



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 07:31 PM UTC

PDB ID : 7ABG / pdb_00007abg
EMDB ID : EMD-11695
Title : Human pre-Bact-1 spliceosome
Authors : Townsend, C.; Kastner, B.; Leelaram, M.N.; Bertram, K.; Stark, H.;
Luehrmann, R.
Deposited on : 2020-09-07
Resolution : 7.80 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

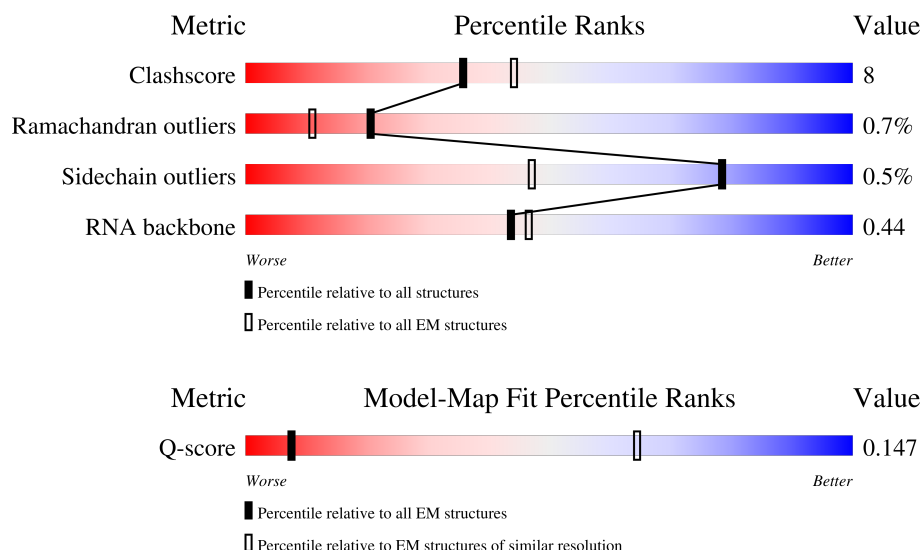
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 7.80 Å.

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



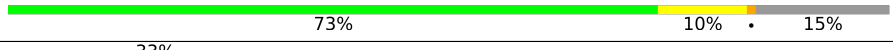
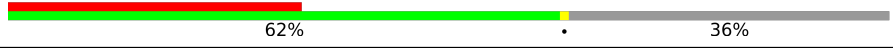
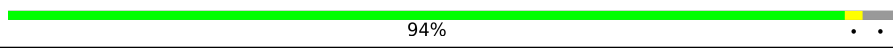
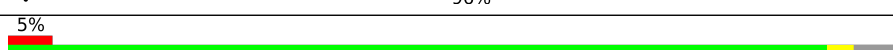
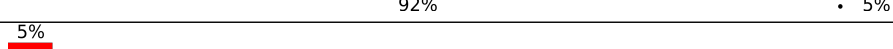
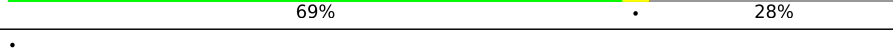
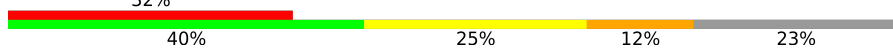
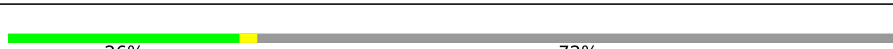
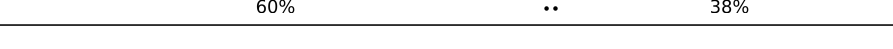
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	370 (7.30 - 8.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A5	790	
2	A2	103	
3	Z	125	

