 (0.2%)
13	L	0.28	0/510	0.76	2/710 (0.3%)
14	O	0.27	0/1259	0.74	4/1758 (0.2%)
15	P	0.29	0/1411	0.71	0/1962
16	Q	0.28	0/682	0.73	1/949 (0.1%)
17	R	0.29	0/505	0.77	2/702 (0.3%)
18	S	0.20	0/162	0.61	0/221
19	V	0.19	0/774	0.52	1/1070 (0.1%)
20	Y	0.25	0/469	0.59	0/652
21	Z	0.13	0/1129	0.30	0/1752
22	s	0.28	0/858	0.72	0/1190
23	t	0.26	0/846	0.67	0/1173
24	u	0.28	0/4355	0.68	2/6065 (0.0%)
25	v	0.26	0/5857	0.66	0/8142
26	x	0.22	0/390	0.59	0/542
27	y	0.17	0/489	0.50	0/677
28	N	0.38	0/499	1.09	1/694 (0.1%)
28	z	0.29	0/499	0.71	0/694
29	0	0.98	0/765	1.68	10/1064 (0.9%)
30	9	0.54	0/2131	0.97	8/2958 (0.3%)
31	F	0.75	1/1470 (0.1%)	1.09	4/2042 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	G	0.14	0/658	0.37	0/919
32	H	0.16	0/673	0.41	0/940
32	I	0.13	0/668	0.38	0/933
32	J	0.16	0/673	0.51	1/940 (0.1%)
33	K	0.39	0/1058	0.78	1/1476 (0.1%)
34	M	0.43	1/3662 (0.0%)	0.55	3/5107 (0.1%)
35	T	0.58	1/2290 (0.0%)	0.97	7/3192 (0.2%)
36	U	0.37	0/6582	0.86	1/9171 (0.0%)
37	W	0.97	0/803	2.24	42/1119 (3.8%)
38	X	1.23	0/841	1.82	14/1166 (1.2%)
39	a	0.87	0/439	1.12	2/610 (0.3%)
39	h	1.07	0/484	1.21	2/673 (0.3%)
40	b	0.91	0/355	1.19	1/490 (0.2%)
40	i	1.07	0/360	1.22	1/497 (0.2%)
41	c	1.00	0/385	1.17	1/535 (0.2%)
41	j	1.03	0/390	1.22	0/542
42	d	0.98	0/357	1.27	5/494 (1.0%)
42	k	0.80	0/362	1.04	0/501
43	e	0.86	0/433	1.13	2/601 (0.3%)
43	l	0.74	0/408	1.00	0/566
44	f	0.93	0/438	1.18	5/608 (0.8%)
44	m	0.72	0/347	0.97	0/479
45	g	1.02	1/459 (0.2%)	1.29	3/637 (0.5%)
45	n	0.87	0/405	1.07	0/563
46	o	0.77	0/1115	0.86	0/1539
47	p	0.58	0/867	4.00	7/1206 (0.6%)
48	q	0.68	0/3090	1.60	23/4304 (0.5%)
49	r	0.55	0/8529	1.11	27/11891 (0.2%)
50	w	1.48	0/275	1.51	0/381
All	All	0.48	6/89317 (0.0%)	0.97	202/125358 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	3	0	1
8	A	0	2
9	B	0	6
11	D	0	1
14	O	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
15	P	0	1
19	V	0	1
24	u	0	1
25	v	0	5
28	z	0	2
29	0	0	1
30	9	0	2
32	J	1	0
33	K	0	3
34	M	0	2
39	h	0	1
47	p	0	4
49	r	0	1
All	All	1	36

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	M	208	ARG	C-N	24.29	1.67	1.33
35	T	616	LEU	C-N	6.58	1.49	1.33
31	F	102	TYR	CA-C	6.06	1.55	1.52
8	A	733	THR	C-N	5.39	1.40	1.34
9	B	566	THR	C-N	5.36	1.44	1.33
45	g	34	VAL	CA-CB	5.25	1.61	1.54

All (202) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	p	232	GLU	O-C-N	-78.64	18.00	122.59
47	p	222	PRO	O-C-N	-72.46	24.82	122.64
47	p	236	PRO	O-C-N	-72.36	24.95	122.64
47	p	235	ASN	O-C-N	-17.12	106.80	121.35
34	M	208	ARG	O-C-N	-16.33	100.80	122.19
32	J	100	ARG	N-CA-CB	-9.64	95.33	110.28
45	g	83	VAL	N-CA-C	8.54	118.56	110.53
37	W	5	THR	N-CA-CB	-8.50	98.30	111.05
37	W	99	SER	N-CA-C	7.96	122.77	112.26
37	W	16	THR	CA-C-O	-7.94	111.86	120.36
37	W	47	ILE	N-CA-CB	7.90	123.05	111.52
36	U	1379	TYR	N-CA-C	7.70	122.78	112.30
37	W	117	TYR	CA-C-O	7.54	128.32	120.40
49	r	1044	VAL	CA-C-N	7.27	126.78	118.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	r	1044	VAL	C-N-CA	7.27	126.78	118.85
49	r	1666	THR	N-CA-C	7.21	121.52	112.87
37	W	71	VAL	CA-C-N	7.12	131.49	120.75
37	W	71	VAL	C-N-CA	7.12	131.49	120.75
38	X	175	PRO	N-CA-C	7.10	127.09	112.47
49	r	533	VAL	N-CA-C	7.03	118.90	112.29
48	q	483	ARG	CA-C-N	-6.99	111.27	122.66
48	q	483	ARG	C-N-CA	-6.99	111.27	122.66
35	T	448	THR	CA-C-N	-6.97	112.16	122.41
35	T	448	THR	C-N-CA	-6.97	112.16	122.41
37	W	4	LEU	N-CA-C	-6.93	97.92	108.67
38	X	56	PHE	CA-C-O	-6.82	112.82	120.32
37	W	58	ASP	N-CA-CB	-6.77	100.54	111.24
37	W	121	LEU	CA-C-O	6.76	128.74	121.44
48	q	853	SER	N-CA-C	-6.75	105.16	113.19
42	d	6	PRO	N-CA-C	6.69	118.86	110.70
29	0	361	GLY	CA-C-N	6.64	134.23	121.54
29	0	361	GLY	C-N-CA	6.64	134.23	121.54
48	q	1024	ASP	O-C-N	6.63	126.82	121.38
17	R	201	VAL	CA-C-N	6.56	138.06	126.45
17	R	201	VAL	C-N-CA	6.56	138.06	126.45
8	A	1773	SER	CA-C-N	6.56	131.72	122.08
8	A	1773	SER	C-N-CA	6.56	131.72	122.08
34	M	208	ARG	CA-C-N	6.45	133.87	121.54
34	M	208	ARG	C-N-CA	6.45	133.87	121.54
48	q	435	GLN	CA-C-N	6.43	133.83	121.54
48	q	435	GLN	C-N-CA	6.43	133.83	121.54
31	F	336	HIS	CA-C-N	6.40	126.09	119.56
31	F	336	HIS	C-N-CA	6.40	126.09	119.56
3	3	587	VAL	N-CA-C	6.34	113.00	106.21
37	W	87	LEU	CA-C-N	6.32	126.23	119.28
37	W	87	LEU	C-N-CA	6.32	126.23	119.28
37	W	40	THR	CA-C-N	6.27	131.50	122.40
37	W	40	THR	C-N-CA	6.27	131.50	122.40
8	A	1513	MET	CA-C-N	6.25	133.48	121.54
8	A	1513	MET	C-N-CA	6.25	133.48	121.54
29	0	277	ARG	N-CA-C	6.24	118.16	111.36
30	9	471	TRP	CA-C-N	6.23	132.92	121.70
30	9	471	TRP	C-N-CA	6.23	132.92	121.70
45	g	87	VAL	N-CA-C	6.17	116.34	110.42
29	0	367	TYR	CA-C-N	6.16	131.04	123.10
29	0	367	TYR	C-N-CA	6.16	131.04	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	W	73	ASN	N-CA-C	6.11	119.78	111.17
38	X	174	PHE	CA-C-N	6.09	127.46	119.84
38	X	174	PHE	C-N-CA	6.09	127.46	119.84
30	9	418	GLY	CA-C-N	6.05	125.44	118.85
30	9	418	GLY	C-N-CA	6.05	125.44	118.85
38	X	49	MET	N-CA-C	-5.98	104.67	111.07
49	r	1006	LYS	CA-C-N	5.96	126.11	119.32
49	r	1006	LYS	C-N-CA	5.96	126.11	119.32
48	q	668	ALA	N-CA-C	-5.95	102.68	110.53
37	W	75	ARG	N-CA-CB	-5.94	102.71	111.51
35	T	460	TYR	N-CA-C	-5.90	106.08	113.28
37	W	113	LYS	N-CA-C	5.88	118.45	111.33
44	f	85	PRO	CA-C-N	-5.87	114.33	120.38
44	f	85	PRO	C-N-CA	-5.87	114.33	120.38
29	0	360	PHE	N-CA-C	5.85	119.48	112.93
49	r	1135	LEU	CA-C-N	5.85	125.79	119.76
49	r	1135	LEU	C-N-CA	5.85	125.79	119.76
37	W	118	LEU	CA-C-N	-5.84	114.53	122.77
37	W	118	LEU	C-N-CA	-5.84	114.53	122.77
37	W	27	ARG	CB-CA-C	-5.84	98.80	109.54
24	u	1103	VAL	CA-C-N	5.81	132.64	121.54
24	u	1103	VAL	C-N-CA	5.81	132.64	121.54
38	X	182	LEU	CA-C-N	-5.79	116.99	123.02
38	X	182	LEU	C-N-CA	-5.79	116.99	123.02
30	9	483	SER	O-C-N	-5.79	116.80	122.99
48	q	978	PHE	CA-C-N	-5.78	113.24	121.50
48	q	978	PHE	C-N-CA	-5.78	113.24	121.50
9	B	816	VAL	CA-C-N	-5.76	111.95	122.38
9	B	816	VAL	C-N-CA	-5.76	111.95	122.38
48	q	666	PRO	N-CA-C	5.72	119.48	110.50
49	r	1291	LEU	CA-C-N	5.71	126.03	119.92
49	r	1291	LEU	C-N-CA	5.71	126.03	119.92
37	W	149	LYS	CB-CA-C	-5.71	101.94	110.16
37	W	27	ARG	CA-C-N	5.70	128.72	120.11
37	W	27	ARG	C-N-CA	5.70	128.72	120.11
37	W	50	SER	CA-C-O	5.70	127.59	121.55
29	0	268	GLU	CA-C-N	5.68	128.98	120.69
29	0	268	GLU	C-N-CA	5.68	128.98	120.69
48	q	807	GLY	N-CA-C	-5.68	107.15	115.72
12	E	146	HIS	CA-C-N	5.67	132.38	121.54
12	E	146	HIS	C-N-CA	5.67	132.38	121.54
8	A	705	LYS	CA-C-N	5.67	132.37	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	705	LYS	C-N-CA	5.67	132.37	121.54
49	r	782	PHE	N-CA-C	5.67	118.03	109.41
13	L	91	ARG	CA-C-N	5.64	132.32	121.54
13	L	91	ARG	C-N-CA	5.64	132.32	121.54
49	r	1048	VAL	N-CA-C	-5.59	106.34	113.22
37	W	34	ILE	CA-C-O	-5.57	114.17	120.74
33	K	213	HIS	CB-CA-C	-5.53	109.21	115.79
29	0	246	TYR	N-CA-CB	5.52	119.82	110.49
29	0	362	PHE	N-CA-C	5.52	122.56	110.80
14	O	445	LYS	CA-C-N	5.51	132.06	121.54
14	O	445	LYS	C-N-CA	5.51	132.06	121.54
37	W	159	GLU	N-CA-C	-5.50	104.93	111.69
47	p	221	PRO	CB-CA-C	5.49	120.53	110.10
43	e	75	ASP	N-CA-C	5.49	117.34	111.36
14	O	389	HIS	CA-C-N	5.48	132.00	121.54
14	O	389	HIS	C-N-CA	5.48	132.00	121.54
48	q	441	GLY	CA-C-N	5.46	127.86	120.38
48	q	441	GLY	C-N-CA	5.46	127.86	120.38
8	A	413	LEU	CA-C-N	5.46	131.97	121.54
8	A	413	LEU	C-N-CA	5.46	131.97	121.54
37	W	71	VAL	O-C-N	-5.46	115.74	122.57
49	r	2096	ALA	CA-C-N	5.46	125.66	120.31
49	r	2096	ALA	C-N-CA	5.46	125.66	120.31
37	W	16	THR	O-C-N	5.45	129.44	123.22
35	T	569	LYS	CA-C-N	-5.44	114.95	122.30
35	T	569	LYS	C-N-CA	-5.44	114.95	122.30
48	q	475	GLY	N-CA-C	-5.43	107.86	114.92
48	q	594	GLU	CB-CA-C	-5.40	101.82	110.79
47	p	222	PRO	CB-CA-C	5.40	120.47	111.56
42	d	35	ASP	CA-C-N	5.40	125.22	119.28
42	d	35	ASP	C-N-CA	5.40	125.22	119.28
8	A	1207	PHE	CA-C-N	5.39	130.00	122.08
8	A	1207	PHE	C-N-CA	5.39	130.00	122.08
37	W	40	THR	N-CA-C	-5.39	106.21	112.89
40	i	6	ASN	N-CA-C	5.38	116.32	110.13
47	p	236	PRO	CB-CA-C	5.38	120.44	111.56
37	W	125	VAL	CA-C-N	5.37	128.01	120.28
37	W	125	VAL	C-N-CA	5.37	128.01	120.28
49	r	1228	VAL	CB-CA-C	-5.36	105.01	112.04
48	q	957	ARG	N-CA-C	-5.36	104.85	111.33
49	r	749	GLY	N-CA-C	-5.36	108.32	114.69
37	W	146	ASP	CA-C-N	5.35	130.16	122.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	W	146	ASP	C-N-CA	5.35	130.16	122.40
48	q	636	LEU	N-CA-C	-5.35	105.35	111.07
37	W	33	VAL	N-CA-CB	-5.35	103.71	111.52
48	q	978	PHE	N-CA-C	-5.32	105.38	111.07
48	q	440	GLU	N-CA-C	5.31	116.87	111.14
49	r	1228	VAL	N-CA-C	5.30	116.67	110.62
37	W	88	PRO	CB-CA-C	-5.30	103.94	112.21
43	e	61	VAL	N-CA-C	5.30	115.53	108.27
37	W	32	PRO	CA-C-N	5.29	130.34	122.99
37	W	32	PRO	C-N-CA	5.29	130.34	122.99
38	X	9	ASN	N-CA-CB	-5.29	101.69	111.53
19	V	10	GLN	N-CA-C	5.29	118.93	110.73
49	r	811	SER	N-CA-C	5.29	115.11	108.45
41	c	47	ILE	N-CA-C	5.29	115.82	108.84
38	X	184	PRO	N-CA-C	-5.28	106.84	114.18
49	r	1127	CYS	CA-C-N	5.28	125.59	119.47
49	r	1127	CYS	C-N-CA	5.28	125.59	119.47
8	A	902	TYR	CA-C-N	5.25	131.56	121.54
8	A	902	TYR	C-N-CA	5.25	131.56	121.54
39	a	54	GLY	N-CA-C	5.24	117.66	110.69
38	X	23	LYS	N-CA-C	5.24	117.40	111.11
42	d	68	ILE	CB-CA-C	-5.22	105.55	111.55
49	r	1693	ARG	CA-C-N	5.21	125.01	119.28
49	r	1693	ARG	C-N-CA	5.21	125.01	119.28
42	d	56	ASN	N-CA-C	5.20	116.05	107.20
31	F	281	VAL	N-CA-C	5.20	115.80	108.36
31	F	156	SER	N-CA-C	5.19	116.73	108.79
49	r	1875	VAL	CA-C-N	5.18	124.63	119.24
49	r	1875	VAL	C-N-CA	5.18	124.63	119.24
44	f	52	LYS	CA-C-N	5.17	126.30	119.84
44	f	52	LYS	C-N-CA	5.17	126.30	119.84
44	f	90	THR	N-CA-C	-5.17	105.34	110.97
10	C	186	VAL	N-CA-C	-5.16	107.78	112.12
49	r	488	LEU	N-CA-C	5.16	119.68	113.17
38	X	54	GLN	N-CA-C	5.16	117.52	109.52
39	h	56	VAL	CB-CA-C	-5.14	104.11	111.31
16	Q	106	ILE	N-CA-C	-5.13	107.42	113.42
49	r	572	ASP	N-CA-C	-5.12	103.38	110.35
39	h	84	LYS	N-CA-C	5.11	117.37	110.06
35	T	467	LEU	CA-C-N	5.09	131.27	121.54
35	T	467	LEU	C-N-CA	5.09	131.27	121.54
38	X	51	MET	N-CA-C	5.09	119.49	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	b	66	CYS	N-CA-C	5.09	118.98	112.87
37	W	90	LEU	CA-C-O	-5.07	113.25	120.51
30	9	484	GLY	N-CA-C	-5.06	101.18	113.18
37	W	28	GLY	N-CA-C	5.06	120.87	113.48
37	W	99	SER	N-CA-CB	-5.06	102.88	111.17
38	X	41	VAL	O-C-N	5.05	127.03	121.83
48	q	619	GLN	CB-CA-C	-5.03	102.98	110.88
8	A	1514	LYS	N-CA-C	-5.03	100.09	110.80
45	g	43	VAL	N-CA-C	5.03	115.15	108.11
37	W	83	LEU	N-CA-C	5.02	117.40	111.33
49	r	574	GLN	N-CA-C	5.02	117.86	111.69
48	q	948	TYR	N-CA-C	5.02	119.38	113.16
30	9	440	ILE	CA-C-N	5.01	125.01	119.89
30	9	440	ILE	C-N-CA	5.01	125.01	119.89
38	X	86	TYR	CA-C-O	-5.01	115.33	121.05
39	a	107	ILE	CB-CA-C	-5.01	106.65	111.06
48	q	1012	VAL	CA-C-N	-5.01	117.43	122.74
48	q	1012	VAL	C-N-CA	-5.01	117.43	122.74
28	N	58	GLY	N-CA-C	-5.00	108.41	114.92
37	W	90	LEU	O-C-N	5.00	129.24	122.59

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
32	J	100	ARG	CA

All (36) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
29	0	238	THR	Peptide
3	3	568	GLY	Peptide
30	9	483	SER	Mainchain
30	9	484	GLY	Peptide
8	A	1213	VAL	Peptide
8	A	1457	HIS	Peptide
9	B	318	PHE	Peptide
9	B	352	LYS	Peptide
9	B	441	PRO	Peptide
9	B	469	ASP	Peptide
9	B	65	TYR	Peptide
9	B	750	LEU	Peptide
11	D	383	ARG	Peptide

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Mol	Chain	Res	Type	Group
33	K	211	GLN	Peptide
33	K	65	ILE	Peptide
33	K	89	LEU	Peptide
34	M	48	ALA	Peptide
34	M	517	THR	Peptide
14	O	390	ALA	Peptide
14	O	391	TYR	Peptide
15	P	276	THR	Peptide
19	V	10	GLN	Peptide
39	h	112	ASN	Peptide
47	p	222	PRO	Mainchain
47	p	232	GLU	Mainchain
47	p	235	ASN	Mainchain
47	p	236	PRO	Mainchain
49	r	430	LEU	Peptide
24	u	464	LEU	Peptide
25	v	259	LYS	Peptide
25	v	522	ASP	Peptide
25	v	582	GLU	Peptide
25	v	584	SER	Peptide
25	v	913	LEU	Peptide
28	z	32	ALA	Peptide
28	z	83	CYS	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	601	0	261	1	0
2	2	1262	0	631	118	0
3	3	584	0	263	1	0
4	5	1470	0	746	7	0
5	6	2035	0	1028	5	0
6	7	457	0	218	1	0
7	8	714	0	302	0	0
8	A	11093	0	4788	41	0
9	B	4456	0	1937	30	0
10	C	1418	0	659	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	D	1578	0	717	5	0
12	E	642	0	292	8	0
13	L	511	0	239	0	0
14	O	1260	0	561	39	0
15	P	1413	0	615	3	0
16	Q	683	0	290	1	0
17	R	507	0	218	0	0
18	S	163	0	74	0	0
19	V	775	0	358	0	0
20	Y	470	0	202	0	0
21	Z	1013	0	515	2	0
22	s	859	0	382	0	0
23	t	849	0	368	1	0
24	u	4357	0	1976	44	0
25	v	5862	0	2629	63	0
26	x	391	0	173	0	0
27	y	490	0	217	0	0
28	N	500	0	172	112	0
28	z	500	0	155	108	0
29	o	766	0	328	0	0
30	9	2139	0	929	357	0
31	F	1471	0	669	13	0
32	G	659	0	296	7	0
32	H	674	0	301	14	0
32	I	669	0	299	9	0
32	J	674	0	301	18	0
33	K	1059	0	478	23	0
34	M	3665	0	1652	186	0
35	T	2292	0	990	32	0
36	U	6588	0	2836	149	0
37	W	804	0	346	51	0
38	X	844	0	374	69	0
39	a	440	0	181	9	0
39	h	485	0	198	86	0
40	b	356	0	157	3	0
40	i	361	0	158	1	0
41	c	386	0	161	7	0
41	j	391	0	163	2	0
42	d	358	0	158	5	0
42	k	363	0	160	1	0
43	e	434	0	188	26	0
43	l	409	0	180	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	f	439	0	188	10	0
44	m	349	0	141	54	0
45	g	461	0	190	7	0
45	n	406	0	169	41	0
46	o	1119	0	518	66	0
47	p	870	0	376	45	0
48	q	3091	0	1402	19	0
49	r	8530	0	3747	33	0
50	w	276	0	120	22	0
51	2	1	0	0	0	0
51	P	3	0	0	0	0
51	Q	3	0	0	0	0
51	Z	1	0	0	0	0
51	y	3	0	0	0	0
52	6	4	0	0	0	0
52	r	1	0	0	0	0
53	A	36	0	6	0	0
54	B	32	0	12	0	0
55	r	54	0	24	1	0
All	All	88879	0	39382	1177	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 9.