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Mol	Chain	Length	Quality of chain
4	F	464	
5	D	357	
6	W	255	
7	B	225	
8	s	2136	
9	Q	144	
10	A1	156	
11	5	116	
12	L	802	
13	R	229	
14	V	95	
15	9	102	
16	C	139	
17	H	91	
18	J	80	
19	2	188	
20	A3	96	
21	K	439	
22	y	110	
23	G	514	
24	Z	230	
25	A	2335	
26	I	312	
27	P	420	
28	p	793	

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Mol	Chain	Length	Quality of chain
29	4	501	
30	A4	1098	
31	u	1304	
32	T	895	
33	E	1217	
34	w	424	
35	x	86	
36	v	536	
37	0	396	
38	N	199	
39	r	972	
40	Y	904	
41	6	106	
42	A6	248	
43	a	118	
43	h	118	
44	b	86	
44	i	86	
45	f	240	
45	m	240	
46	e	126	
46	l	126	
47	d	76	
47	k	76	
48	c	92	

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Mol	Chain	Length	Quality of chain
48	j	92	
49	g	119	
49	n	119	
50	q	73	
51	X	641	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
53	GTP	r	1500	-	-	X	-

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 73818 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 Nuclear cap-binding protein subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A5	732	Total	C	N	O	0	0
			3723	2259	732	732		

- Molecule 2 is a protein called U6 snRNA-associated Sm-like protein LSm7.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	A2	79	Total	C	N	O	0	0
			393	235	79	79		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
3	z	108	Total	C	N	O	0	0
			544	328	108	108		

- Molecule 4 is a protein called Splicing factor 3A subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	F	49	Total	C	N	O	0	0
			242	144	49	49		

- Molecule 5 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	D	302	Total	C	N	O	0	0
			1506	902	302	302		

- Molecule 6 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	W	162	Total	C	N	O	0	0
			816	492	162	162		

- Molecule 7 is a protein called U2 small nuclear ribonucleoprotein B”.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	B	169	Total	C	N	O	0	0
			851	513	169	169		

- Molecule 8 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	s	1722	Total	C	N	O	0	0
			8688	5244	1722	1722		

- Molecule 9 is a protein called Protein BUD31 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	Q	138	Total	C	N	O	0	0
			695	419	138	138		

- Molecule 10 is a protein called Nuclear cap-binding protein subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	A1	148	Total	C	N	O	0	0
			724	428	148	148		

- Molecule 11 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	5	114	Total	C	N	O	P	0	0
			2397	1074	399	810	114		

- Molecule 12 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	L	103	Total	C	N	O	0	0
			517	311	103	103		

- Molecule 13 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	R	9	Total	C	N	O	0	0
			45	27	9	9		

- Molecule 14 is a protein called U6 snRNA-associated Sm-like protein LSm2.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	V	90	Total	C	N	O	0	0
			453	273	90	90		

- Molecule 15 is a protein called U6 snRNA-associated Sm-like protein LSm3.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	9	73	Total	C	N	O	0	0
			369	223	73	73		

- Molecule 16 is a protein called U6 snRNA-associated Sm-like protein LSm4.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	C	80	Total	C	N	O	0	0
			404	244	80	80		

- Molecule 17 is a protein called U6 snRNA-associated Sm-like protein LSm5.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	H	76	Total	C	N	O	0	0
			380	228	76	76		

- Molecule 18 is a protein called U6 snRNA-associated Sm-like protein LSm6.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	J	69	Total	C	N	O	0	0
			342	204	69	69		

- Molecule 19 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	2	145	Total	C	N	O	P	0	0
			3077	1374	533	1025	145		

- Molecule 20 is a protein called U6 snRNA-associated Sm-like protein LSm8.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	A3	62	Total	C	N	O	0	0
			304	180	62	62		

- Molecule 21 is a protein called Microfibrillar-associated protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	K	123	Total	C	N	O	0	0
			614	368	123	123		

- Molecule 22 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	y	100	Total	C	N	O	0	0
			498	298	100	100		

- Molecule 23 is a protein called Pleiotropic regulator 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	G	320	Total	C	N	O	0	0
			1604	964	320	320		

- Molecule 24 is a RNA chain called MINX M3 pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	47	Total	C	N	O	P	0	0
			998	447	177	327	47		

- Molecule 25 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	A	2174	Total	C	N	O	0	0
			11024	6676	2174	2174		

- Molecule 26 is a protein called Pre-mRNA-splicing factor 38A.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	I	176	Total	C	N	O	0	0
			883	531	176	176		

- Molecule 27 is a protein called Pre-mRNA-splicing factor RBM22.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	P	162	Total	C	N	O	0	0
			825	501	162	162		

- Molecule 28 is a protein called Splicing factor 3A subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	p	60	Total	C	N	O	0	0
			301	181	60	60		

- Molecule 29 is a protein called Splicing factor 3A subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	4	421	Total	C	N	O	0	0
			2110	1268	421	421		

- Molecule 30 is a protein called Transcription elongation regulator 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	A4	405	Total	C	N	O	0	0
			2034	1224	405	405		

- Molecule 31 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	u	836	Total	C	N	O	0	0
			4207	2535	836	836		

- Molecule 32 is a protein called Splicing factor 3B subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	T	183	Total	C	N	O	0	0
			942	576	183	183		

- Molecule 33 is a protein called Splicing factor 3B subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	E	1177	Total	C	N	O	0	0
			5926	3572	1177	1177		

- Molecule 34 is a protein called Splicing factor 3B subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	w	78	Total	C	N	O	0	0
			391	235	78	78		

- Molecule 35 is a protein called Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	x	79	Total	C	N	O	0	0
			397	239	79	79		

- Molecule 36 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	v	119	Total	C	N	O	0	0
			605	367	119	119		

- Molecule 37 is a protein called Smad nuclear-interacting protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	0	150	Total	C	N	O	0	0
			761	461	150	150		

- Molecule 38 is a protein called Zinc finger matrin-type protein 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	N	56	Total	C	N	O	0	0
			277	165	56	56		

- Molecule 39 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	r	844	Total	C	N	O	0	0
			4265	2577	844	844		

- Molecule 40 is a protein called Serine/arginine repetitive matrix protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	Y	95	Total	C	N	O	0	0
			478	288	95	95		

- Molecule 41 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	6	78	Total	C	N	O	P	0	0
			1672	747	309	538	78		

- Molecule 42 is a protein called Serine/arginine-rich splicing factor 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	A6	74	Total	C	N	O	0	0
			368	220	74	74		

- Molecule 43 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	h	95	Total	C	N	O	0	0
			482	292	95	95		
43	a	78	Total	C	N	O	0	0
			393	237	78	78		

- Molecule 44 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	i	72	Total	C	N	O	0	0
			359	215	72	72		
44	b	73	Total	C	N	O	0	0
			364	218	73	73		

- Molecule 45 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	m	82	Total	C	N	O	0	0
			413	249	82	82		
45	f	64	Total	C	N	O	0	0
			319	191	64	64		

- Molecule 46 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	l	83	Total	C	N	O	0	0
			415	249	83	83		
46	e	78	Total	C	N	O	0	0
			390	234	78	78		

- Molecule 47 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	k	73	Total	C	N	O	0	0
			364	218	73	73		
47	d	69	Total	C	N	O	0	0
			344	206	69	69		

- Molecule 48 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	j	81	Total	C	N	O	0	0
			403	241	81	81		
48	c	78	Total	C	N	O	0	0
			388	232	78	78		

- Molecule 49 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	n	80	Total	C	N	O	0	0
			402	242	80	80		
49	g	93	Total	C	N	O	0	0
			469	283	93	93		