All (1177) 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:v:898:ASN:CB	38:X:191:PHE:CB	1.75	1.63
46:o:2:ALA:CA	46:o:263:VAL:CB	1.78	1.61
34:M:109:MET:CB	36:U:938:TYR:CB	1.75	1.60
25:v:942:LYS:CB	38:X:213:THR:CA	1.77	1.60
36:U:485:ILE:HA	36:U:565:ILE:CA	1.13	1.60
36:U:485:ILE:CA	36:U:565:ILE:HA	1.16	1.57
34:M:96:ASN:CB	36:U:946:GLU:CB	1.82	1.57
30:9:338:ARG:HA	39:h:99:MET:CB	1.32	1.56
46:o:2:ALA:HA	46:o:263:VAL:CB	1.17	1.56
36:U:426:LEU:CB	36:U:636:GLN:CB	1.75	1.56
36:U:485:ILE:CB	36:U:591:TYR:C	1.82	1.53
30:9:38:ASN:H	34:M:730:VAL:CB	1.21	1.52
30:9:128:VAL:H	45:n:15:VAL:CB	1.20	1.52
30:9:338:ARG:CA	39:h:99:MET:CB	1.86	1.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:9:127:LEU:HA	45:n:69:ILE:C	1.30	1.51
30:9:496:LYS:CB	38:X:157:ASN:CA	1.85	1.50
34:M:208:ARG:C	34:M:209:PHE:N	1.67	1.50
36:U:485:ILE:CA	36:U:565:ILE:CA	1.75	1.49
30:9:128:VAL:N	45:n:15:VAL:CB	1.73	1.48
30:9:334:LEU:HA	39:h:70:VAL:CA	1.19	1.48
2:2:59:A:H61	30:9:443:THR:CB	1.24	1.48
34:M:350:LEU:CB	34:M:365:ALA:CA	1.79	1.46
8:A:358:PRO:CB	35:T:333:GLN:CB	1.91	1.46
30:9:334:LEU:CB	39:h:71:LYS:C	1.89	1.46
2:2:60:U:H4'	30:9:428:GLU:N	1.25	1.45
2:2:52:G:O6	30:9:436:ARG:CA	1.66	1.44
36:U:485:ILE:C	36:U:565:ILE:CB	1.91	1.44
28:z:31:THR:N	28:N:31:THR:CA	1.76	1.43
36:U:529:GLU:CB	36:U:1047:HIS:CB	1.97	1.43
34:M:350:LEU:CB	34:M:365:ALA:HA	1.00	1.43
24:u:480:VAL:O	30:9:393:PRO:CB	1.65	1.42
34:M:309:ALA:CB	36:U:354:SER:HA	1.13	1.41
36:U:489:VAL:CB	36:U:567:VAL:H	1.32	1.41
37:W:37:LEU:CB	44:m:48:PHE:CB	1.99	1.41
46:o:28:PRO:CA	46:o:63:ALA:HB1	1.50	1.40
2:2:53:U:H5''	30:9:462:LEU:CB	1.51	1.40
34:M:309:ALA:CB	36:U:354:SER:CA	1.92	1.39
2:2:51:A:C6	30:9:438:LEU:N	1.88	1.39
24:u:477:LYS:CB	30:9:395:TRP:O	1.65	1.37
34:M:309:ALA:HB2	36:U:354:SER:CB	1.53	1.37
2:2:53:U:C2	30:9:442:ASN:O	1.75	1.36
2:2:51:A:N7	30:9:436:ARG:O	1.58	1.36
30:9:136:TYR:O	45:n:72:ASP:CB	1.72	1.36
24:u:493:LYS:CB	30:9:420:LYS:C	1.83	1.35
30:9:132:ASP:O	39:h:96:ILE:CB	1.75	1.34
46:o:23:HIS:O	46:o:31:ASP:CB	1.75	1.34
37:W:38:GLY:O	44:m:26:ILE:CB	1.75	1.33
34:M:104:VAL:O	36:U:939:GLN:CB	1.75	1.32
30:9:496:LYS:CA	38:X:157:ASN:CB	2.07	1.32
46:o:28:PRO:CB	46:o:63:ALA:CA	2.07	1.32
14:O:465:ARG:CB	34:M:547:LEU:N	1.93	1.31
24:u:491:GLU:C	30:9:420:LYS:H	1.36	1.31
28:z:31:THR:CA	28:N:31:THR:HA	1.36	1.31
2:2:60:U:H5''	30:9:428:GLU:C	1.57	1.30
34:M:354:PRO:HA	34:M:361:HIS:CB	1.62	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:9:232:GLU:CB	30:9:253:GLU:O	1.78	1.30
24:u:480:VAL:C	30:9:393:PRO:CB	1.79	1.29
25:v:600:GLN:CB	49:r:860:GLN:O	1.78	1.29
36:U:491:ARG:O	36:U:513:PRO:CB	1.79	1.29
30:9:34:ARG:CB	34:M:730:VAL:O	1.79	1.29
30:9:38:ASN:N	34:M:730:VAL:CB	1.94	1.29
34:M:103:PHE:O	36:U:939:GLN:CB	1.80	1.28
24:u:489:PRO:O	30:9:421:ALA:HB3	1.19	1.28
24:u:493:LYS:CB	30:9:420:LYS:O	1.76	1.28
2:2:60:U:C4'	30:9:428:GLU:H	1.45	1.28
44:m:75:GLU:HA	45:n:57:THR:O	1.28	1.27
30:9:331:VAL:CB	39:h:51:LYS:O	1.82	1.27
34:M:206:ASP:N	36:U:1052:LEU:O	1.63	1.27
36:U:485:ILE:HA	36:U:565:ILE:C	1.59	1.27
2:2:53:U:O2'	30:9:445:HIS:CB	1.82	1.27
25:v:942:LYS:CA	38:X:213:THR:CB	2.12	1.27
34:M:205:ASN:C	36:U:1052:LEU:C	1.91	1.27
2:2:51:A:C2	30:9:438:LEU:CB	2.18	1.26
2:2:53:U:C5'	30:9:462:LEU:CB	2.14	1.26
30:9:127:LEU:CA	45:n:69:ILE:C	2.09	1.26
30:9:128:VAL:CA	45:n:15:VAL:CB	2.06	1.26
37:W:9:ILE:O	44:m:45:CYS:C	1.78	1.26
46:o:2:ALA:N	46:o:263:VAL:CB	1.96	1.25
30:9:127:LEU:HA	45:n:69:ILE:CA	1.48	1.25
36:U:529:GLU:CA	36:U:1047:HIS:CB	2.14	1.25
46:o:23:HIS:C	46:o:31:ASP:CB	2.09	1.24
24:u:487:LEU:O	30:9:403:ASN:HA	1.36	1.23
34:M:355:HIS:HA	34:M:359:GLU:CB	1.59	1.23
37:W:9:ILE:O	44:m:45:CYS:CA	1.86	1.23
30:9:343:GLU:O	45:n:80:LEU:CB	1.78	1.23
34:M:354:PRO:CB	34:M:362:LYS:HA	1.69	1.23
14:O:448:ALA:O	47:p:87:ASN:C	1.79	1.22
36:U:485:ILE:CA	36:U:591:TYR:O	1.88	1.22
2:2:60:U:C4'	30:9:428:GLU:N	2.02	1.22
34:M:135:ARG:HA	36:U:941:MET:CB	1.69	1.22
36:U:485:ILE:CB	36:U:566:THR:H	1.53	1.21
30:9:334:LEU:CA	39:h:70:VAL:CA	2.16	1.21
14:O:448:ALA:C	47:p:87:ASN:C	1.87	1.20
14:O:452:PHE:N	47:p:89:PRO:N	1.89	1.19
34:M:355:HIS:H	34:M:361:HIS:CB	1.53	1.19
24:u:489:PRO:HA	30:9:416:TYR:CB	1.72	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:9:32:THR:O	34:M:732:ALA:HB3	1.43	1.17
30:9:334:LEU:HA	39:h:70:VAL:C	1.68	1.17
46:o:23:HIS:CA	46:o:31:ASP:CB	2.23	1.17
2:2:53:U:N3	30:9:442:ASN:O	1.76	1.17
14:O:448:ALA:O	47:p:87:ASN:O	1.63	1.17
30:9:34:ARG:CB	34:M:734:TYR:H	1.57	1.17
46:o:179:GLU:O	50:w:45:TRP:N	1.76	1.16
28:z:79:GLY:H	28:N:79:GLY:CA	1.56	1.16
30:9:133:GLU:CB	39:h:94:ARG:CB	2.24	1.16
34:M:621:ARG:CB	47:p:106:ALA:N	2.07	1.16
30:9:32:THR:O	34:M:732:ALA:CB	1.93	1.15
46:o:30:GLY:HA2	46:o:52:VAL:CB	1.75	1.15
2:2:59:A:N6	30:9:443:THR:CB	2.09	1.15
8:A:360:SER:CB	35:T:322:ILE:HA	1.75	1.15
34:M:350:LEU:CB	34:M:364:VAL:O	1.95	1.15
37:W:40:THR:HA	44:m:46:ASP:O	1.46	1.14
8:A:2266:ARG:O	49:r:1261:PRO:CB	1.96	1.14
37:W:10:GLU:HA	44:m:45:CYS:HA	1.27	1.14
46:o:23:HIS:HA	46:o:31:ASP:CA	1.78	1.13
2:2:51:A:H2'	30:9:439:GLY:O	1.46	1.13
2:2:63:G:OP2	30:9:410:ILE:O	1.65	1.13
28:z:71:LYS:O	28:N:75:ASP:CB	1.97	1.13
36:U:489:VAL:CB	36:U:567:VAL:N	2.11	1.13
46:o:28:PRO:CA	46:o:63:ALA:CB	2.11	1.13
30:9:338:ARG:CB	39:h:99:MET:CB	2.26	1.13
8:A:362:ARG:N	35:T:327:GLU:HA	1.64	1.12
30:9:341:THR:CB	39:h:58:ALA:HB3	1.79	1.12
30:9:334:LEU:CB	39:h:71:LYS:N	2.13	1.12
30:9:129:GLU:CB	45:n:14:THR:C	2.23	1.11
30:9:334:LEU:HA	39:h:70:VAL:HA	1.23	1.11
36:U:485:ILE:CA	36:U:566:THR:N	2.14	1.11
34:M:104:VAL:C	36:U:939:GLN:CB	2.23	1.11
2:2:60:U:H4'	30:9:427:ALA:C	1.75	1.11
37:W:25:ASP:N	44:m:66:VAL:C	1.85	1.10
2:2:62:U:OP2	30:9:431:HIS:HA	1.52	1.10
30:9:129:GLU:CB	45:n:14:THR:O	2.00	1.10
36:U:426:LEU:C	36:U:636:GLN:CB	2.23	1.10
37:W:14:GLN:CB	44:m:67:LEU:CB	2.28	1.10
36:U:485:ILE:O	36:U:565:ILE:C	1.94	1.10
2:2:51:A:C5	30:9:436:ARG:O	1.84	1.09
2:2:52:G:C6	30:9:436:ARG:HA	1.87	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:62:U:OP1	30:9:411:CYS:CB	2.00	1.09
34:M:136:ALA:HA	36:U:937:LEU:CB	1.82	1.09
46:o:181:GLY:H	50:w:43:GLU:N	1.49	1.09
30:9:135:GLY:O	39:h:97:SER:CB	1.87	1.09
37:W:41:LEU:CB	44:m:19:CYS:O	1.99	1.09
2:2:61:C:OP2	30:9:432:ALA:N	1.56	1.08
37:W:47:ILE:HA	44:m:65:ARG:CB	1.83	1.08
30:9:128:VAL:CB	45:n:15:VAL:CB	2.30	1.08
30:9:334:LEU:CB	39:h:70:VAL:C	2.25	1.08
36:U:491:ARG:CB	36:U:512:GLN:C	2.28	1.07
2:2:60:U:H3'	30:9:432:ALA:HB2	1.35	1.07
25:v:974:LYS:CB	38:X:219:LYS:O	2.03	1.06
30:9:341:THR:CB	39:h:58:ALA:CB	2.33	1.06
8:A:362:ARG:H	35:T:327:GLU:HA	1.14	1.06
30:9:490:LYS:CB	38:X:162:THR:CA	2.33	1.06
30:9:334:LEU:CB	39:h:71:LYS:CA	2.34	1.06
30:9:35:ASP:HA	34:M:730:VAL:H	1.20	1.05
30:9:490:LYS:CB	38:X:162:THR:N	2.19	1.05
30:9:329:GLU:HA	39:h:43:LEU:CB	1.84	1.05
34:M:136:ALA:CA	36:U:937:LEU:CB	2.31	1.05
2:2:52:G:O6	30:9:436:ARG:HA	0.88	1.05
2:2:60:U:C3'	30:9:428:GLU:H	1.68	1.05
36:U:485:ILE:CA	36:U:566:THR:H	1.68	1.05
46:o:179:GLU:CB	50:w:46:ARG:CB	2.34	1.05
34:M:355:HIS:N	34:M:361:HIS:CB	2.20	1.04
46:o:23:HIS:HA	46:o:31:ASP:CB	1.84	1.04
30:9:334:LEU:CB	39:h:72:GLU:N	2.18	1.04
30:9:339:HIS:HA	39:h:100:PHE:CA	1.68	1.04
9:B:194:LYS:CB	43:e:11:HIS:CB	2.36	1.04
30:9:125:GLN:O	45:n:15:VAL:CB	2.06	1.04
34:M:206:ASP:N	36:U:1052:LEU:C	2.09	1.04
2:2:61:C:OP1	30:9:431:HIS:N	1.86	1.03
30:9:490:LYS:CB	38:X:162:THR:CB	2.35	1.03
46:o:1:MET:C	46:o:263:VAL:CB	2.24	1.03
24:u:487:LEU:O	30:9:403:ASN:CA	2.05	1.03
30:9:343:GLU:CB	45:n:76:LEU:O	2.07	1.03
34:M:310:LYS:N	36:U:353:LEU:O	1.91	1.02
28:z:31:THR:N	28:N:31:THR:HA	1.28	1.02
25:v:979:ARG:HA	38:X:164:GLU:O	1.59	1.02
30:9:334:LEU:CA	39:h:70:VAL:C	2.29	1.02
14:O:465:ARG:CB	34:M:543:ARG:O	2.07	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:9:38:ASN:CB	34:M:726:ILE:O	2.07	1.01
28:z:66:ASP:HA	28:N:66:ASP:CB	1.77	1.01
34:M:621:ARG:CB	47:p:106:ALA:O	2.08	1.01
30:9:337:GLN:CB	39:h:68:GLU:C	2.34	1.01
28:z:36:TYR:CB	28:N:33:GLU:HA	1.91	1.01
34:M:308:ALA:HB1	36:U:351:PHE:C	1.83	1.01
25:v:974:LYS:CB	38:X:219:LYS:C	2.34	1.01
28:z:79:GLY:H	28:N:79:GLY:HA3	1.23	1.01
2:2:61:C:H3'	30:9:431:HIS:O	1.59	1.00
24:u:489:PRO:O	30:9:421:ALA:CB	2.08	1.00
25:v:600:GLN:CB	49:r:860:GLN:C	2.33	1.00
2:2:53:U:OP1	30:9:462:LEU:CB	2.09	1.00
34:M:354:PRO:CA	34:M:361:HIS:CB	2.38	1.00
24:u:491:GLU:C	30:9:420:LYS:N	2.20	1.00
30:9:125:GLN:N	45:n:10:LEU:CB	2.24	1.00
25:v:975:LYS:CB	38:X:210:PHE:CB	2.39	1.00
34:M:309:ALA:HB3	36:U:354:SER:HA	1.01	0.99
36:U:426:LEU:CA	36:U:636:GLN:CB	2.40	0.99
36:U:491:ARG:C	36:U:513:PRO:CB	2.34	0.99
33:K:210:LYS:O	33:K:213:HIS:O	1.79	0.99
37:W:37:LEU:O	44:m:48:PHE:CB	2.10	0.99
25:v:896:PHE:HA	38:X:182:LEU:O	1.61	0.99
30:9:133:GLU:O	39:h:95:TYR:O	1.79	0.99
30:9:35:ASP:HA	34:M:730:VAL:N	1.77	0.98
28:z:79:GLY:N	28:N:79:GLY:CA	2.25	0.98
34:M:138:ARG:O	36:U:933:GLY:HA2	1.64	0.98
34:M:354:PRO:CB	34:M:362:LYS:CA	2.22	0.98
2:2:60:U:C5'	30:9:428:GLU:O	2.11	0.98
34:M:206:ASP:C	36:U:1052:LEU:HA	1.89	0.98
46:o:1:MET:CB	46:o:235:SER:HA	1.94	0.98
28:z:31:THR:N	28:N:31:THR:CB	2.26	0.97
36:U:426:LEU:CB	36:U:636:GLN:CA	2.42	0.97
30:9:493:GLU:HA	38:X:157:ASN:C	1.86	0.97
36:U:485:ILE:C	36:U:565:ILE:CA	2.27	0.97
30:9:339:HIS:HA	39:h:100:PHE:HA	1.45	0.97
36:U:427:TYR:CB	36:U:637:ASP:HA	1.95	0.97
28:z:73:ALA:HB2	28:N:73:ALA:HB2	0.98	0.97
34:M:355:HIS:CA	34:M:359:GLU:CB	2.42	0.97
34:M:618:ARG:O	47:p:106:ALA:O	1.82	0.97
36:U:485:ILE:CB	36:U:591:TYR:O	0.67	0.97
34:M:622:ALA:HB2	47:p:106:ALA:HA	1.47	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:I:73:ALA:O	32:I:77:ALA:HB3	1.64	0.96
2:2:60:U:H5'	30:9:428:GLU:O	1.64	0.96
28:z:69:ASP:HA	28:N:72:ASN:CB	1.95	0.96
34:M:309:ALA:HB3	36:U:354:SER:CA	1.74	0.96
36:U:485:ILE:HA	36:U:566:THR:N	1.77	0.95
37:W:47:ILE:HA	44:m:65:ARG:CA	1.95	0.95
8:A:1706:ASP:O	8:A:1710:ASN:HA	1.65	0.95
30:9:34:ARG:CA	34:M:730:VAL:O	1.97	0.95
46:o:30:GLY:CA	46:o:52:VAL:CB	2.44	0.95
28:z:69:ASP:O	28:N:73:ALA:N	2.00	0.95
30:9:334:LEU:N	39:h:53:LEU:N	2.05	0.95
37:W:38:GLY:C	44:m:26:ILE:CB	2.39	0.95
30:9:127:LEU:CA	45:n:69:ILE:O	2.13	0.95
36:U:491:ARG:CB	36:U:513:PRO:N	2.30	0.95
36:U:485:ILE:CA	36:U:565:ILE:C	2.27	0.94
36:U:527:ILE:O	36:U:1051:LYS:CB	2.14	0.94
2:2:51:A:C2	30:9:440:ILE:N	2.34	0.94
2:2:61:C:P	30:9:428:GLU:O	2.25	0.94
30:9:334:LEU:N	39:h:53:LEU:H	1.66	0.94
30:9:342:HIS:CB	45:n:76:LEU:HA	1.98	0.94
30:9:490:LYS:H	38:X:161:GLU:N	1.66	0.94
36:U:529:GLU:HA	36:U:1047:HIS:CB	1.96	0.94
34:M:308:ALA:CB	36:U:351:PHE:O	2.16	0.94
8:A:2268:LEU:CB	49:r:1263:PRO:HA	1.96	0.94
9:B:117:ASP:CA	43:e:88:ASN:N	2.10	0.94
8:A:360:SER:CB	35:T:322:ILE:CA	2.46	0.93
14:O:465:ARG:CB	34:M:546:SER:C	2.42	0.93
34:M:309:ALA:HB2	36:U:354:SER:CA	1.75	0.93
2:2:53:U:O2	30:9:442:ASN:O	1.84	0.93
30:9:331:VAL:C	39:h:51:LYS:C	2.34	0.93
36:U:485:ILE:O	36:U:565:ILE:CB	2.14	0.92
24:u:491:GLU:CA	30:9:420:LYS:N	2.32	0.92
30:9:333:ILE:O	39:h:54:GLY:HA3	1.69	0.92
36:U:489:VAL:HA	36:U:654:ASN:CB	1.99	0.92
2:2:51:A:N1	30:9:438:LEU:CB	2.32	0.92
30:9:338:ARG:C	39:h:99:MET:CB	2.35	0.92
46:o:180:LYS:C	50:w:41:LYS:O	2.09	0.92
30:9:334:LEU:H	39:h:53:LEU:H	1.14	0.92
46:o:23:HIS:HA	46:o:31:ASP:HA	1.50	0.92
30:9:337:GLN:CA	39:h:68:GLU:N	2.25	0.92
30:9:493:GLU:H	38:X:159:PRO:CA	1.82	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:M:138:ARG:O	36:U:932:ALA:O	1.88	0.92
34:M:308:ALA:CB	36:U:351:PHE:C	2.43	0.91
37:W:10:GLU:HA	44:m:45:CYS:CA	1.95	0.91
46:o:181:GLY:N	50:w:43:GLU:N	2.17	0.91
30:9:331:VAL:CB	39:h:51:LYS:C	2.41	0.91
30:9:34:ARG:CB	34:M:734:TYR:N	2.32	0.91
30:9:334:LEU:CA	39:h:71:LYS:N	2.33	0.91
34:M:136:ALA:C	36:U:937:LEU:CB	2.44	0.91
2:2:60:U:C3'	30:9:428:GLU:O	2.18	0.91
2:2:60:U:C5'	30:9:428:GLU:C	2.44	0.90
28:z:31:THR:CA	28:N:31:THR:CB	2.49	0.90
28:z:105:LYS:C	28:N:107:GLU:H	1.74	0.90
36:U:485:ILE:C	36:U:565:ILE:C	2.39	0.90
30:9:490:LYS:CB	38:X:162:THR:H	1.82	0.90
34:M:350:LEU:CB	34:M:365:ALA:C	2.43	0.90
34:M:350:LEU:CB	34:M:364:VAL:C	2.44	0.90
14:O:452:PHE:H	47:p:88:ASP:C	1.79	0.90
14:O:452:PHE:H	47:p:89:PRO:N	1.61	0.89
24:u:480:VAL:N	30:9:393:PRO:CB	2.14	0.89
28:z:73:ALA:CB	28:N:73:ALA:HB2	1.50	0.89
34:M:206:ASP:CA	36:U:1052:LEU:O	2.20	0.89
24:u:491:GLU:CA	30:9:420:LYS:H	1.86	0.89
30:9:127:LEU:HA	45:n:69:ILE:O	1.69	0.89
30:9:331:VAL:HA	39:h:71:LYS:O	1.73	0.89
24:u:760:GLU:HA	48:q:957:ARG:HA	1.54	0.89
37:W:37:LEU:C	44:m:48:PHE:CB	2.46	0.89
37:W:46:ALA:O	44:m:65:ARG:CB	2.20	0.89
2:2:53:U:C2	30:9:442:ASN:C	2.47	0.88
2:2:61:C:C6	30:9:431:HIS:C	2.50	0.88
24:u:480:VAL:H	30:9:393:PRO:CB	1.82	0.88
30:9:329:GLU:O	39:h:53:LEU:CB	2.22	0.88
36:U:485:ILE:N	36:U:565:ILE:HA	1.55	0.88
34:M:621:ARG:HA	47:p:104:GLY:C	1.96	0.88
8:A:2266:ARG:O	49:r:1261:PRO:CA	2.21	0.88
2:2:62:U:O4	30:9:436:ARG:N	1.80	0.88
2:2:51:A:N1	30:9:438:LEU:N	2.22	0.88
25:v:600:GLN:CA	49:r:860:GLN:O	2.20	0.88
34:M:347:SER:N	34:M:368:GLN:CB	2.17	0.87
30:9:337:GLN:HA	39:h:68:GLU:N	1.49	0.87
44:m:75:GLU:CA	45:n:57:THR:O	2.20	0.87
36:U:489:VAL:HA	36:U:654:ASN:C	1.99	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:51:A:N1	30:9:438:LEU:CA	2.35	0.86
37:W:47:ILE:HA	44:m:65:ARG:HA	1.56	0.86
8:A:2314:PHE:CB	49:r:1125:SER:CB	2.53	0.86
30:9:342:HIS:CB	45:n:76:LEU:CB	2.51	0.86
43:e:87:LYS:HA	44:f:94:ARG:O	1.75	0.86
2:2:61:C:H6	30:9:431:HIS:C	1.84	0.86
30:9:331:VAL:CA	39:h:51:LYS:O	2.24	0.86
30:9:493:GLU:H	38:X:159:PRO:HA	1.38	0.86
37:W:40:THR:CA	44:m:46:ASP:O	2.23	0.86
25:v:600:GLN:N	49:r:860:GLN:O	2.08	0.86
37:W:9:ILE:O	44:m:46:ASP:N	2.08	0.86
2:2:51:A:C6	30:9:437:CYS:C	2.53	0.85
37:W:9:ILE:O	44:m:45:CYS:HA	1.74	0.85
30:9:32:THR:O	34:M:732:ALA:HB1	1.76	0.85
36:U:488:SER:H	36:U:565:ILE:CB	1.89	0.85
25:v:940:LEU:O	38:X:216:HIS:CB	2.25	0.85
28:z:31:THR:H	28:N:31:THR:CB	1.88	0.85
30:9:134:GLU:C	39:h:95:TYR:O	2.18	0.85
34:M:350:LEU:CB	34:M:365:ALA:N	2.38	0.85
36:U:492:MET:HA	36:U:513:PRO:CB	2.06	0.85
28:z:31:THR:CA	28:N:31:THR:CA	2.12	0.85
28:z:77:LEU:O	28:N:79:GLY:N	2.08	0.85
37:W:10:GLU:CA	44:m:45:CYS:HA	2.05	0.85
30:9:35:ASP:CA	34:M:730:VAL:N	2.39	0.85
2:2:61:C:C6	30:9:431:HIS:O	2.30	0.85
24:u:489:PRO:HA	30:9:416:TYR:CA	1.88	0.85
30:9:490:LYS:N	38:X:161:GLU:N	2.24	0.85
36:U:485:ILE:C	36:U:566:THR:N	2.34	0.84
25:v:942:LYS:CB	38:X:213:THR:N	2.40	0.84
2:2:61:C:OP2	30:9:428:GLU:O	1.95	0.84
30:9:338:ARG:HA	39:h:99:MET:CA	2.07	0.84
2:2:51:A:C5	30:9:438:LEU:N	2.43	0.84
28:z:31:THR:CB	28:N:31:THR:CB	2.55	0.83
34:M:135:ARG:CA	36:U:941:MET:CB	2.54	0.83
30:9:496:LYS:CB	38:X:157:ASN:C	2.50	0.83
32:I:112:ALA:HB1	33:K:36:VAL:HA	1.59	0.83
34:M:309:ALA:CB	36:U:354:SER:CB	2.33	0.83
34:M:355:HIS:C	34:M:359:GLU:N	2.35	0.83
28:z:73:ALA:CB	28:N:73:ALA:CB	0.83	0.83
25:v:599:GLU:N	49:r:862:ASP:C	2.35	0.83
2:2:51:A:H2'	30:9:439:GLY:C	1.87	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:E:85:TYR:H	31:F:60:MET:CB	1.91	0.83
25:v:599:GLU:H	49:r:862:ASP:C	1.81	0.82
37:W:38:GLY:HA2	44:m:26:ILE:CB	2.09	0.82
30:9:490:LYS:N	38:X:161:GLU:H	1.75	0.82
25:v:895:ARG:O	38:X:184:PRO:CB	2.26	0.82
2:2:60:U:H4'	30:9:427:ALA:CA	2.09	0.82
36:U:485:ILE:CB	36:U:566:THR:N	2.37	0.82
14:O:464:ASP:O	34:M:515:ILE:HA	1.78	0.82
30:9:128:VAL:HA	45:n:16:THR:C	2.04	0.82
28:z:43:GLY:N	28:N:40:GLY:O	2.11	0.82
30:9:37:ILE:N	34:M:730:VAL:CB	2.42	0.81
28:z:68:PHE:O	28:N:72:ASN:N	2.12	0.81
34:M:138:ARG:O	36:U:933:GLY:CA	2.25	0.81
28:z:70:ALA:CB	28:N:70:ALA:HB2	1.38	0.81
37:W:37:LEU:CA	44:m:48:PHE:CB	2.59	0.81
36:U:529:GLU:N	36:U:1047:HIS:CB	2.44	0.81
34:M:308:ALA:N	36:U:352:ALA:O	1.95	0.81
46:o:28:PRO:CB	46:o:63:ALA:HB3	1.30	0.80
2:2:52:G:N1	30:9:435:MET:C	2.40	0.80
2:2:51:A:C5	30:9:437:CYS:C	2.60	0.80
36:U:485:ILE:O	36:U:566:THR:N	2.14	0.80
30:9:490:LYS:H	38:X:161:GLU:H	1.27	0.80
28:z:73:ALA:HB3	28:N:73:ALA:CB	0.70	0.80
28:z:70:ALA:HB2	28:N:70:ALA:HB2	0.90	0.80
30:9:342:HIS:CB	45:n:76:LEU:CA	2.60	0.80
30:9:493:GLU:CA	38:X:157:ASN:C	2.55	0.80
46:o:179:GLU:O	50:w:44:LYS:C	2.25	0.79
34:M:104:VAL:O	36:U:935:PHE:O	2.00	0.79
24:u:489:PRO:C	30:9:421:ALA:HB3	2.06	0.79
28:z:77:LEU:O	28:N:80:PHE:N	2.12	0.79
46:o:28:PRO:N	46:o:63:ALA:HB1	1.97	0.79
14:O:465:ARG:CB	34:M:547:LEU:H	1.89	0.79
25:v:599:GLU:C	49:r:860:GLN:O	2.26	0.79
30:9:331:VAL:CB	39:h:73:MET:H	1.96	0.79
36:U:489:VAL:HA	36:U:654:ASN:CA	2.11	0.79
9:B:117:ASP:HA	43:e:88:ASN:N	1.95	0.79
28:z:31:THR:O	28:N:31:THR:O	1.94	0.78
28:z:108:GLU:O	28:N:110:LEU:N	1.84	0.78
30:9:334:LEU:H	39:h:53:LEU:N	1.72	0.78
30:9:127:LEU:N	45:n:69:ILE:C	2.33	0.78
30:9:129:GLU:CB	45:n:15:VAL:N	2.30	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:W:13:ALA:HA	44:m:68:GLY:HA3	1.65	0.78
2:2:60:U:H3'	30:9:432:ALA:CB	2.14	0.78
2:2:61:C:OP2	30:9:429:TRP:O	2.00	0.78
28:z:79:GLY:N	28:N:79:GLY:C	2.40	0.78
34:M:622:ALA:N	47:p:106:ALA:C	2.42	0.78
37:W:9:ILE:O	44:m:45:CYS:N	2.16	0.78
2:2:52:G:O6	30:9:436:ARG:N	2.17	0.78
28:z:31:THR:H	28:N:31:THR:CA	1.93	0.78
37:W:47:ILE:CA	44:m:65:ARG:HA	2.10	0.78
30:9:331:VAL:CB	39:h:51:LYS:CB	2.63	0.78
2:2:51:A:N6	30:9:438:LEU:N	2.32	0.77
46:o:179:GLU:HA	50:w:42:ALA:O	1.83	0.77
24:u:489:PRO:CB	30:9:416:TYR:C	2.52	0.77
30:9:496:LYS:CB	38:X:157:ASN:CB	0.77	0.77
24:u:477:LYS:CB	30:9:399:LEU:CB	2.62	0.77
28:z:73:ALA:HB1	28:N:73:ALA:HB1	0.77	0.77
30:9:34:ARG:CB	34:M:734:TYR:CB	2.63	0.77
34:M:307:ILE:C	36:U:352:ALA:O	2.27	0.77
9:B:112:THR:O	43:e:83:LEU:HA	1.85	0.77
37:W:38:GLY:CA	44:m:26:ILE:CB	2.61	0.77
25:v:896:PHE:CA	38:X:182:LEU:O	2.08	0.77
30:9:133:GLU:C	39:h:95:TYR:O	2.27	0.77
46:o:179:GLU:C	50:w:42:ALA:O	2.28	0.77
2:2:53:U:H5'	30:9:462:LEU:CB	2.12	0.77
14:O:452:PHE:CA	47:p:89:PRO:N	2.42	0.77
25:v:979:ARG:CA	38:X:164:GLU:O	2.32	0.76
28:z:63:VAL:CB	28:N:63:VAL:CB	0.77	0.76
2:2:61:C:C4	30:9:432:ALA:O	2.29	0.76
25:v:979:ARG:CB	38:X:165:MET:HA	2.14	0.76
8:A:2268:LEU:CB	49:r:1263:PRO:CA	2.63	0.76
30:9:33:LEU:O	34:M:732:ALA:HB3	1.86	0.76
28:z:73:ALA:HB3	28:N:73:ALA:HB3	0.76	0.76
28:z:108:GLU:O	28:N:109:GLN:CB	2.20	0.76
28:z:70:ALA:HB3	28:N:70:ALA:HB3	0.76	0.76
25:v:942:LYS:O	38:X:213:THR:N	2.19	0.76
34:M:205:ASN:O	36:U:1052:LEU:CA	2.32	0.76
36:U:426:LEU:CB	36:U:636:GLN:HA	2.16	0.76
28:z:70:ALA:CB	28:N:70:ALA:CB	0.76	0.76
30:9:38:ASN:H	34:M:730:VAL:CA	1.98	0.76
34:M:103:PHE:C	36:U:939:GLN:CB	2.59	0.76
37:W:41:LEU:CB	44:m:27:PHE:CB	2.63	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:o:1:MET:CB	46:o:235:SER:CA	2.63	0.76
2:2:60:U:C4'	30:9:427:ALA:HA	2.16	0.75
36:U:488:SER:CB	36:U:565:ILE:H	1.99	0.75
44:f:79:SER:HA	45:g:59:SER:O	1.85	0.75
2:2:50:C:C5	30:9:437:CYS:CB	2.41	0.75
2:2:51:A:C6	30:9:438:LEU:CA	2.64	0.75
24:u:760:GLU:CA	48:q:957:ARG:HA	2.17	0.75
28:z:33:GLU:H	28:N:31:THR:CB	1.99	0.75
34:M:354:PRO:C	34:M:362:LYS:N	2.44	0.75
24:u:489:PRO:CB	30:9:416:TYR:O	2.33	0.75
30:9:331:VAL:C	39:h:51:LYS:O	2.29	0.75
36:U:491:ARG:C	36:U:513:PRO:CA	2.58	0.75
46:o:179:GLU:O	50:w:42:ALA:O	2.04	0.75
28:z:87:LEU:O	28:N:79:GLY:HA2	1.85	0.75
24:u:487:LEU:O	30:9:403:ASN:N	2.18	0.75
2:2:60:U:O3'	30:9:428:GLU:O	2.04	0.75
14:O:451:LEU:H	47:p:87:ASN:C	1.95	0.75
46:o:4:THR:O	46:o:242:ASN:CB	2.34	0.75
2:2:60:U:H4'	30:9:427:ALA:HA	1.69	0.74
37:W:47:ILE:CA	44:m:65:ARG:CB	2.64	0.74
14:O:448:ALA:O	47:p:88:ASP:N	2.20	0.74
34:M:206:ASP:O	36:U:1052:LEU:HA	1.85	0.74
43:e:15:GLY:N	43:e:32:LEU:O	2.19	0.74
30:9:337:GLN:CB	39:h:68:GLU:O	2.35	0.74
32:J:31:GLU:O	32:J:35:ALA:HB2	1.87	0.74
37:W:9:ILE:O	44:m:44:ASP:C	2.21	0.74
30:9:349:GLN:O	30:9:350:ALA:HB3	1.84	0.74
25:v:977:LEU:O	38:X:166:MET:O	2.04	0.74
36:U:527:ILE:C	36:U:1051:LYS:CB	2.60	0.74
37:W:41:LEU:O	44:m:25:ARG:CB	2.29	0.74
2:2:53:U:P	30:9:462:LEU:CB	2.76	0.73
14:O:465:ARG:HA	34:M:542:GLU:O	1.86	0.73
24:u:489:PRO:CA	30:9:416:TYR:CB	2.62	0.73
34:M:206:ASP:O	36:U:1052:LEU:CA	2.36	0.73
30:9:332:GLU:CA	39:h:44:ILE:H	1.66	0.73
32:H:73:ALA:O	32:H:77:ALA:HB3	1.89	0.73
37:W:13:ALA:CA	44:m:68:GLY:HA3	2.18	0.73
28:z:37:ASP:N	28:N:33:GLU:O	2.21	0.73
34:M:622:ALA:H	47:p:106:ALA:C	1.94	0.73
35:T:609:GLN:O	35:T:611:PHE:N	2.21	0.73
12:E:143:LEU:CB	31:F:348:ASP:O	2.37	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:u:495:ARG:O	30:9:400:HIS:HA	1.89	0.73
14:O:465:ARG:CB	34:M:547:LEU:CA	2.66	0.73
34:M:205:ASN:O	36:U:1052:LEU:C	2.31	0.73
46:o:4:THR:O	46:o:242:ASN:HA	1.89	0.73
2:2:51:A:N6	30:9:438:LEU:H	1.85	0.72
32:H:31:GLU:O	32:H:35:ALA:HB2	1.89	0.72
2:2:61:C:H3'	30:9:431:HIS:C	2.14	0.72
37:W:24:LEU:H	44:m:65:ARG:CB	2.01	0.72
30:9:496:LYS:CB	38:X:157:ASN:HA	2.15	0.72
37:W:38:GLY:O	44:m:26:ILE:CA	2.36	0.72
14:O:449:GLN:N	47:p:87:ASN:N	2.38	0.72
30:9:136:TYR:CB	45:n:72:ASP:HA	2.20	0.72
36:U:427:TYR:CB	36:U:637:ASP:CA	2.66	0.72
46:o:179:GLU:O	50:w:46:ARG:N	2.21	0.72
30:9:490:LYS:HA	38:X:159:PRO:O	1.84	0.72
25:v:904:TYR:CB	38:X:188:ASP:H	2.02	0.72
25:v:942:LYS:O	38:X:212:ILE:C	2.32	0.72
9:B:113:VAL:O	43:e:85:SER:CA	2.37	0.72
30:9:337:GLN:CB	39:h:68:GLU:N	2.52	0.71
30:9:332:GLU:HA	39:h:44:ILE:H	1.50	0.71
2:2:60:U:O3'	30:9:428:GLU:N	2.24	0.71
24:u:487:LEU:C	30:9:403:ASN:HA	2.14	0.71
32:J:99:THR:O	32:J:100:ARG:CB	2.39	0.71
33:K:209:ILE:O	33:K:212:GLN:C	2.33	0.71
30:9:332:GLU:HA	39:h:52:LEU:N	2.06	0.71
2:2:51:A:N3	30:9:440:ILE:N	2.33	0.71
30:9:334:LEU:CA	39:h:70:VAL:HA	2.05	0.71
30:9:337:GLN:CB	39:h:68:GLU:CA	2.69	0.71
34:M:354:PRO:C	34:M:361:HIS:CB	2.64	0.71
28:z:70:ALA:HB3	28:N:70:ALA:CB	0.79	0.71
37:W:13:ALA:CA	44:m:68:GLY:CA	2.69	0.71
24:u:491:GLU:CB	30:9:401:GLY:O	2.39	0.71
28:z:79:GLY:N	28:N:78:SER:O	2.05	0.71
2:2:59:A:H61	30:9:443:THR:CA	2.04	0.71
33:K:23:TYR:CB	33:K:27:GLY:HA3	2.21	0.71
2:2:61:C:N4	30:9:432:ALA:O	2.23	0.70
30:9:489:LYS:N	38:X:161:GLU:H	1.78	0.70
2:2:61:C:OP1	30:9:428:GLU:CB	2.40	0.70
30:9:490:LYS:CB	38:X:162:THR:HA	2.22	0.70
2:2:52:G:H1	30:9:435:MET:CB	2.03	0.70
34:M:206:ASP:C	36:U:1052:LEU:CA	2.65	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:M:621:ARG:CB	47:p:106:ALA:C	2.65	0.70
28:z:40:GLY:N	28:N:36:TYR:O	2.25	0.70
30:9:35:ASP:CA	34:M:730:VAL:CA	2.57	0.70
33:K:62:GLU:C	33:K:64:ASP:H	2.00	0.70
33:K:132:CYS:O	33:K:134:ALA:N	2.20	0.70
30:9:496:LYS:C	38:X:157:ASN:CB	2.65	0.70
48:q:665:PRO:O	48:q:668:ALA:HB3	1.92	0.70
30:9:334:LEU:CB	39:h:71:LYS:O	2.40	0.69
28:z:73:ALA:HB1	28:N:73:ALA:CB	1.32	0.69
2:2:53:U:O2	30:9:442:ASN:C	2.33	0.69
34:M:621:ARG:CB	47:p:106:ALA:CA	2.69	0.69
28:z:79:GLY:CA	28:N:79:GLY:C	2.64	0.69
24:u:490:GLU:CB	30:9:419:PRO:O	2.41	0.69
24:u:491:GLU:CB	30:9:418:GLY:HA2	2.23	0.69
46:o:23:HIS:CA	46:o:31:ASP:CA	2.60	0.69
36:U:426:LEU:O	36:U:636:GLN:CB	2.40	0.69
30:9:333:ILE:O	39:h:54:GLY:CA	2.38	0.69
36:U:485:ILE:H	36:U:592:VAL:HA	1.58	0.69
46:o:27:ILE:HA	46:o:67:MET:CB	2.23	0.69
2:2:60:U:H5"	30:9:428:GLU:CA	2.21	0.68
9:B:118:PHE:N	43:e:88:ASN:CB	2.52	0.68
28:z:70:ALA:HB2	28:N:70:ALA:CB	1.17	0.68
28:z:69:ASP:CA	28:N:72:ASN:CB	2.71	0.68
34:M:621:ARG:CA	47:p:106:ALA:O	2.41	0.68
30:9:33:LEU:C	34:M:732:ALA:HB3	2.19	0.68
25:v:968:ARG:CB	38:X:165:MET:CB	2.72	0.68
25:v:957:GLY:O	38:X:182:LEU:O	2.12	0.67
14:O:452:PHE:H	47:p:88:ASP:CA	2.06	0.67
34:M:621:ARG:CB	47:p:106:ALA:H	2.07	0.67
36:U:489:VAL:CB	36:U:566:THR:HA	2.25	0.67
28:z:69:ASP:CB	28:N:42:TYR:O	2.43	0.67
30:9:231:LYS:O	30:9:232:GLU:CB	2.42	0.67
35:T:577:SER:O	35:T:580:ARG:N	2.28	0.67
46:o:28:PRO:CA	46:o:63:ALA:HB2	1.99	0.67
28:z:69:ASP:O	28:N:72:ASN:CB	2.42	0.67
35:T:616:LEU:O	35:T:618:ARG:N	2.28	0.67
36:U:482:ARG:C	36:U:592:VAL:CB	2.68	0.67
44:m:75:GLU:HA	45:n:57:THR:C	2.17	0.67
46:o:180:LYS:O	50:w:41:LYS:HA	1.94	0.67
2:2:52:G:H1	30:9:435:MET:C	2.02	0.66
33:K:209:ILE:O	33:K:212:GLN:O	2.14	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:M:104:VAL:CA	36:U:939:GLN:CB	2.72	0.66
28:z:73:ALA:CB	28:N:73:ALA:HB1	1.19	0.66
36:U:492:MET:CB	36:U:654:ASN:O	2.42	0.66
32:H:68:ALA:N	33:K:66:MET:HA	2.11	0.66
36:U:491:ARG:CB	36:U:513:PRO:CA	2.73	0.66
30:9:344:ASN:CB	39:h:57:LYS:O	2.43	0.66
34:M:622:ALA:CB	47:p:106:ALA:HA	2.21	0.66
2:2:52:G:C6	30:9:435:MET:C	2.74	0.66
28:z:101:MET:O	28:N:101:MET:O	1.68	0.66
30:9:132:ASP:C	39:h:96:ILE:CB	2.67	0.66
37:W:9:ILE:CB	44:m:46:ASP:CB	2.73	0.66
48:q:665:PRO:C	48:q:668:ALA:HB3	2.21	0.66
25:v:942:LYS:O	38:X:212:ILE:CB	2.43	0.66
30:9:331:VAL:CB	39:h:73:MET:N	2.58	0.66
34:M:347:SER:O	34:M:351:ARG:CB	2.44	0.66
37:W:13:ALA:O	44:m:66:VAL:C	2.39	0.66
8:A:2077:ALA:HB3	49:r:1047:PRO:CB	2.26	0.66
14:O:454:ASN:N	47:p:89:PRO:CA	2.31	0.66
28:z:50:VAL:O	28:N:50:VAL:O	0.66	0.66
30:9:128:VAL:CA	45:n:16:THR:C	2.69	0.66
45:g:90:LYS:O	45:g:94:ALA:N	2.25	0.66
46:o:23:HIS:CA	46:o:31:ASP:HA	2.23	0.66
28:z:16:GLU:O	28:N:14:PRO:O	2.13	0.66
32:I:31:GLU:O	32:I:35:ALA:HB2	1.96	0.66
2:2:54:U:H1'	30:9:443:THR:CB	2.26	0.66
30:9:489:LYS:N	38:X:161:GLU:N	2.43	0.66
30:9:35:ASP:H	34:M:731:GLN:CB	1.89	0.65
46:o:181:GLY:H	50:w:43:GLU:CA	2.07	0.65
2:2:60:U:C4'	30:9:428:GLU:O	2.45	0.65
36:U:485:ILE:N	36:U:592:VAL:HA	2.11	0.65
24:u:491:GLU:CB	30:9:419:PRO:CB	2.70	0.65
30:9:340:LEU:CB	39:h:67:LEU:HA	2.27	0.65
34:M:138:ARG:C	36:U:936:PHE:H	2.05	0.65
48:q:666:PRO:C	48:q:668:ALA:H	2.04	0.65
2:2:61:C:P	30:9:428:GLU:C	2.79	0.65
30:9:127:LEU:C	45:n:69:ILE:H	1.97	0.65
34:M:208:ARG:O	34:M:209:PHE:N	2.26	0.65
36:U:485:ILE:CB	36:U:591:TYR:CA	2.72	0.65
30:9:134:GLU:CA	39:h:95:TYR:O	2.44	0.65
30:9:349:GLN:O	30:9:350:ALA:CB	2.42	0.65
28:z:20:ILE:H	28:N:18:ASN:C	2.04	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:62:U:O3'	30:9:410:ILE:HA	1.95	0.65
37:W:13:ALA:O	44:m:67:LEU:N	2.30	0.65
8:A:358:PRO:O	35:T:323:LEU:O	1.85	0.64
14:O:467:GLY:O	34:M:538:PHE:O	2.15	0.64
30:9:34:ARG:C	34:M:730:VAL:N	2.23	0.64
14:O:452:PHE:H	47:p:88:ASP:HA	1.63	0.64
30:9:339:HIS:CA	39:h:100:PHE:HA	2.22	0.64
30:9:331:VAL:CA	39:h:71:LYS:O	2.45	0.64
46:o:28:PRO:CB	46:o:63:ALA:CB	0.65	0.64
32:J:113:ALA:HA	33:K:15:ALA:CB	2.27	0.64
36:U:489:VAL:CA	36:U:654:ASN:C	2.68	0.64
37:W:6:ALA:CB	44:m:83:GLU:CB	2.76	0.64
2:2:52:G:C1'	30:9:440:ILE:HA	2.03	0.64
34:M:309:ALA:HB3	36:U:355:ASN:N	2.13	0.64
34:M:207:GLU:CB	36:U:1052:LEU:HA	2.27	0.64
2:2:61:C:OP2	30:9:432:ALA:CA	2.44	0.63
25:v:940:LEU:C	38:X:216:HIS:CB	2.71	0.63
4:5:24:G:N3	4:5:26:A:N6	2.47	0.63
36:U:491:ARG:C	36:U:513:PRO:HA	2.23	0.63
46:o:4:THR:O	46:o:242:ASN:CA	2.46	0.63
46:o:22:LEU:O	46:o:26:PHE:CB	2.46	0.63
33:K:77:GLN:O	33:K:79:ILE:N	2.32	0.63
37:W:13:ALA:O	44:m:67:LEU:CA	2.44	0.63
24:u:760:GLU:CB	48:q:957:ARG:HA	2.28	0.63
34:M:332:ALA:O	34:M:336:GLN:CB	2.47	0.63
42:d:69:MET:HA	43:e:62:TYR:O	1.99	0.63
33:K:132:CYS:C	33:K:134:ALA:H	2.06	0.62
37:W:9:ILE:C	44:m:45:CYS:HA	2.23	0.62
46:o:179:GLU:CA	50:w:42:ALA:O	2.46	0.62
30:9:330:TYR:O	39:h:71:LYS:O	2.17	0.62
34:M:355:HIS:C	34:M:358:HIS:C	2.67	0.62
28:z:74:CYS:O	28:N:74:CYS:O	0.63	0.62
8:A:2268:LEU:CB	49:r:1264:PRO:N	2.62	0.62
28:z:70:ALA:HB1	28:N:70:ALA:HB1	0.63	0.62
24:u:494:GLU:H	30:9:420:LYS:N	1.89	0.62
30:9:488:ASN:CB	38:X:161:GLU:CB	2.78	0.62
34:M:206:ASP:C	36:U:1052:LEU:O	2.41	0.62
46:o:179:GLU:C	50:w:42:ALA:C	2.56	0.62
32:H:16:CYS:O	32:H:25:TYR:CB	2.48	0.62
12:E:147:GLN:CB	31:F:325:GLY:O	2.48	0.61
25:v:942:LYS:CB	38:X:213:THR:CB	0.62	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:9:34:ARG:C	34:M:729:SER:C	2.68	0.61
34:M:621:ARG:N	47:p:106:ALA:O	2.33	0.61
49:r:1992:GLU:HA	49:r:1995:ALA:HB3	1.80	0.61
28:z:16:GLU:O	28:N:16:GLU:O	2.18	0.61
49:r:508:GLY:HA3	55:r:2201:ADP:H8	1.64	0.61
2:2:60:U:C5'	30:9:428:GLU:N	2.62	0.61
36:U:491:ARG:CB	36:U:512:GLN:O	2.48	0.61
25:v:904:TYR:CB	38:X:188:ASP:N	2.62	0.61
28:z:20:ILE:N	28:N:18:ASN:C	2.57	0.61
9:B:112:THR:O	43:e:83:LEU:CB	2.49	0.61
28:z:70:ALA:CB	28:N:70:ALA:HB1	1.29	0.61
30:9:341:THR:CB	39:h:58:ALA:HB2	2.30	0.60
39:a:108:VAL:HA	40:b:63:LEU:O	2.01	0.60
24:u:760:GLU:O	48:q:957:ARG:O	2.19	0.60
39:a:67:LEU:N	39:a:99:MET:O	2.21	0.60
28:z:14:PRO:O	28:N:15:PRO:HA	2.00	0.60
30:9:36:GLN:C	34:M:730:VAL:CB	2.74	0.60
30:9:493:GLU:N	38:X:159:PRO:CA	2.61	0.60
28:z:56:THR:O	28:N:51:GLY:HA3	2.00	0.60
30:9:496:LYS:CB	38:X:157:ASN:O	2.49	0.60
34:M:309:ALA:HB3	36:U:354:SER:C	2.25	0.60
34:M:99:HIS:HA	36:U:938:TYR:O	2.02	0.60
36:U:484:ASP:CB	36:U:563:PHE:CB	2.79	0.60
12:E:85:TYR:N	31:F:60:MET:CB	2.61	0.60
14:O:466:ARG:O	34:M:542:GLU:N	2.31	0.60
32:J:80:ASP:O	32:J:84:ALA:HB2	2.02	0.60
41:c:21:ILE:O	41:c:24:TYR:CB	2.50	0.60
11:D:416:ILE:HA	11:D:431:ALA:HA	1.84	0.59
23:t:305:GLY:HA2	25:v:632:ALA:HB3	1.82	0.59
8:A:359:ILE:CB	35:T:320:ARG:O	2.50	0.59
34:M:205:ASN:HA	36:U:1050:VAL:O	2.01	0.59
34:M:308:ALA:HB1	36:U:351:PHE:O	1.90	0.59
37:W:13:ALA:C	44:m:68:GLY:CA	2.65	0.59
2:2:61:C:OP2	30:9:432:ALA:CB	2.50	0.59
2:2:12:G:H1	5:6:86:U:H3	1.50	0.59
8:A:2266:ARG:C	49:r:1261:PRO:CB	2.75	0.59
9:B:478:THR:HA	9:B:494:GLY:HA3	1.83	0.59
28:z:73:ALA:HB2	28:N:73:ALA:CB	1.12	0.59
30:9:27:LEU:HA	47:p:247:VAL:CB	2.33	0.59
30:9:43:THR:CB	47:p:248:GLU:HA	2.32	0.59
34:M:206:ASP:O	36:U:1052:LEU:O	2.21	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:U:485:ILE:O	36:U:565:ILE:CA	2.43	0.59
28:z:20:ILE:O	28:N:21:LEU:CB	2.46	0.59
30:9:343:GLU:CA	45:n:76:LEU:O	2.51	0.59
34:M:309:ALA:HB3	36:U:355:ASN:H	1.68	0.59
28:z:59:THR:N	28:N:56:THR:O	2.34	0.59
2:2:61:C:C3'	30:9:431:HIS:O	2.42	0.59
28:z:14:PRO:O	28:N:15:PRO:CA	2.40	0.59
36:U:492:MET:CA	36:U:513:PRO:CB	2.79	0.59
30:9:108:VAL:CB	30:9:119:ASN:H	2.15	0.58
31:F:87:ASP:O	31:F:88:ARG:CB	2.50	0.58
34:M:621:ARG:HA	47:p:104:GLY:O	2.03	0.58
30:9:329:GLU:CA	39:h:43:LEU:CB	2.73	0.58
2:2:54:U:H5'	30:9:445:HIS:CB	2.33	0.58
28:z:107:GLU:O	28:N:106:LYS:O	2.20	0.58
46:o:27:ILE:O	46:o:67:MET:CB	2.52	0.58
31:F:269:PRO:O	31:F:270:LYS:CB	2.51	0.58
30:9:332:GLU:CA	39:h:52:LEU:N	2.64	0.58
33:K:60:ALA:O	33:K:63:THR:N	2.37	0.58
28:N:79:GLY:HA2	28:N:87:LEU:O	2.04	0.58
35:T:500:GLN:O	35:T:501:ARG:C	2.47	0.58
41:c:44:GLU:O	41:c:61:ALA:HA	2.04	0.58
46:o:28:PRO:CB	46:o:63:ALA:HB1	0.65	0.58
36:U:486:GLU:N	36:U:565:ILE:CB	2.60	0.58
37:W:44:PHE:CB	44:m:47:GLU:CB	2.80	0.58
25:v:336:ALA:HA	25:v:351:SER:HA	1.85	0.58
37:W:40:THR:CB	44:m:46:ASP:O	2.51	0.58
9:B:112:THR:O	43:e:83:LEU:CA	2.52	0.58
2:2:63:G:P	30:9:410:ILE:O	2.61	0.57
44:f:16:ARG:HA	44:f:29:GLY:O	2.04	0.57
25:v:978:LEU:CB	38:X:171:PHE:CB	2.82	0.57
34:M:619:ALA:HA	47:p:107:GLN:HA	1.86	0.57
2:2:60:U:H3'	30:9:428:GLU:O	1.99	0.57
8:A:1634:SER:CB	49:r:1146:LYS:CB	2.82	0.57
33:K:62:GLU:C	33:K:64:ASP:N	2.60	0.57
34:M:354:PRO:C	34:M:361:HIS:C	2.69	0.57
2:2:62:U:O2'	30:9:452:ILE:CB	2.52	0.57
34:M:668:CYS:O	34:M:672:ALA:HB2	2.04	0.57
46:o:23:HIS:CB	46:o:31:ASP:CB	2.82	0.57
39:a:71:LYS:HA	39:a:94:ARG:O	2.05	0.57
43:l:80:ALA:HB1	43:l:81:PRO:HA	1.86	0.57
30:9:331:VAL:CB	39:h:73:MET:CB	2.82	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:M:723:MET:O	34:M:727:ARG:CB	2.52	0.57
9:B:113:VAL:O	43:e:85:SER:N	2.37	0.57
36:U:484:ASP:C	36:U:564:LEU:C	2.73	0.57
9:B:117:ASP:CB	43:e:84:LYS:CB	2.82	0.57
45:g:17:ILE:O	45:g:25:VAL:N	2.27	0.57
28:z:44:PRO:O	28:N:43:GLY:C	2.28	0.57
28:z:77:LEU:C	28:N:79:GLY:H	2.12	0.56
30:9:33:LEU:C	34:M:732:ALA:CA	2.71	0.56
34:M:406:GLU:HA	34:M:410:GLN:HA	1.87	0.56
8:A:1367:ASN:H	35:T:465:SER:HA	1.70	0.56
34:M:479:ARG:O	34:M:483:SER:CB	2.53	0.56
14:O:448:ALA:C	47:p:87:ASN:O	2.23	0.56
28:z:71:LYS:O	28:N:75:ASP:N	2.38	0.56
9:B:113:VAL:O	43:e:85:SER:CB	2.53	0.56
32:J:128:ARG:O	32:J:132:ALA:CB	2.53	0.56
34:M:140:LEU:N	36:U:930:GLU:O	2.27	0.56
2:2:52:G:C6	30:9:436:ARG:CA	2.67	0.56
30:9:342:HIS:C	45:n:76:LEU:C	2.61	0.56
30:9:354:GLU:O	30:9:355:GLU:CB	2.53	0.56
32:J:31:GLU:O	32:J:35:ALA:CB	2.53	0.56
48:q:453:GLN:O	48:q:498:THR:HA	2.05	0.56
2:2:61:C:N4	30:9:436:ARG:H	2.04	0.56
28:z:70:ALA:HB1	28:N:70:ALA:CB	1.08	0.56
28:z:79:GLY:N	28:N:79:GLY:N	2.23	0.56
46:o:180:LYS:O	50:w:44:LYS:CB	2.52	0.56
9:B:186:VAL:HA	9:B:534:VAL:HA	1.88	0.56
32:I:73:ALA:O	32:I:77:ALA:CB	2.48	0.56
2:2:61:C:N4	30:9:436:ARG:N	2.53	0.55
8:A:360:SER:H	35:T:326:SER:H	1.54	0.55
8:A:2266:ARG:O	49:r:1261:PRO:C	2.49	0.55
28:z:16:GLU:N	28:N:14:PRO:O	2.35	0.55
34:M:163:GLU:O	34:M:167:ARG:CB	2.54	0.55
34:M:205:ASN:C	36:U:1052:LEU:CA	2.70	0.55
34:M:480:VAL:O	34:M:484:LEU:CB	2.53	0.55
36:U:492:MET:CB	36:U:654:ASN:CB	2.83	0.55
36:U:632:ASN:N	36:U:668:ALA:HB2	2.21	0.55
30:9:341:THR:H	39:h:58:ALA:HB3	1.72	0.55
46:o:180:LYS:C	50:w:40:PRO:O	2.36	0.55
9:B:194:LYS:O	43:e:8:LYS:CB	2.54	0.55
2:2:53:U:C2'	30:9:445:HIS:CB	2.81	0.55
2:2:61:C:N4	30:9:436:ARG:CB	2.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:v:977:LEU:CB	38:X:167:LEU:CB	2.74	0.55
34:M:47:GLY:HA3	34:M:50:LYS:H	1.72	0.55
34:M:52:ARG:O	34:M:56:LEU:CB	2.55	0.55
44:m:77:LEU:O	45:n:56:GLU:N	2.28	0.55
46:o:2:ALA:C	46:o:263:VAL:CB	2.73	0.55
2:2:62:U:O2'	30:9:452:ILE:HA	2.07	0.55
30:9:133:GLU:O	39:h:95:TYR:C	2.50	0.55
4:5:41:U:O4	21:Z:242:G:N2	2.40	0.55
25:v:896:PHE:H	38:X:183:VAL:CB	1.88	0.55
14:O:467:GLY:O	34:M:538:PHE:C	2.50	0.55
28:z:37:ASP:H	28:N:34:GLU:C	2.15	0.55
34:M:355:HIS:CA	34:M:359:GLU:N	2.36	0.55
35:T:535:THR:O	35:T:537:HIS:N	2.40	0.55
9:B:113:VAL:C	43:e:85:SER:CB	2.80	0.55
9:B:120:ALA:HB3	43:e:76:MET:N	2.21	0.55
30:9:126:ASN:O	45:n:15:VAL:HA	2.07	0.55
49:r:1048:VAL:O	49:r:1050:GLU:N	2.40	0.55
14:O:391:TYR:O	14:O:395:ALA:N	2.37	0.54
14:O:449:GLN:CB	47:p:85:ASN:CB	2.81	0.54
36:U:488:SER:N	36:U:565:ILE:CB	2.66	0.54
46:o:23:HIS:CB	46:o:31:ASP:HA	2.37	0.54
36:U:489:VAL:N	36:U:565:ILE:O	2.40	0.54
5:6:25:C:H41	15:P:64:ARG:HA	1.72	0.54
25:v:428:GLY:HA3	25:v:433:SER:HA	1.88	0.54
28:z:41:LYS:N	28:N:37:ASP:O	2.41	0.54
39:a:61:ARG:C	39:a:63:CYS:H	2.15	0.54
8:A:362:ARG:N	35:T:327:GLU:CA	2.53	0.54
34:M:139:ALA:HB1	36:U:930:GLU:O	2.07	0.54
34:M:342:PRO:C	34:M:344:LEU:H	2.16	0.54
25:v:699:VAL:HA	25:v:715:MET:O	2.07	0.54
28:z:73:ALA:O	28:N:77:LEU:N	2.37	0.54
30:9:128:VAL:HA	45:n:17:ILE:N	2.22	0.54
30:9:107:SER:HA	30:9:115:LYS:O	2.07	0.54
36:U:491:ARG:CB	36:U:513:PRO:HA	2.37	0.54
48:q:480:TYR:HA	48:q:496:TYR:O	2.08	0.54
32:J:15:PRO:HA	32:J:25:TYR:O	2.08	0.54
34:M:619:ALA:CA	47:p:107:GLN:HA	2.33	0.54
28:z:99:GLN:O	28:N:99:GLN:O	0.53	0.53
30:9:35:ASP:N	34:M:730:VAL:N	2.40	0.53
32:J:27:ARG:O	32:J:31:GLU:CB	2.57	0.53
34:M:138:ARG:H	36:U:937:LEU:CB	2.20	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:9:35:ASP:C	34:M:727:ARG:HA	2.34	0.53
44:f:15:TYR:O	44:f:31:PHE:N	2.41	0.53
46:o:30:GLY:HA3	46:o:52:VAL:CB	2.35	0.53
24:u:492:GLN:H	30:9:418:GLY:HA3	1.74	0.53
28:z:43:GLY:O	28:N:40:GLY:O	2.27	0.53
25:v:894:CYS:CB	38:X:184:PRO:CB	2.87	0.53
4:5:19:A:O2'	4:5:21:A:N1	2.42	0.53
30:9:332:GLU:N	39:h:52:LEU:N	2.50	0.53
34:M:231:ASN:O	34:M:233:ASP:N	2.41	0.53
25:v:801:GLU:O	25:v:864:SER:HA	2.08	0.53
42:d:18:SER:N	42:d:71:GLU:O	2.23	0.53
32:G:31:GLU:O	32:G:35:ALA:HB2	2.09	0.53
33:K:196:GLU:O	33:K:199:ILE:N	2.39	0.53
25:v:898:ASN:CB	38:X:191:PHE:CA	2.79	0.53
41:j:15:VAL:O	42:k:33:GLY:HA3	2.09	0.53
48:q:851:ASN:C	48:q:853:SER:H	2.15	0.52
28:z:58:GLY:O	28:N:58:GLY:O	0.52	0.52
28:z:69:ASP:C	28:N:72:ASN:CB	2.82	0.52
30:9:126:ASN:C	45:n:15:VAL:CB	2.82	0.52
34:M:355:HIS:N	34:M:361:HIS:CA	2.72	0.52
36:U:487:ASP:N	36:U:565:ILE:CB	2.73	0.52
2:2:60:U:C3'	30:9:432:ALA:HB2	2.24	0.52
32:J:75:LEU:O	32:J:79:GLN:CB	2.57	0.52
8:A:360:SER:N	35:T:326:SER:H	2.07	0.52
28:z:59:THR:CB	28:N:56:THR:O	2.58	0.52
34:M:519:GLN:O	34:M:523:ASN:N	2.33	0.52
39:a:65:MET:O	39:a:100:PHE:HA	2.08	0.52
34:M:355:HIS:C	34:M:358:HIS:CA	2.83	0.52
28:z:70:ALA:O	28:N:70:ALA:O	0.52	0.52
30:9:33:LEU:C	34:M:732:ALA:N	2.61	0.52
32:I:27:ARG:O	32:I:31:GLU:CB	2.57	0.52
37:W:39:ALA:HA	44:m:18:ARG:HA	1.91	0.52
25:v:974:LYS:CB	38:X:220:ILE:CA	2.88	0.52
30:9:35:ASP:C	34:M:730:VAL:C	2.76	0.52
35:T:529:PHE:O	35:T:532:GLN:N	2.39	0.52
9:B:113:VAL:O	43:e:85:SER:HA	2.09	0.52
25:v:942:LYS:O	38:X:212:ILE:CA	2.57	0.52