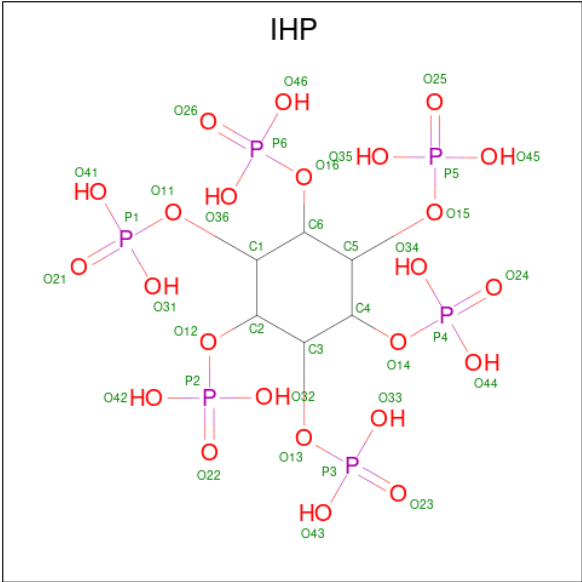
- Molecule 50 is a protein called Ubiquitin-like protein 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	q	73	Total	C	N	O	0	0
			360	214	73	73		

- Molecule 51 is a protein called WW domain-binding protein 11.

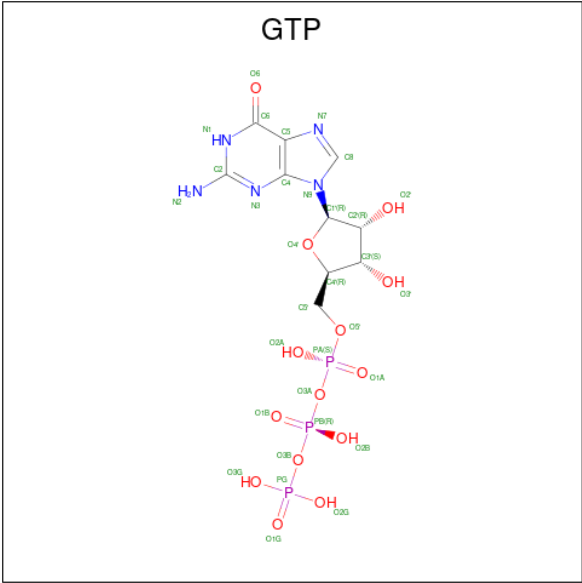
Mol	Chain	Residues	Atoms				AltConf	Trace
51	X	36	Total	C	N	O	0	0
			182	110	36	36		

- Molecule 52 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$).



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

- Molecule 53 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

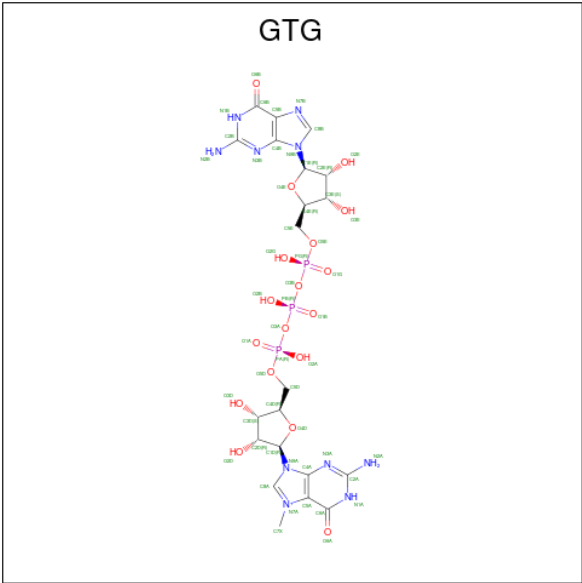


Mol	Chain	Residues	Atoms					AltConf
53	r	1	Total	C	N	O	P	0
			32	10	5	14	3	

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

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

- Molecule 55 is 7-METHYL-GUANOSINE-5'-TRIPHOSPHATE-5'-GUANOSINE (CCD ID: GTG) (formula: C₂₁H₃₀N₁₀O₁₈P₃).