30:9:471:TRP:HA	30:9:472:GLN:CB	2.39	0.52
46:o:4:THR:CB	46:o:242:ASN:HA	2.41	0.52
30:9:332:GLU:HA	39:h:52:LEU:H	1.72	0.51
32:H:30:ILE:O	32:H:34:ILE:CB	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:2268:LEU:O	49:r:1264:PRO:CB	2.59	0.51
32:G:82:TRP:O	32:G:86:MET:CB	2.58	0.51
2:2:63:G:N7	30:9:434:GLY:HA2	2.25	0.51
8:A:119:LEU:N	8:A:128:PHE:O	2.38	0.51
14:O:451:LEU:N	47:p:87:ASN:C	2.67	0.51
28:z:37:ASP:CB	28:N:33:GLU:O	2.58	0.51
30:9:32:THR:C	34:M:732:ALA:HB3	2.30	0.51
32:G:73:ALA:O	32:G:77:ALA:CB	2.58	0.51
32:H:3:LEU:N	32:J:63:PRO:O	2.42	0.51
33:K:210:LYS:O	33:K:213:HIS:C	2.49	0.51
32:J:80:ASP:O	32:J:84:ALA:CB	2.58	0.51
3:3:535:LEU:CB	35:T:537:HIS:CB	2.88	0.51
30:9:33:LEU:C	34:M:732:ALA:CB	2.84	0.51
46:o:28:PRO:CB	46:o:63:ALA:HB2	0.99	0.51
4:5:12:U:H3	4:5:65:G:H1	1.59	0.51
14:O:454:ASN:N	47:p:89:PRO:HA	2.23	0.51
32:J:113:ALA:HA	33:K:15:ALA:HB3	1.91	0.51
34:M:207:GLU:N	36:U:1052:LEU:HA	2.26	0.51
11:D:479:THR:O	11:D:486:ILE:HA	2.12	0.50
25:v:974:LYS:CB	38:X:220:ILE:N	2.74	0.50
36:U:485:ILE:HA	36:U:565:ILE:HA	0.68	0.50
48:q:642:GLU:O	48:q:668:ALA:HA	2.11	0.50
9:B:113:VAL:CB	43:e:78:LYS:CB	2.90	0.50
14:O:448:ALA:O	47:p:88:ASP:CA	2.59	0.50
35:T:607:THR:C	35:T:609:GLN:H	2.20	0.50
10:C:291:LEU:O	10:C:294:ALA:HB3	2.11	0.50
34:M:307:ILE:C	36:U:352:ALA:C	2.72	0.50
37:W:41:LEU:CA	44:m:19:CYS:O	2.56	0.50
30:9:337:GLN:O	39:h:67:LEU:N	2.37	0.50
34:M:138:ARG:O	36:U:932:ALA:C	2.55	0.50
39:a:27:GLY:HA3	40:b:35:SER:CB	2.41	0.50
31:F:255:MET:C	31:F:257:ASN:H	2.20	0.50
32:I:74:ILE:O	32:I:78:LEU:CB	2.60	0.50
9:B:117:ASP:CB	43:e:88:ASN:N	2.73	0.50
24:u:491:GLU:HA	30:9:420:LYS:N	2.10	0.50
48:q:476:ASN:O	48:q:492:THR:HA	2.12	0.50
30:9:127:LEU:C	45:n:69:ILE:O	2.54	0.50
34:M:328:GLU:O	34:M:332:ALA:CB	2.60	0.50
34:M:355:HIS:C	34:M:358:HIS:HA	2.37	0.50
33:K:209:ILE:O	33:K:210:LYS:C	2.54	0.49
9:B:832:TYR:HA	9:B:900:VAL:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:K:207:TYR:HA	33:K:220:ASN:CB	2.42	0.49
33:K:209:ILE:O	33:K:212:GLN:N	2.45	0.49
32:H:73:ALA:O	32:H:77:ALA:CB	2.60	0.49
36:U:485:ILE:N	36:U:591:TYR:O	2.44	0.49
46:o:23:HIS:HA	46:o:31:ASP:N	2.25	0.49
28:z:83:CYS:O	28:N:84:ASN:O	1.94	0.49
32:H:31:GLU:O	32:H:35:ALA:CB	2.57	0.49
34:M:206:ASP:C	36:U:1052:LEU:C	2.81	0.49
39:a:47:ARG:N	39:a:105:SER:O	2.46	0.49
2:2:52:G:C6	30:9:435:MET:O	2.65	0.49
2:2:60:U:O3'	30:9:428:GLU:CA	2.61	0.49
4:5:9:G:N2	4:5:10:U:O4	2.43	0.49
36:U:492:MET:N	36:U:513:PRO:HA	2.27	0.49
46:o:27:ILE:CA	46:o:67:MET:CB	2.90	0.49
2:2:62:U:P	30:9:431:HIS:HA	2.50	0.49
8:A:972:GLU:HA	8:A:1101:PHE:O	2.12	0.49
9:B:115:GLU:O	43:e:85:SER:HA	2.11	0.49
30:9:340:LEU:CB	39:h:67:LEU:CA	2.54	0.49
34:M:615:VAL:O	34:M:619:ALA:CB	2.60	0.49
25:v:667:GLY:HA2	25:v:672:VAL:HA	1.93	0.49
28:z:80:PHE:O	28:N:79:GLY:O	2.30	0.49
30:9:34:ARG:CB	34:M:734:TYR:CA	2.90	0.49
33:K:209:ILE:O	33:K:213:HIS:O	2.30	0.49
37:W:24:LEU:N	44:m:65:ARG:CB	2.73	0.49
2:2:51:A:H2	30:9:438:LEU:CB	2.10	0.49
2:2:61:C:H3'	30:9:431:HIS:CA	2.42	0.49
24:u:489:PRO:O	30:9:418:GLY:CA	2.59	0.49
28:z:38:ILE:C	28:N:37:ASP:O	2.52	0.49
30:9:493:GLU:N	38:X:159:PRO:HA	2.17	0.49
32:G:31:GLU:O	32:G:35:ALA:CB	2.61	0.49
36:U:527:ILE:CB	36:U:1051:LYS:CB	2.91	0.49
8:A:361:HIS:CA	35:T:326:SER:O	2.37	0.49
11:D:467:ALA:HB3	11:D:480:ALA:HB3	1.95	0.49
30:9:341:THR:N	39:h:58:ALA:HB3	2.28	0.49
8:A:360:SER:CB	35:T:322:ILE:C	2.71	0.48
14:O:449:GLN:CB	47:p:85:ASN:N	2.72	0.48
30:9:331:VAL:CB	39:h:51:LYS:CA	2.91	0.48
28:z:69:ASP:CB	28:N:43:GLY:HA3	2.43	0.48
32:J:128:ARG:O	32:J:132:ALA:HB2	2.14	0.48
34:M:456:LEU:O	34:M:460:THR:CB	2.62	0.48
28:z:67:ILE:O	28:N:70:ALA:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:U:526:ASN:CB	36:U:1048:ASP:CB	2.91	0.48
44:f:79:SER:CA	45:g:59:SER:O	2.59	0.48
28:N:26:LEU:O	28:N:58:GLY:HA2	2.12	0.48
8:A:1016:VAL:HA	8:A:1025:THR:HA	1.94	0.48
36:U:489:VAL:CB	36:U:566:THR:CA	2.91	0.48
28:z:20:ILE:N	28:N:18:ASN:O	2.46	0.48
30:9:337:GLN:HA	39:h:68:GLU:H	1.64	0.48
32:H:128:ARG:O	32:H:132:ALA:CB	2.61	0.48
8:A:1726:ILE:HA	8:A:1729:ALA:HB3	1.95	0.48
25:v:978:LEU:O	38:X:167:LEU:CB	2.57	0.48
30:9:342:HIS:C	45:n:76:LEU:O	2.56	0.48
33:K:210:LYS:C	33:K:213:HIS:O	2.53	0.48
41:c:66:SER:C	41:c:68:THR:H	2.22	0.48
6:7:56:CYS:O	6:7:60:LEU:N	2.46	0.48
14:O:449:GLN:CB	47:p:82:ASN:O	2.62	0.48
49:r:441:GLY:O	49:r:693:THR:N	2.36	0.48
14:O:452:PHE:CB	47:p:88:ASP:HA	2.44	0.48
34:M:259:TRP:O	34:M:263:ALA:HB2	2.14	0.48
8:A:2266:ARG:HA	49:r:1261:PRO:CB	2.44	0.48
1:1:63:VAL:N	1:1:83:CYS:O	2.47	0.48
11:D:333:VAL:HA	11:D:349:SER:HA	1.95	0.48
42:d:22:ASN:C	42:d:24:GLY:N	2.71	0.48
8:A:609:LYS:O	8:A:613:TYR:N	2.42	0.47
46:o:29:PHE:O	46:o:53:GLU:O	2.32	0.47
30:9:38:ASN:CA	34:M:730:VAL:CB	2.89	0.47
30:9:490:LYS:CA	38:X:162:THR:H	2.27	0.47
32:H:128:ARG:O	32:H:132:ALA:HB2	2.13	0.47
32:I:29:LEU:O	32:I:33:TYR:CB	2.62	0.47
34:M:351:ARG:HA	34:M:365:ALA:HB1	1.86	0.47
37:W:47:ILE:CB	44:m:65:ARG:CB	2.85	0.47
12:E:85:TYR:HA	31:F:61:LEU:H	1.20	0.47
32:I:31:GLU:O	32:I:35:ALA:CB	2.60	0.47
44:f:12:HIS:O	44:f:15:TYR:CB	2.62	0.47
32:G:30:ILE:O	32:G:34:ILE:CB	2.63	0.47
32:H:74:ILE:O	32:H:78:LEU:CB	2.62	0.47
45:g:45:MET:O	45:g:52:PRO:HA	2.14	0.47
46:o:180:LYS:O	50:w:41:LYS:O	2.32	0.47
24:u:487:LEU:CB	30:9:403:ASN:CB	2.93	0.47
30:9:393:PRO:C	28:N:55:GLU:CB	2.57	0.47
32:G:73:ALA:O	32:G:77:ALA:HB3	2.14	0.47
2:2:52:G:C6	30:9:436:ARG:N	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:z:17:VAL:O	28:N:16:GLU:O	2.28	0.47
30:9:339:HIS:CA	39:h:100:PHE:CA	2.64	0.47
30:9:341:THR:CA	39:h:58:ALA:HB3	2.43	0.47
31:F:157:CYS:HA	31:F:168:CYS:O	2.15	0.47
46:o:4:THR:CB	46:o:242:ASN:CA	2.93	0.47
28:z:87:LEU:O	28:N:86:TYR:C	2.45	0.47
33:K:210:LYS:CB	33:K:220:ASN:CB	2.93	0.47
42:d:22:ASN:O	42:d:24:GLY:N	2.47	0.47
2:2:52:G:O6	30:9:436:ARG:CB	2.53	0.47
2:2:60:U:O3'	30:9:428:GLU:C	2.58	0.47
25:v:972:LEU:CB	38:X:189:ILE:C	2.88	0.47
30:9:334:LEU:N	39:h:71:LYS:N	2.63	0.47
41:c:62:GLU:HA	41:c:73:GLN:HA	1.98	0.46
14:O:452:PHE:N	47:p:89:PRO:CA	2.70	0.46
30:9:136:TYR:CB	39:h:98:LYS:N	2.78	0.46
25:v:942:LYS:N	38:X:212:ILE:O	2.46	0.46
30:9:37:ILE:C	34:M:730:VAL:CB	2.81	0.46
30:9:127:LEU:N	45:n:70:LEU:N	2.62	0.46
37:W:9:ILE:C	44:m:46:ASP:N	2.73	0.46
9:B:194:LYS:O	43:e:8:LYS:HA	2.15	0.46
32:J:100:ARG:CB	32:J:103:LEU:CB	2.94	0.46
12:E:143:LEU:HA	31:F:348:ASP:CB	2.46	0.46
49:r:1349:GLY:HA2	49:r:1491:SER:O	2.16	0.46
24:u:495:ARG:O	30:9:400:HIS:CA	2.61	0.46
25:v:480:ASN:HA	25:v:504:PRO:HA	1.97	0.46
25:v:568:MET:HA	25:v:574:LEU:HA	1.98	0.46
34:M:308:ALA:HB3	36:U:351:PHE:O	2.10	0.46
35:T:601:ALA:O	35:T:604:LYS:N	2.48	0.46
30:9:490:LYS:CA	38:X:159:PRO:O	2.50	0.46
30:9:38:ASN:CB	34:M:730:VAL:CB	2.94	0.46
46:o:181:GLY:C	50:w:39:LEU:O	2.57	0.46
32:J:30:ILE:O	32:J:34:ILE:CB	2.64	0.45
35:T:571:SER:CB	35:T:574:THR:H	2.29	0.45
12:E:118:ALA:CB	31:F:66:GLU:O	2.64	0.45
15:P:280:ALA:O	15:P:283:ALA:HB3	2.16	0.45
48:q:852:ASN:C	48:q:854:ILE:H	2.24	0.45
30:9:480:GLU:O	30:9:483:SER:O	2.35	0.45
34:M:622:ALA:CA	47:p:106:ALA:HA	2.46	0.45
8:A:719:CYS:O	8:A:724:ILE:N	2.50	0.45
24:u:720:GLY:N	25:v:216:GLY:O	2.48	0.45
28:z:22:TYR:O	28:N:89:VAL:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:G:27:ARG:O	32:G:31:GLU:CB	2.64	0.45
32:J:111:ASP:O	32:J:115:ARG:CB	2.65	0.45
34:M:206:ASP:O	36:U:1052:LEU:CB	2.65	0.45
14:O:450:GLU:CB	47:p:87:ASN:HA	2.46	0.45
14:O:465:ARG:CA	34:M:543:ARG:O	2.54	0.45
43:e:27:VAL:O	43:e:48:VAL:HA	2.15	0.45
28:z:66:ASP:C	28:N:69:ASP:H	2.25	0.45
9:B:114:TYR:N	43:e:85:SER:CB	2.79	0.45
34:M:207:GLU:CB	36:U:1052:LEU:CA	2.95	0.45
37:W:61:PRO:O	37:W:86:ALA:HB1	2.16	0.45
44:m:77:LEU:O	45:n:56:GLU:CB	2.65	0.45
46:o:22:LEU:O	46:o:26:PHE:N	2.49	0.45
46:o:179:GLU:C	50:w:44:LYS:C	2.74	0.45
2:2:52:G:H1'	30:9:440:ILE:HA	1.93	0.45
28:z:83:CYS:O	28:N:82:VAL:O	2.34	0.45
9:B:834:VAL:HA	9:B:898:LEU:O	2.17	0.45
14:O:448:ALA:O	47:p:88:ASP:HA	2.17	0.45
25:v:605:LEU:O	25:v:616:ILE:HA	2.16	0.45
28:z:69:ASP:O	28:N:72:ASN:CA	2.64	0.45
39:a:59:PHE:HA	39:a:64:ASN:O	2.16	0.45
28:z:105:LYS:C	28:N:107:GLU:N	2.55	0.45
28:z:107:GLU:C	28:N:106:LYS:O	2.52	0.45
44:f:34:PHE:HA	44:f:39:ASN:O	2.17	0.45
44:f:44:ASP:N	44:f:68:GLY:O	2.50	0.45
49:r:419:GLY:C	49:r:421:HIS:H	2.25	0.44
9:B:756:LYS:HA	9:B:760:GLY:HA3	1.99	0.44
25:v:972:LEU:CB	38:X:190:ALA:N	2.54	0.44
30:9:33:LEU:O	34:M:732:ALA:CB	2.62	0.44
30:9:393:PRO:O	28:N:55:GLU:CB	2.64	0.44
42:d:22:ASN:C	42:d:24:GLY:H	2.25	0.44
49:r:721:VAL:HA	49:r:825:THR:O	2.17	0.44
2:2:53:U:OP1	30:9:462:LEU:C	2.60	0.44
24:u:490:GLU:HA	30:9:421:ALA:CB	2.37	0.44
30:9:480:GLU:HA	30:9:483:SER:O	2.16	0.44
36:U:492:MET:N	36:U:513:PRO:CB	2.77	0.44
46:o:218:LYS:HA	46:o:244:ASN:O	2.17	0.44
2:2:51:A:N6	30:9:435:MET:C	2.30	0.44
25:v:661:PHE:N	25:v:678:VAL:O	2.51	0.44
35:T:585:ILE:O	35:T:589:GLU:CB	2.65	0.44
30:9:133:GLU:O	39:h:95:TYR:N	2.51	0.44
35:T:604:LYS:O	35:T:606:GLU:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:a:44:ILE:O	39:a:51:LYS:HA	2.17	0.44
46:o:180:LYS:H	50:w:43:GLU:CB	2.06	0.44
48:q:852:ASN:C	48:q:854:ILE:N	2.74	0.44
15:P:167:PHE:O	15:P:172:GLU:N	2.48	0.44
30:9:343:GLU:N	45:n:76:LEU:O	2.51	0.44
41:c:64:ILE:HA	41:c:70:SER:HA	1.98	0.44
46:o:49:PHE:O	46:o:50:ALA:HB2	2.18	0.44
32:H:29:LEU:O	32:H:33:TYR:CB	2.66	0.44
2:2:52:G:N1	30:9:435:MET:O	2.49	0.43
36:U:485:ILE:H	36:U:592:VAL:CA	2.28	0.43
2:2:60:U:O4'	30:9:427:ALA:HA	2.17	0.43
30:9:125:GLN:CA	45:n:10:LEU:CB	2.95	0.43
36:U:482:ARG:CA	36:U:592:VAL:CB	2.65	0.43
28:z:59:THR:CA	28:N:56:THR:O	2.67	0.43
36:U:498:GLU:HA	36:U:499:TYR:HA	1.74	0.43
34:M:206:ASP:O	36:U:1052:LEU:C	2.61	0.43
9:B:850:LEU:O	9:B:855:GLY:N	2.51	0.43
2:2:61:C:C3'	30:9:431:HIS:C	2.85	0.43
32:I:40:ASP:N	32:I:45:GLN:O	2.44	0.43
8:A:2266:ARG:O	49:r:1261:PRO:HA	2.16	0.43
28:z:79:GLY:C	28:N:79:GLY:O	2.45	0.43
30:9:136:TYR:CB	39:h:98:LYS:H	2.31	0.43
34:M:135:ARG:CB	36:U:941:MET:CB	2.96	0.43
31:F:255:MET:O	31:F:257:ASN:N	2.52	0.43
34:M:683:ARG:O	34:M:687:ILE:CB	2.67	0.43
46:o:179:GLU:HA	50:w:42:ALA:C	2.42	0.43
5:6:2:U:H2'	5:6:3:G:C8	2.54	0.43
9:B:495:ARG:HA	9:B:549:TRP:HA	2.01	0.43
30:9:35:ASP:O	34:M:727:ARG:HA	2.18	0.43
4:5:50:G:O6	4:5:51:A:N6	2.52	0.43
8:A:91:ALA:HB2	8:A:125:ALA:HB1	2.01	0.43
9:B:196:LYS:C	43:e:12:GLU:CB	2.59	0.43
28:z:79:GLY:CA	28:N:79:GLY:O	2.67	0.43
30:9:136:TYR:O	45:n:72:ASP:CA	2.58	0.43
34:M:560:TYR:O	34:M:564:PHE:CB	2.67	0.43
2:2:53:U:H5'	30:9:459:TRP:HA	2.01	0.42
2:2:60:U:C1'	30:9:427:ALA:HA	2.49	0.42
2:2:61:C:OP2	30:9:432:ALA:HB3	2.17	0.42
8:A:895:GLY:O	8:A:909:TYR:HA	2.19	0.42
8:A:1640:SER:HA	8:A:1652:MET:HA	2.01	0.42
25:v:901:GLU:C	38:X:186:ARG:N	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:T:535:THR:C	35:T:537:HIS:H	2.27	0.42
14:O:465:ARG:CB	34:M:543:ARG:C	2.85	0.42
21:Z:240:A:H2'	21:Z:241:A:C8	2.54	0.42
25:v:971:ASP:O	38:X:167:LEU:CB	2.67	0.42
36:U:484:ASP:CB	36:U:564:LEU:O	2.67	0.42
24:u:489:PRO:O	30:9:418:GLY:N	2.40	0.42
24:u:490:GLU:HA	30:9:421:ALA:HB3	2.00	0.42
34:M:259:TRP:O	34:M:263:ALA:CB	2.67	0.42
35:T:601:ALA:O	35:T:605:ASP:N	2.38	0.42
35:T:606:GLU:O	35:T:608:LEU:N	2.52	0.42
41:c:63:GLU:O	41:c:71:ARG:N	2.52	0.42
49:r:1583:ASP:C	49:r:1585:GLN:H	2.26	0.42
2:2:62:U:OP2	30:9:431:HIS:CA	2.44	0.42
34:M:264:ASP:O	34:M:268:ARG:CB	2.67	0.42
24:u:760:GLU:HA	48:q:957:ARG:CA	2.37	0.42
34:M:138:ARG:C	36:U:932:ALA:O	2.61	0.42
8:A:1514:LYS:O	8:A:1516:LYS:N	2.52	0.42
30:9:337:GLN:CB	39:h:70:VAL:CB	2.97	0.42
32:H:8:SER:C	32:H:10:GLU:H	2.27	0.42
48:q:851:ASN:C	48:q:853:SER:N	2.77	0.42
28:z:83:CYS:O	28:N:85:ARG:N	2.18	0.42
30:9:490:LYS:N	38:X:162:THR:H	2.17	0.42
44:f:89:ASP:O	44:f:93:ALA:HB2	2.20	0.42
14:O:452:PHE:N	47:p:88:ASP:C	2.50	0.42
28:z:19:ARG:O	28:N:20:ILE:CB	2.63	0.42
30:9:329:GLU:C	39:h:53:LEU:CB	2.92	0.42
34:M:452:ALA:O	34:M:456:LEU:CB	2.68	0.42
44:f:78:VAL:O	45:g:60:ILE:HA	2.19	0.42
8:A:645:THR:O	8:A:649:GLU:CB	2.68	0.42
11:D:195:LYS:O	11:D:489:TYR:HA	2.20	0.42
28:z:73:ALA:O	28:z:77:LEU:CB	2.68	0.42
28:z:104:LYS:N	28:N:102:ASP:O	2.53	0.42
30:9:339:HIS:C	39:h:100:PHE:HA	2.45	0.42
32:J:128:ARG:O	32:J:132:ALA:HB3	2.20	0.42
35:T:507:PHE:C	35:T:509:LEU:H	2.27	0.42
36:U:1338:PHE:HA	36:U:1339:PRO:HA	1.86	0.42
48:q:666:PRO:C	48:q:668:ALA:N	2.75	0.42
8:A:896:ILE:HA	8:A:908:VAL:O	2.20	0.41
34:M:205:ASN:O	36:U:1052:LEU:HA	2.17	0.41
36:U:484:ASP:O	36:U:564:LEU:C	2.49	0.41
49:r:1481:ILE:C	49:r:1483:ARG:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:v:78:ILE:O	25:v:89:ILE:HA	2.21	0.41
30:9:490:LYS:H	38:X:161:GLU:CA	2.32	0.41
34:M:597:LEU:O	34:M:601:GLN:CB	2.68	0.41
28:z:38:ILE:O	28:N:39:PHE:C	2.61	0.41
34:M:615:VAL:O	34:M:619:ALA:HB3	2.21	0.41
40:i:5:LEU:O	41:j:49:GLY:HA3	2.20	0.41
48:q:434:PRO:C	48:q:436:TYR:H	2.27	0.41
8:A:2265:ASP:O	49:r:1261:PRO:CB	2.69	0.41
25:v:599:GLU:H	49:r:862:ASP:CA	2.32	0.41
25:v:1212:ARG:HA	25:v:1216:ALA:HB3	2.03	0.41
45:g:71:PRO:C	45:g:73:SER:H	2.28	0.41
46:o:179:GLU:O	50:w:42:ALA:C	2.60	0.41
2:2:59:A:N6	30:9:443:THR:CA	2.73	0.41
9:B:197:SER:N	43:e:12:GLU:CB	2.84	0.41
25:v:974:LYS:CB	38:X:220:ILE:CB	2.99	0.41
28:z:18:ASN:O	28:N:19:ARG:CB	2.68	0.41
30:9:136:TYR:CB	39:h:98:LYS:CB	2.98	0.41
34:M:543:ARG:O	34:M:547:LEU:CB	2.68	0.41
36:U:489:VAL:CB	36:U:566:THR:C	2.87	0.41
9:B:238:ASN:O	9:B:242:LEU:CB	2.69	0.41
32:H:68:ALA:H	33:K:66:MET:CA	2.33	0.41
37:W:160:LYS:O	37:W:161:MET:C	2.63	0.41
41:c:61:ALA:O	41:c:74:LEU:N	2.52	0.41
28:z:21:LEU:O	28:N:62:VAL:N	2.54	0.41
28:z:37:ASP:N	28:N:34:GLU:O	2.54	0.41
30:9:139:TYR:CB	39:h:95:TYR:CB	2.99	0.41
30:9:395:TRP:N	28:N:55:GLU:O	2.54	0.41
34:M:326:ASP:C	34:M:328:GLU:H	2.29	0.41
34:M:550:TRP:O	34:M:552:ASN:N	2.48	0.41
2:2:52:G:N7	30:9:439:GLY:C	2.56	0.41
4:5:46:U:O4	4:5:47:A:N6	2.54	0.41
5:6:57:U:H2'	5:6:58:G:H8	1.86	0.41
40:b:39:TYR:O	40:b:41:ASN:N	2.54	0.41
46:o:10:VAL:O	46:o:49:PHE:CB	2.68	0.41
48:q:642:GLU:O	48:q:668:ALA:HB1	2.19	0.41
25:v:135:ILE:O	25:v:167:VAL:N	2.54	0.41
36:U:484:ASP:CB	36:U:564:LEU:N	2.84	0.41
12:E:118:ALA:HB1	31:F:66:GLU:O	2.21	0.40
32:J:109:GLN:O	32:J:113:ALA:CB	2.70	0.40
34:M:328:GLU:O	34:M:332:ALA:HB2	2.21	0.40
39:h:68:GLU:HA	39:h:97:SER:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:465:ARG:CB	34:M:546:SER:CA	2.98	0.40
16:Q:13:ASP:HA	16:Q:14:GLY:HA2	1.74	0.40
25:v:677:THR:N	25:v:685:ASP:O	2.54	0.40
28:z:63:VAL:HA	28:N:19:ARG:O	2.21	0.40
34:M:622:ALA:N	47:p:106:ALA:O	2.52	0.40
35:T:607:THR:O	35:T:609:GLN:N	2.54	0.40
36:U:484:ASP:H	36:U:592:VAL:CB	2.34	0.40
10:C:300:GLU:O	10:C:304:MET:N	2.45	0.40
49:r:538:ILE:O	49:r:585:ILE:HA	2.21	0.40
8:A:360:SER:H	35:T:326:SER:N	2.19	0.40
49:r:577:LYS:O	49:r:581:SER:N	2.54	0.40
2:2:61:C:OP2	30:9:429:TRP:C	2.65	0.40
5:6:49:G:H2'	5:6:50:A:H8	1.87	0.40
25:v:475:ILE:HA	25:v:484:VAL:HA	2.03	0.40
35:T:529:PHE:C	35:T:532:GLN:H	2.29	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	120/322 (37%)	109 (91%)	11 (9%)	0	100	100
3	3	116/619 (19%)	96 (83%)	20 (17%)	0	100	100
6	7	91/464 (20%)	84 (92%)	7 (8%)	0	100	100
7	8	142/895 (16%)	127 (89%)	15 (11%)	0	100	100
8	A	2232/2335 (96%)	1989 (89%)	243 (11%)	0	100	100
9	B	900/972 (93%)	769 (85%)	131 (15%)	0	100	100
10	C	282/536 (53%)	232 (82%)	50 (18%)	0	100	100
11	D	318/514 (62%)	283 (89%)	33 (10%)	2 (1%)	21	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	E	126/579 (22%)	115 (91%)	11 (9%)	0	100	100
13	L	101/802 (13%)	88 (87%)	13 (13%)	0	100	100
14	O	251/848 (30%)	227 (90%)	24 (10%)	0	100	100
15	P	282/420 (67%)	247 (88%)	35 (12%)	0	100	100
16	Q	136/144 (94%)	121 (89%)	15 (11%)	0	100	100
17	R	98/229 (43%)	78 (80%)	20 (20%)	0	100	100
18	S	32/2752 (1%)	27 (84%)	5 (16%)	0	100	100
19	V	157/166 (95%)	151 (96%)	6 (4%)	0	100	100
20	Y	93/904 (10%)	92 (99%)	1 (1%)	0	100	100
22	s	173/472 (37%)	155 (90%)	18 (10%)	0	100	100
23	t	166/343 (48%)	140 (84%)	26 (16%)	0	100	100
24	u	877/1304 (67%)	812 (93%)	64 (7%)	1 (0%)	48	83
25	v	1179/1217 (97%)	1055 (90%)	122 (10%)	2 (0%)	43	77
26	x	77/86 (90%)	70 (91%)	7 (9%)	0	100	100
27	y	98/110 (89%)	92 (94%)	6 (6%)	0	100	100
28	N	99/125 (79%)	76 (77%)	21 (21%)	2 (2%)	6	31
28	z	99/125 (79%)	88 (89%)	11 (11%)	0	100	100
29	0	153/396 (39%)	133 (87%)	14 (9%)	6 (4%)	2	18
30	9	416/501 (83%)	375 (90%)	31 (8%)	10 (2%)	4	27
31	F	297/357 (83%)	273 (92%)	17 (6%)	7 (2%)	4	27
32	G	130/504 (26%)	120 (92%)	9 (7%)	1 (1%)	16	53
32	H	133/504 (26%)	119 (90%)	13 (10%)	1 (1%)	16	53
32	I	132/504 (26%)	123 (93%)	9 (7%)	0	100	100
32	J	133/504 (26%)	116 (87%)	14 (10%)	3 (2%)	5	28
33	K	211/225 (94%)	178 (84%)	30 (14%)	3 (1%)	9	39
34	M	732/855 (86%)	623 (85%)	103 (14%)	6 (1%)	16	53
35	T	458/908 (50%)	417 (91%)	34 (7%)	7 (2%)	8	38
36	U	1317/1485 (89%)	1292 (98%)	25 (2%)	0	100	100
37	W	160/255 (63%)	146 (91%)	12 (8%)	2 (1%)	9	41
38	X	165/225 (73%)	158 (96%)	4 (2%)	3 (2%)	6	33
39	a	87/118 (74%)	76 (87%)	10 (12%)	1 (1%)	11	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	h	96/118 (81%)	92 (96%)	4 (4%)	0	100	100
40	b	71/86 (83%)	66 (93%)	4 (6%)	1 (1%)	9	39
40	i	72/86 (84%)	69 (96%)	3 (4%)	0	100	100
41	c	76/92 (83%)	67 (88%)	8 (10%)	1 (1%)	9	41
41	j	77/92 (84%)	75 (97%)	2 (3%)	0	100	100
42	d	71/76 (93%)	64 (90%)	6 (8%)	1 (1%)	9	39
42	k	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
43	e	86/126 (68%)	83 (96%)	2 (2%)	1 (1%)	10	43
43	l	81/126 (64%)	80 (99%)	1 (1%)	0	100	100
44	f	87/240 (36%)	81 (93%)	6 (7%)	0	100	100
44	m	67/240 (28%)	66 (98%)	1 (2%)	0	100	100
45	g	89/119 (75%)	81 (91%)	8 (9%)	0	100	100
45	n	80/119 (67%)	77 (96%)	3 (4%)	0	100	100
46	o	221/301 (73%)	203 (92%)	15 (7%)	3 (1%)	9	39
47	p	169/793 (21%)	164 (97%)	3 (2%)	2 (1%)	10	43
48	q	623/1041 (60%)	598 (96%)	21 (3%)	4 (1%)	21	58
49	r	1720/2136 (80%)	1632 (95%)	85 (5%)	3 (0%)	43	77
50	w	54/285 (19%)	52 (96%)	0	2 (4%)	2	20
All	All	16581/30776 (54%)	15092 (91%)	1414 (8%)	75 (0%)	26	63

All (75) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	D	384	HIS
29	0	246	TYR
29	0	267	ASP
29	0	270	LEU
29	0	362	PHE
30	9	232	GLU
30	9	350	ALA
30	9	485	ASN
31	F	193	THR
34	M	720	ILE
38	X	175	PRO
46	o	28	PRO
49	r	957	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
49	r	1584	ILE
28	N	104	LYS
30	9	227	PRO
30	9	230	PRO
31	F	88	ARG
32	G	57	VAL
32	H	55	ILE
33	K	133	ASN
34	M	49	PRO
35	T	468	ASP
35	T	608	LEU
37	W	160	LYS
38	X	176	GLY
43	e	80	ALA
48	q	483	ARG
50	w	63	ALA
11	D	385	TYR
25	v	585	ALA
30	9	472	GLN
31	F	256	ASP
32	J	7	ILE
32	J	55	ILE
32	J	61	ILE
34	M	385	VAL
35	T	617	PRO
40	b	40	MET
48	q	993	THR
30	9	442	ASN
31	F	159	PRO
31	F	162	ARG
33	K	79	ILE
34	M	357	VAL
35	T	501	ARG
35	T	607	THR
35	T	619	ASP
37	W	32	PRO
42	d	23	GLY
46	o	48	GLY
48	q	637	GLY
28	N	85	ARG
25	v	583	MET
29	0	271	PRO

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Mol	Chain	Res	Type
30	9	305	PRO
30	9	443	THR
31	F	149	GLY
34	M	337	LEU
34	M	585	ASP
35	T	536	ILE
39	a	89	PRO
48	q	436	TYR
29	0	355	LYS
33	K	90	PRO
38	X	213	THR
46	o	25	ALA
30	9	104	VAL
47	p	222	PRO
47	p	236	PRO
41	c	16	GLN
50	w	64	GLY
24	u	465	PRO
31	F	324	PRO
49	r	585	ILE

### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	2	57/188 (30%)	12 (21%)	1 (1%)
21	Z	46/369 (12%)	18 (39%)	1 (2%)
4	5	69/116 (59%)	27 (39%)	1 (1%)
5	6	94/107 (87%)	25 (26%)	1 (1%)
All	All	266/780 (34%)	82 (30%)	4 (1%)

All (82) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	2	13	C
2	2	16	U
2	2	17	U
2	2	18	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	2	19	G
2	2	23	A
2	2	24	A
2	2	25	G
2	2	30	A
2	2	31	G
2	2	49	U
2	2	58	U
4	5	8	G
4	5	9	G
4	5	10	U
4	5	14	U
4	5	15	C
4	5	17	U
4	5	19	A
4	5	20	G
4	5	21	A
4	5	23	C
4	5	25	C
4	5	26	A
4	5	27	U
4	5	34	U
4	5	36	C
4	5	40	U
4	5	41	U
4	5	44	A
4	5	45	C
4	5	47	A
4	5	52	U
4	5	53	U
4	5	61	A
4	5	62	G
4	5	68	C
4	5	69	A
4	5	72	U
5	6	6	C
5	6	7	G
5	6	9	U
5	6	21	U
5	6	22	A
5	6	24	A
5	6	25	C

*Continued on next page...*

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Mol	Chain	Res	Type
5	6	26	U
5	6	28	A
5	6	29	A
5	6	30	A
5	6	31	U
5	6	34	G
5	6	36	A
5	6	44	G
5	6	49	G
5	6	54	G
5	6	56	A
5	6	59	G
5	6	61	C
5	6	69	A
5	6	74	U
5	6	78	A
5	6	83	A
5	6	84	A
21	Z	235	C
21	Z	236	C
21	Z	239	C
21	Z	243	G
21	Z	244	U
21	Z	246	U
21	Z	247	G
21	Z	251	C
21	Z	253	A
21	Z	254	G
21	Z	255	C
21	Z	258	A
21	Z	259	C
21	Z	262	G
21	Z	385	U
21	Z	388	U
21	Z	394	A
21	Z	397	U

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	2	23	A
4	5	26	A

*Continued on next page...*

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Mol	Chain	Res	Type
5	6	58	G
21	Z	261	A

## 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 20 ligands modelled in this entry, 16 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
55	ADP	r	2201	-	28,29,29	1.44	5 (17%)	43,45,45	1.78	7 (16%)
55	ADP	r	2202	52	28,29,29	1.38	4 (14%)	43,45,45	1.86	9 (20%)
54	GTP	B	1500	-	33,34,34	0.95	1 (3%)	50,54,54	1.58	9 (18%)
53	IHP	A	3001	-	36,36,36	1.57	6 (16%)	60,60,60	0.93	2 (3%)

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
55	ADP	r	2201	-	-	8/16/32/32	0/3/3/3
55	ADP	r	2202	52	-	2/16/32/32	0/3/3/3
54	GTP	B	1500	-	-	6/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	IHP	A	3001	-	-	3/30/54/54	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	r	2201	ADP	C5-C4	4.62	1.47	1.39
55	r	2202	ADP	C5-C4	4.53	1.47	1.39
53	A	3001	IHP	P2-O12	3.70	1.66	1.59
53	A	3001	IHP	P1-O11	3.35	1.65	1.59
53	A	3001	IHP	P3-O13	3.32	1.65	1.59
53	A	3001	IHP	P4-O14	3.27	1.65	1.59
53	A	3001	IHP	P5-O15	3.24	1.65	1.59
53	A	3001	IHP	P6-O16	3.20	1.65	1.59
55	r	2202	ADP	C5-C6	2.62	1.48	1.41
55	r	2201	ADP	C5-C6	2.54	1.48	1.41
55	r	2202	ADP	C5-N7	-2.48	1.34	1.39
55	r	2201	ADP	C5-N7	-2.43	1.34	1.39
55	r	2202	ADP	C8-N7	2.40	1.36	1.31
55	r	2201	ADP	C8-N7	2.40	1.36	1.31
55	r	2201	ADP	PA-O3A	2.39	1.62	1.59
54	B	1500	GTP	C2-N3	2.21	1.38	1.33

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	r	2202	ADP	C5-C4-N3	-6.37	117.94	126.72
55	r	2201	ADP	C5-C4-N3	-5.79	118.75	126.72
54	B	1500	GTP	C5-C4-N3	-5.03	120.39	128.39
55	r	2202	ADP	N3-C4-N9	4.83	135.39	127.17
54	B	1500	GTP	C2-N3-C4	4.66	120.33	112.30
55	r	2201	ADP	N3-C4-N9	4.54	134.89	127.17
55	r	2202	ADP	C2-N3-C4	3.90	121.36	111.83
55	r	2201	ADP	C2-N3-C4	3.68	120.81	111.83
55	r	2202	ADP	C4-C5-N7	-3.58	106.49	110.58
55	r	2201	ADP	N3-C2-N1	-3.27	123.64	128.58
53	A	3001	IHP	O12-C2-C1	3.24	115.66	108.76
54	B	1500	GTP	N9-C4-N3	3.18	132.32	125.95
55	r	2201	ADP	C4-C5-N7	-3.15	106.98	110.58
55	r	2202	ADP	N3-C2-N1	-3.00	124.04	128.58
54	B	1500	GTP	C2-N1-C6	-2.87	119.90	125.11
54	B	1500	GTP	N9-C8-N7	-2.63	108.53	113.40
55	r	2202	ADP	C5-N7-C8	2.53	107.43	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	B	1500	GTP	C5-C6-N1	2.53	119.69	113.25
54	B	1500	GTP	C8-N7-C5	2.52	108.75	104.26
54	B	1500	GTP	O6-C6-C5	-2.38	120.25	126.53
55	r	2201	ADP	C5-N7-C8	2.27	107.02	103.45
55	r	2202	ADP	C3'-C2'-C1'	2.25	105.72	101.46
55	r	2202	ADP	C4-N9-C8	2.25	108.10	105.74
55	r	2201	ADP	C4-N9-C8	2.23	108.08	105.74
54	B	1500	GTP	C3'-C2'-C1'	2.14	105.50	101.46
53	A	3001	IHP	P3-O13-C3	-2.13	117.74	123.43
55	r	2202	ADP	C6-C5-N7	2.00	135.95	132.09

There are no chirality outliers.

All (19) torsion outliers are listed below:

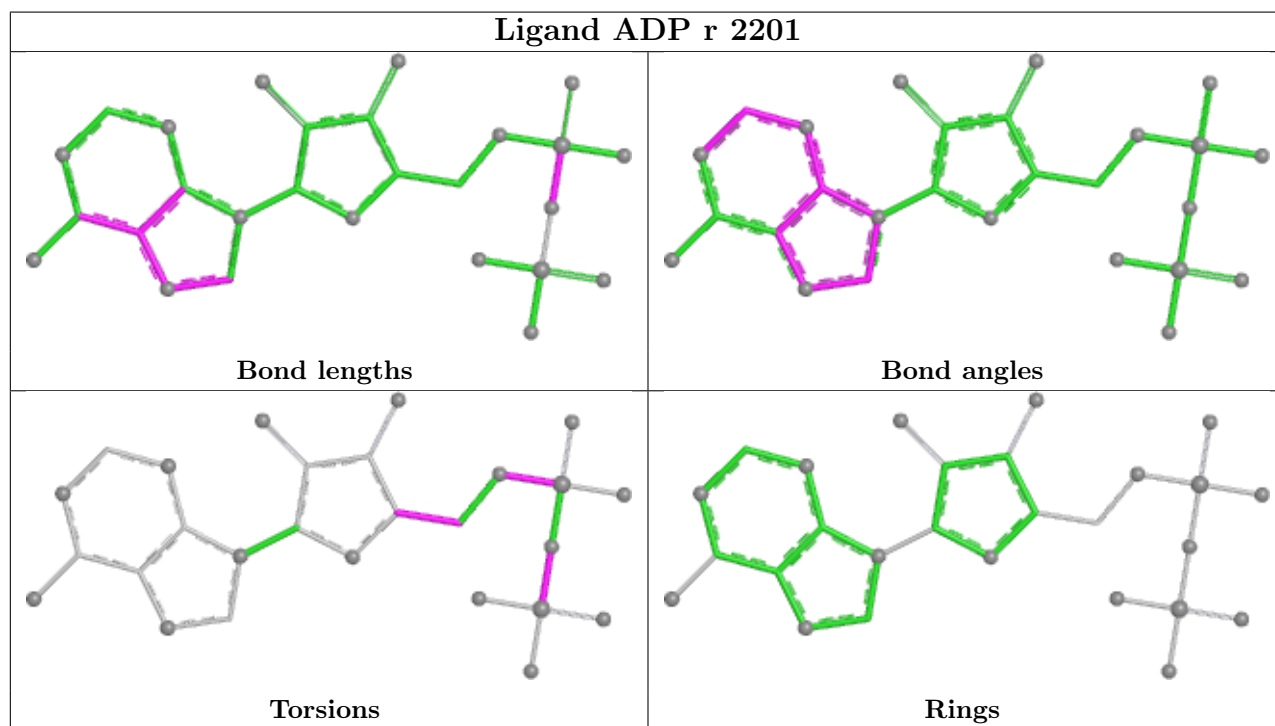
Mol	Chain	Res	Type	Atoms
53	A	3001	IHP	C1-C2-O12-P2
54	B	1500	GTP	C5'-O5'-PA-O3A
55	r	2201	ADP	PA-O3A-PB-O2B
55	r	2201	ADP	C5'-O5'-PA-O1A
55	r	2201	ADP	C5'-O5'-PA-O2A
55	r	2201	ADP	C5'-O5'-PA-O3A
55	r	2201	ADP	C3'-C4'-C5'-O5'
55	r	2201	ADP	O4'-C4'-C5'-O5'
55	r	2202	ADP	C3'-C4'-C5'-O5'
53	A	3001	IHP	C4-O14-P4-O24
55	r	2202	ADP	O4'-C4'-C5'-O5'
54	B	1500	GTP	PB-O3A-PA-O5'
53	A	3001	IHP	C3-C2-O12-P2
54	B	1500	GTP	C5'-O5'-PA-O1A
54	B	1500	GTP	C4'-C5'-O5'-PA
54	B	1500	GTP	PA-O3A-PB-O1B
55	r	2201	ADP	PA-O3A-PB-O1B
55	r	2201	ADP	PA-O3A-PB-O3B
54	B	1500	GTP	PG-O3B-PB-O2B

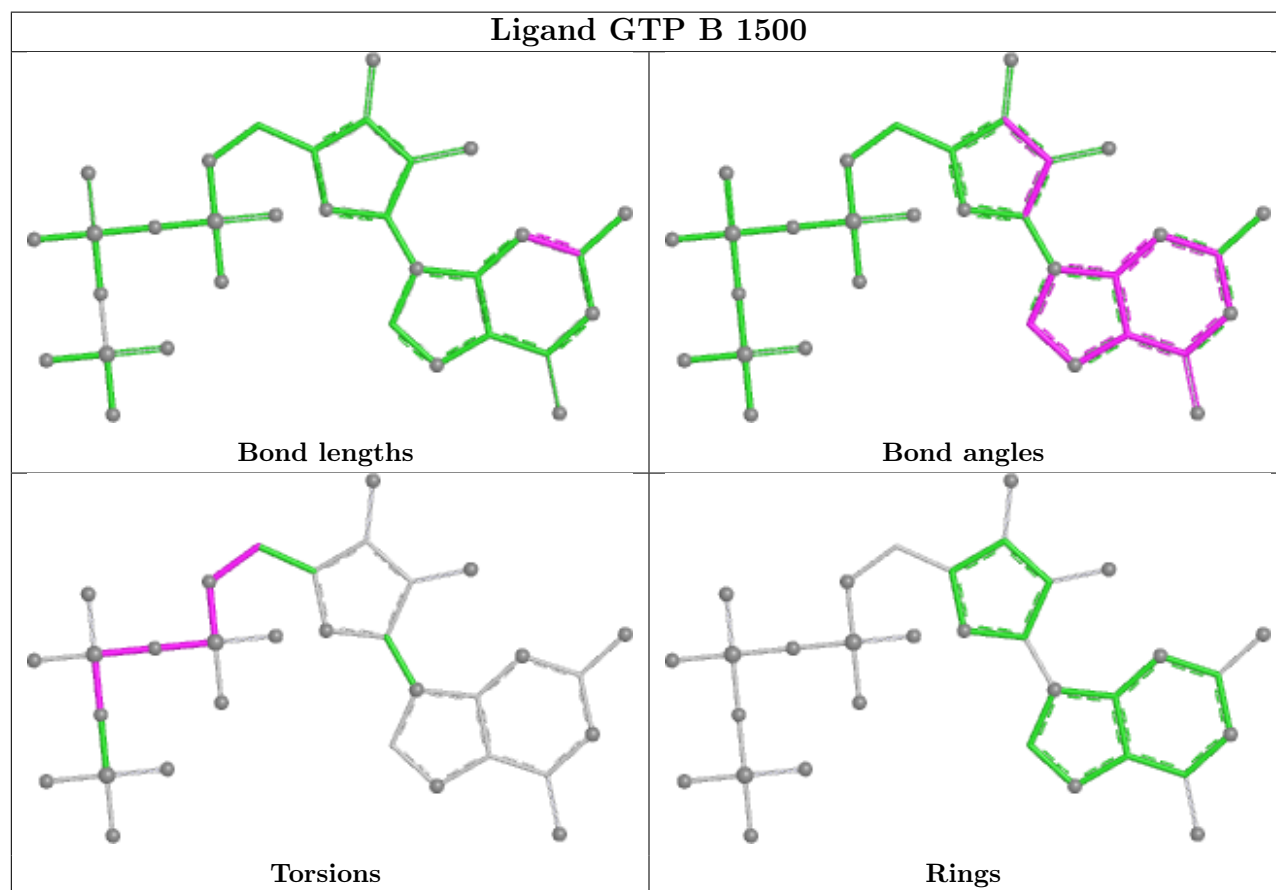
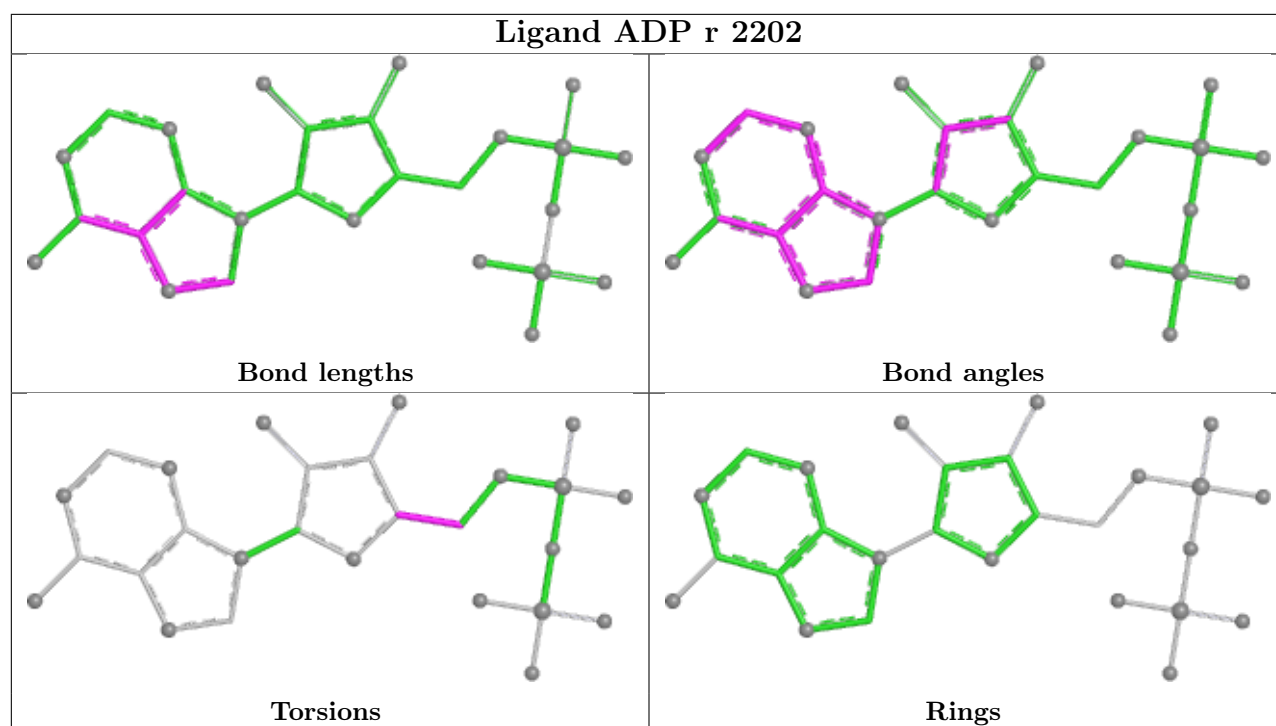
There are no ring outliers.

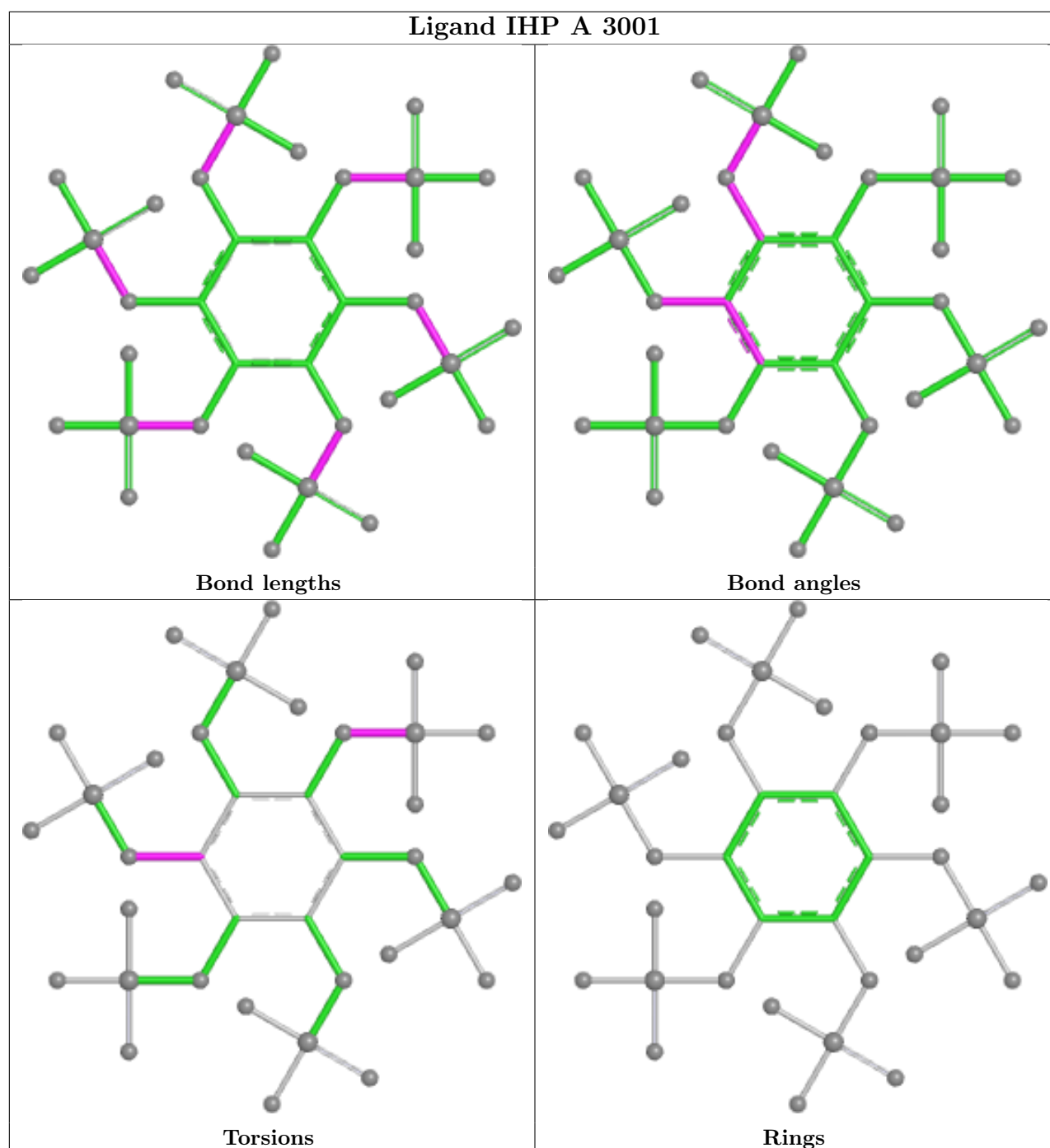
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	r	2201	ADP	1	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
30	9	5
34	M	3
38	X	1
36	U	1
2	2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	9	124:ALA	C	125:GLN	N	48.62
1	X	163:ASN	C	164:GLU	N	43.68
1	9	96:ARG	C	97:LYS	N	22.97
1	9	30:LYS	C	31:SER	N	15.71
1	9	172:ASP	C	173:ILE	N	11.06
1	U	492:MET	C	493:LYS	N	9.55
1	9	63:ASP	C	64:LYS	N	7.82
1	M	355:HIS	C	356:HIS	N	5.18
1	M	33:PHE	C	34:SER	N	4.52
1	2	59:A	O3'	60:U	P	4.29
1	M	208:ARG	C	209:PHE	N	1.67

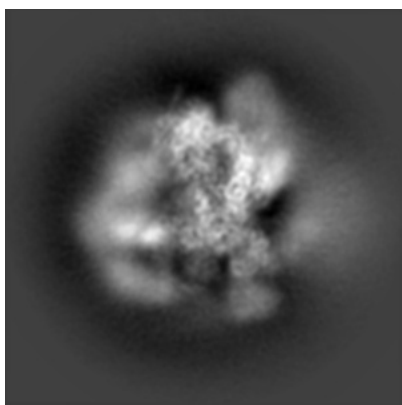
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4240. These allow visual inspection of the internal detail of the map and identification of artifacts.

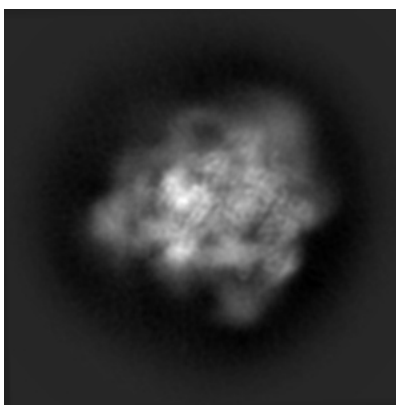
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

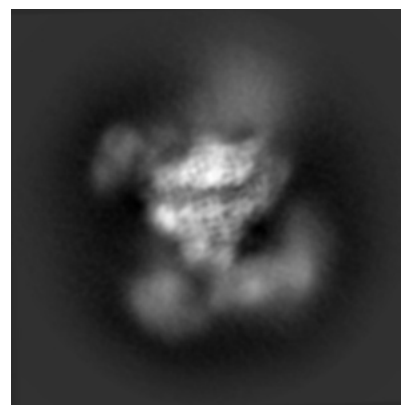
#### 6.1.1 Primary map



X



Y

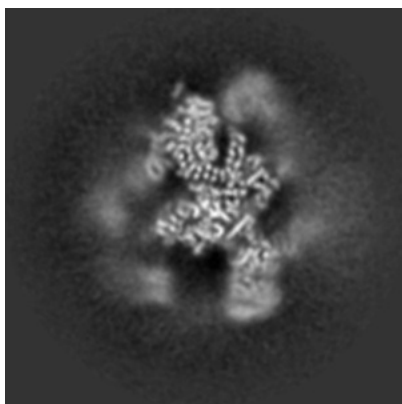


Z

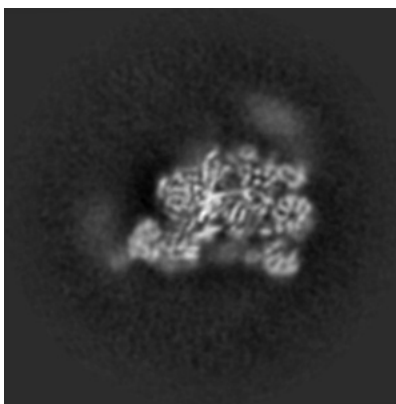
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

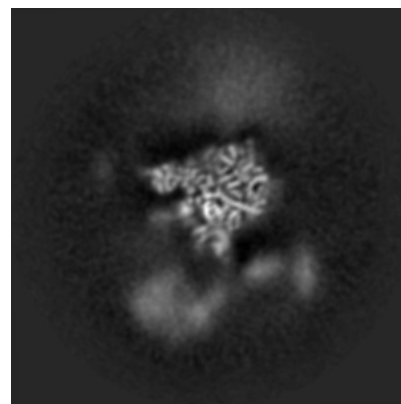
#### 6.2.1 Primary map



X Index: 210



Y Index: 210

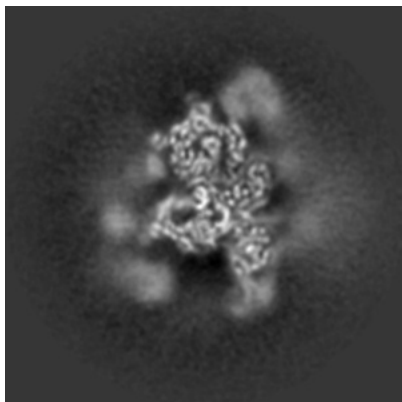


Z Index: 210

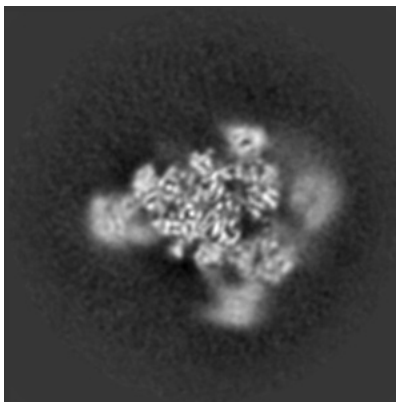
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

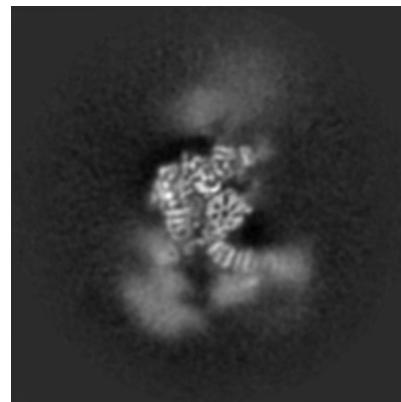
### 6.3.1 Primary map



X Index: 218



Y Index: 249

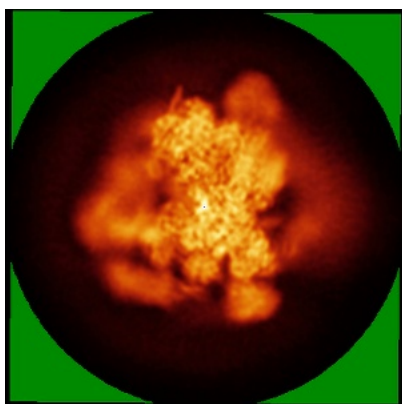


Z Index: 184

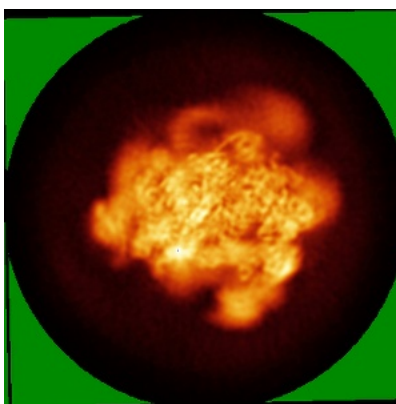
The images above show the largest variance slices of the map in three orthogonal directions.

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

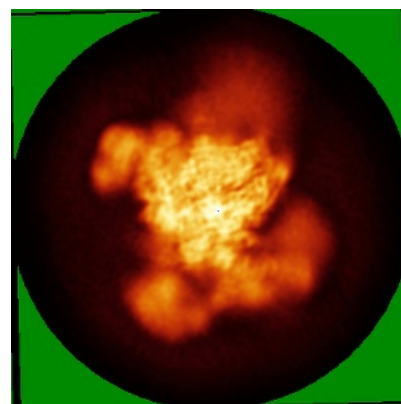
### 6.4.1 Primary map



X



Y

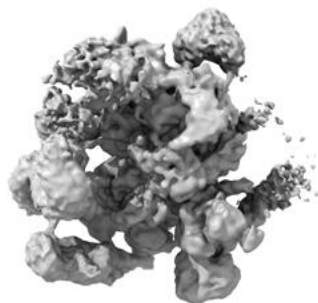


Z

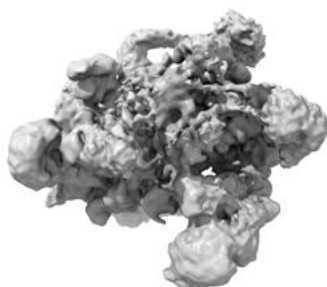
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.013. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

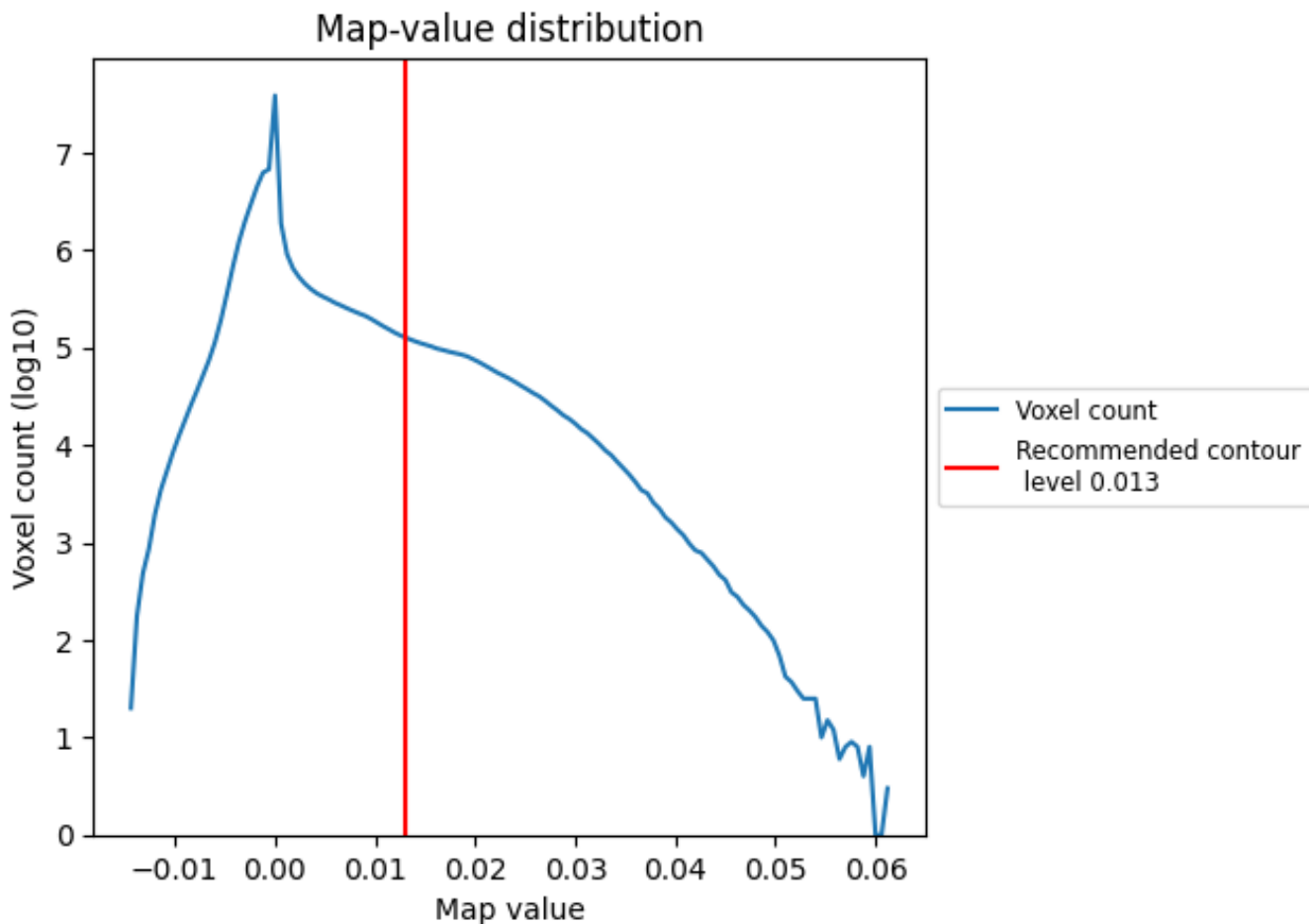
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

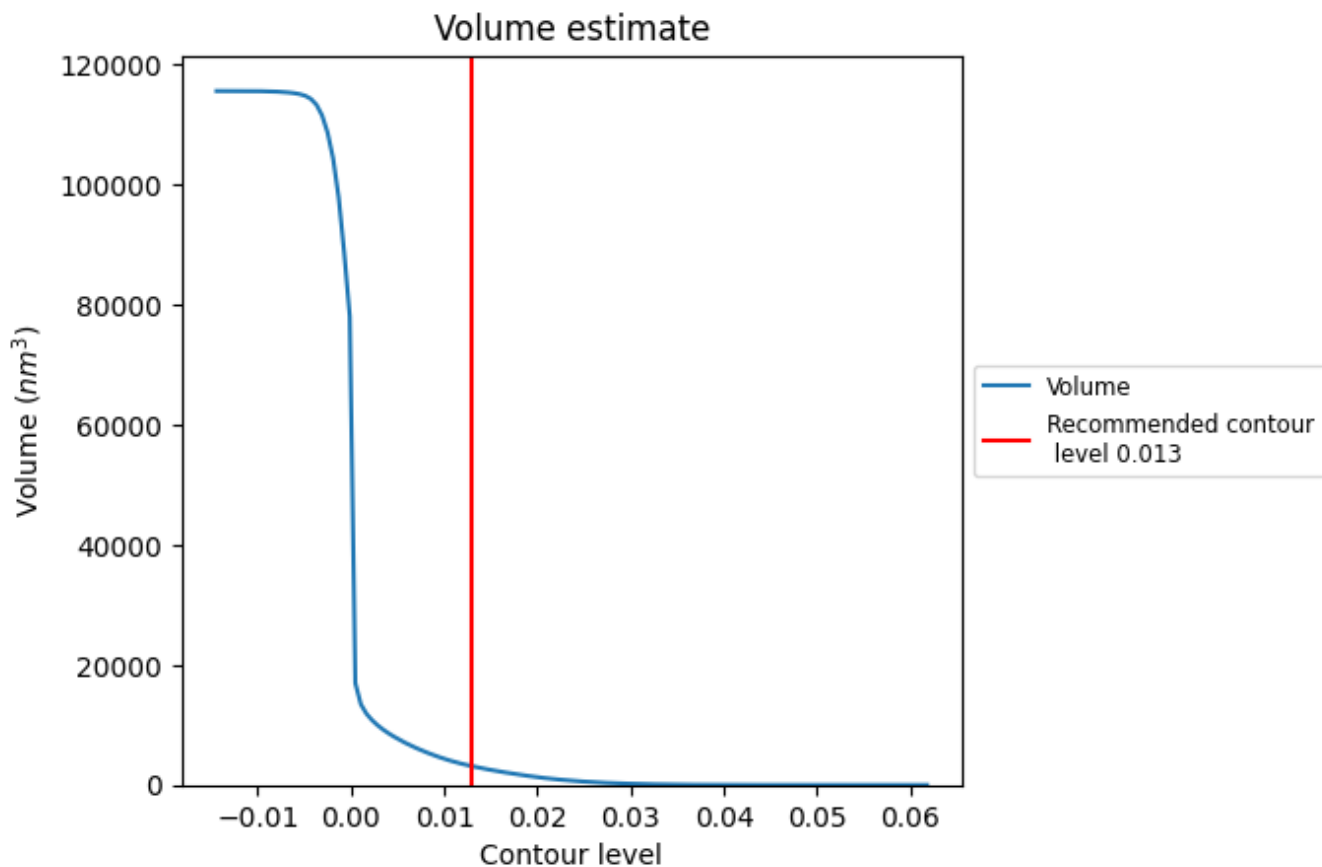
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

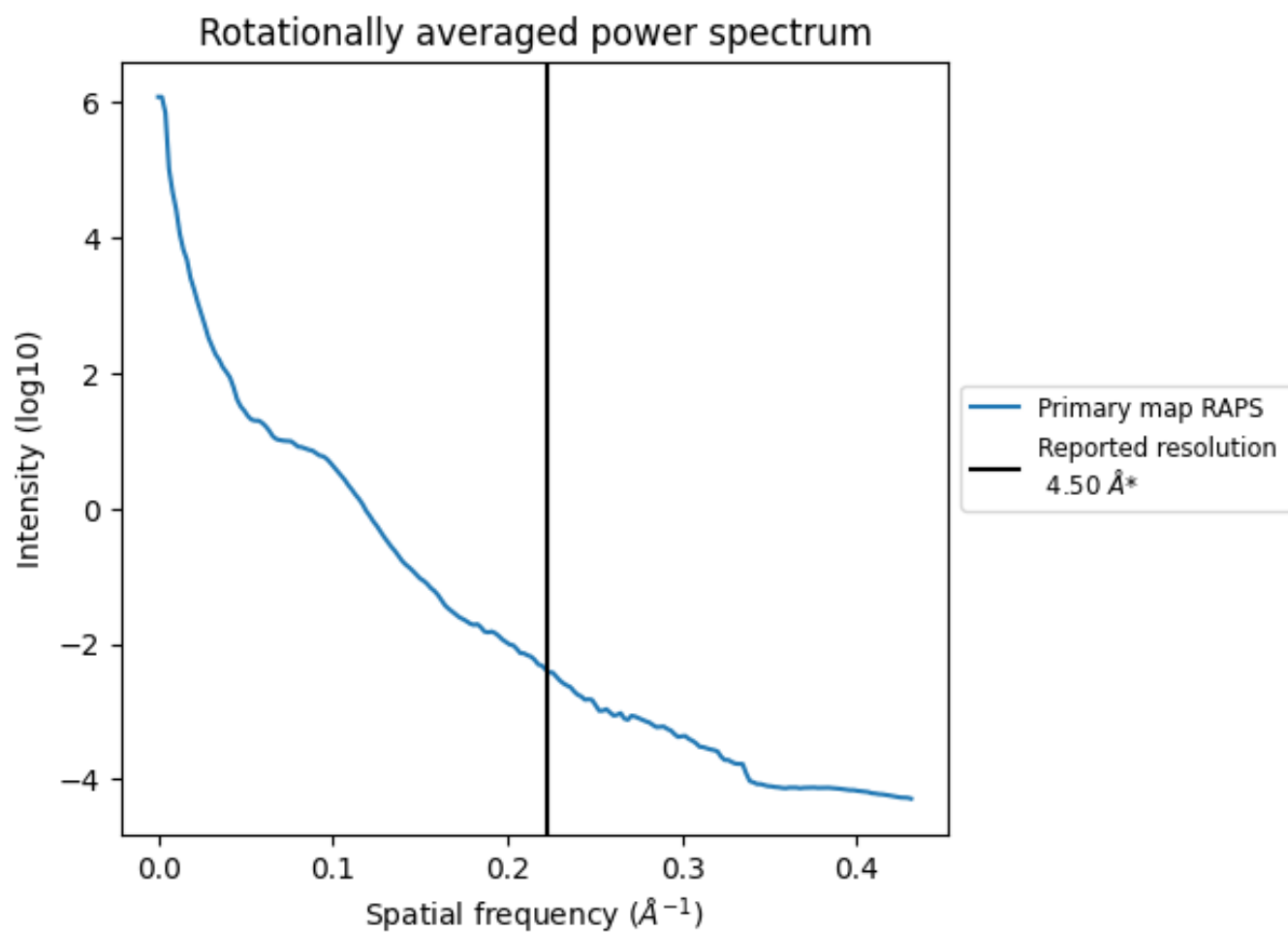
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is  $31270 \text{ nm}^3$ ; this corresponds to an approximate mass of 2825 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 [i](#)



\*Reported resolution corresponds to spatial frequency of 0.222 Å<sup>-1</sup>

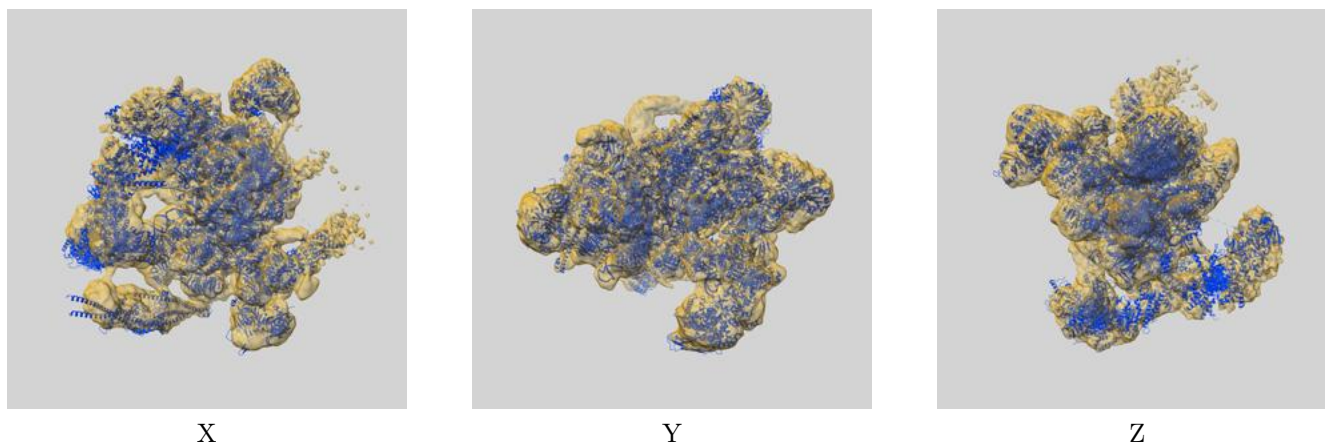
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

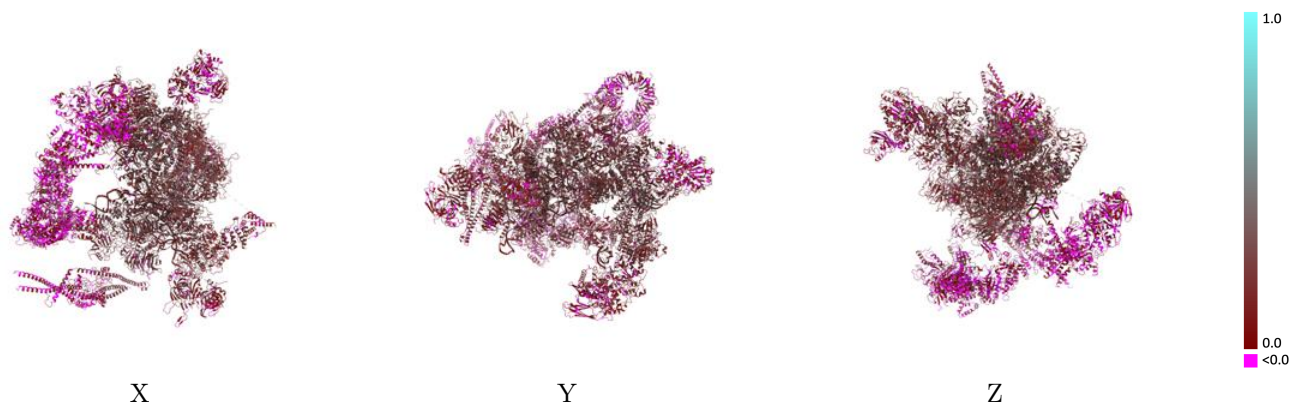
This section contains information regarding the fit between EMDB map EMD-4240 and PDB model 6FF7. Per-residue inclusion information can be found in section 3 on page 16.

### 9.1 Map-model overlay [i](#)



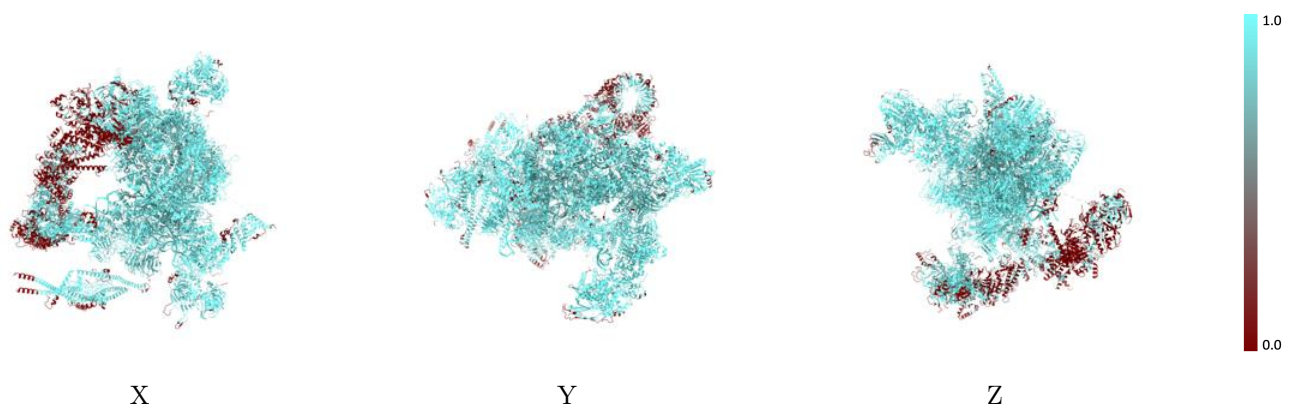
The images above show the 3D surface view of the map at the recommended contour level 0.013 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



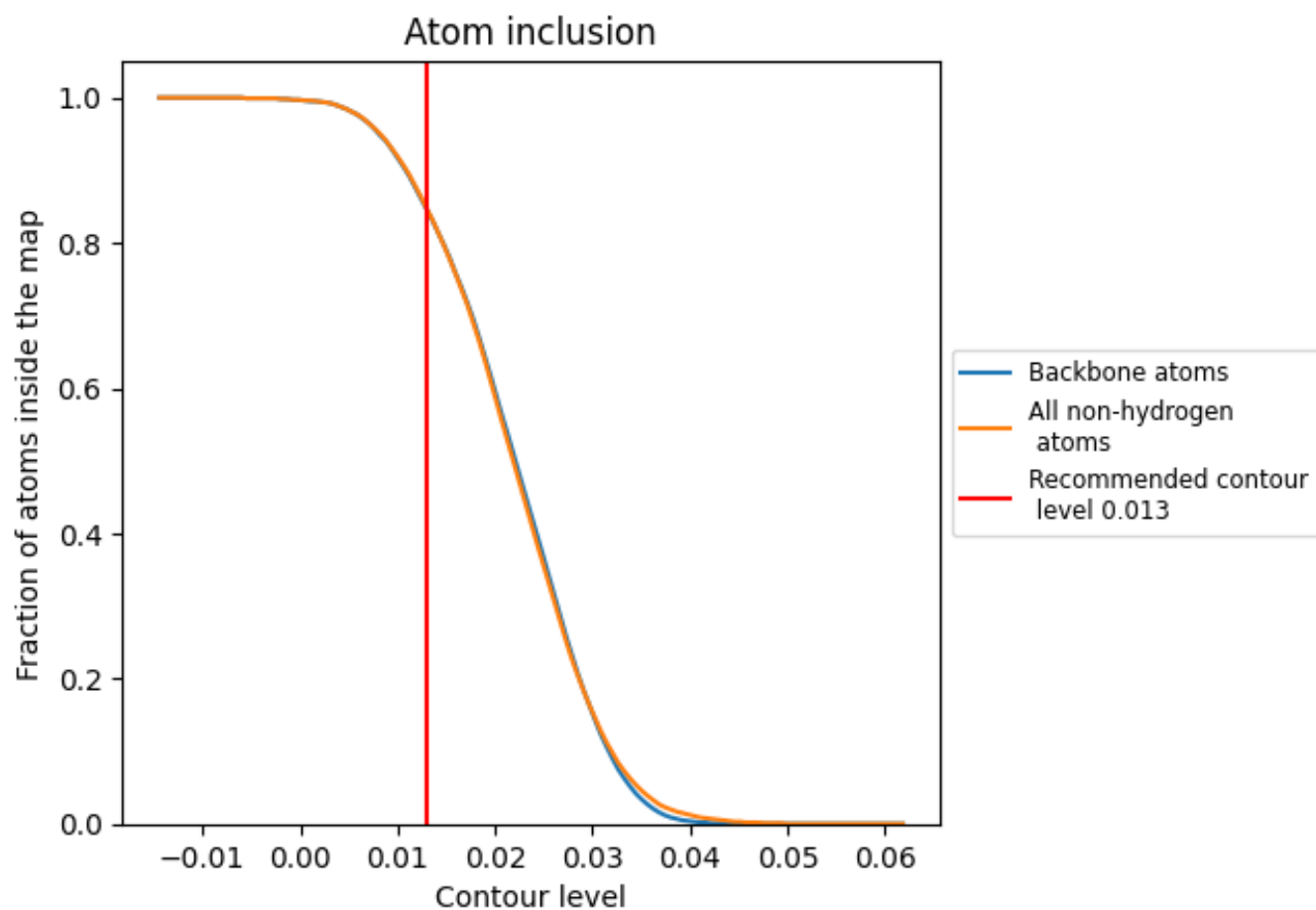
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.013).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 85% 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 (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8470	 0.1670
0	 0.9190	 0.1610
1	 0.9470	 0.2430
2	 0.9820	 0.2000
3	 0.8580	 0.2320
5	 0.9910	 0.2150
6	 0.9930	 0.2100
7	 0.9230	 0.2390
8	 0.9850	 0.2750
9	 0.1750	 0.0230
A	 0.9760	 0.2600
B	 0.9810	 0.2160
C	 0.9080	 0.2540
D	 0.9930	 0.2600
E	 0.9830	 0.1800
F	 0.9720	 0.1660
G	 0.7480	 0.0420
H	 0.7800	 0.0320
I	 0.9660	 0.1100
J	 0.6940	 0.0850
K	 0.6830	 0.0980
L	 0.9790	 0.2650
M	 0.5650	 0.0120
N	 0.9780	 0.2510
O	 0.9820	 0.2320
P	 0.9340	 0.1790
Q	 0.9970	 0.2310
R	 0.9450	 0.2360
S	 0.7360	 0.1650
T	 0.8670	 0.1900
U	 0.6890	 0.0370
V	 0.9920	 0.1600
W	 0.0850	 -0.0140
X	 0.3680	 0.0470
Y	 0.9980	 0.2330



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Chain	Atom inclusion	Q-score
Z	 0.9960	 0.2180
a	 0.9160	 0.1150
b	 0.9470	 0.0820
c	 0.9330	 0.0960
d	 0.8970	 0.1460
e	 0.8920	 0.1560
f	 0.7990	 0.1180
g	 0.9630	 0.1490
h	 0.3130	 0.0120
i	 0.6650	 0.0260
j	 0.6320	 0.0420
k	 0.6530	 0.0480
l	 0.5060	 0.0720
m	 0.1430	 0.0170
n	 0.2760	 -0.0040
o	 0.2110	 0.0070
p	 0.2550	 0.0250
q	 0.9000	 0.0760
r	 0.9410	 0.1590
s	 0.9800	 0.2590
t	 0.9270	 0.2440
u	 0.9790	 0.2660
v	 0.9920	 0.2410
w	 0.0000	 0.0580
x	 0.9870	 0.2510
y	 0.9860	 0.2370
z	 0.9660	 0.3160