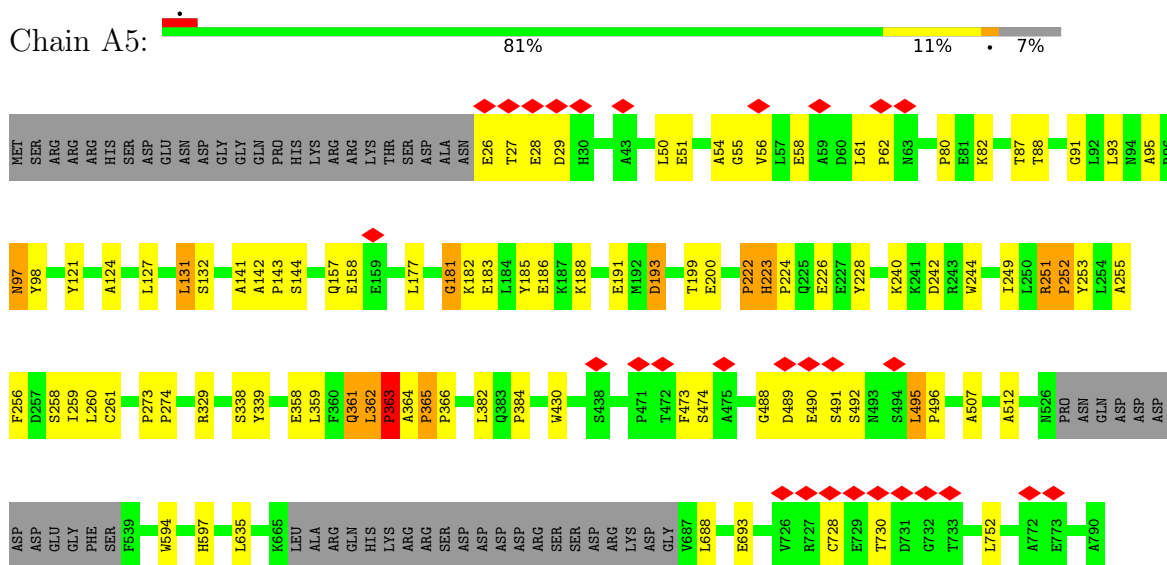


Mol	Chain	Residues	Atoms					AltConf
55	A6	1	Total	C	N	O	P	0
			52	21	10	18	3	

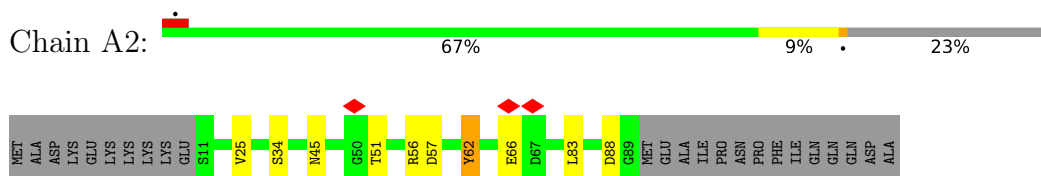
3 Residue-property plots

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

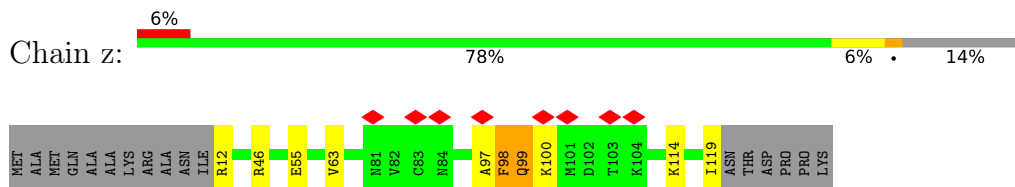
- Molecule 1: Nuclear cap-binding protein subunit 1



- Molecule 2: U6 snRNA-associated Sm-like protein LSm7

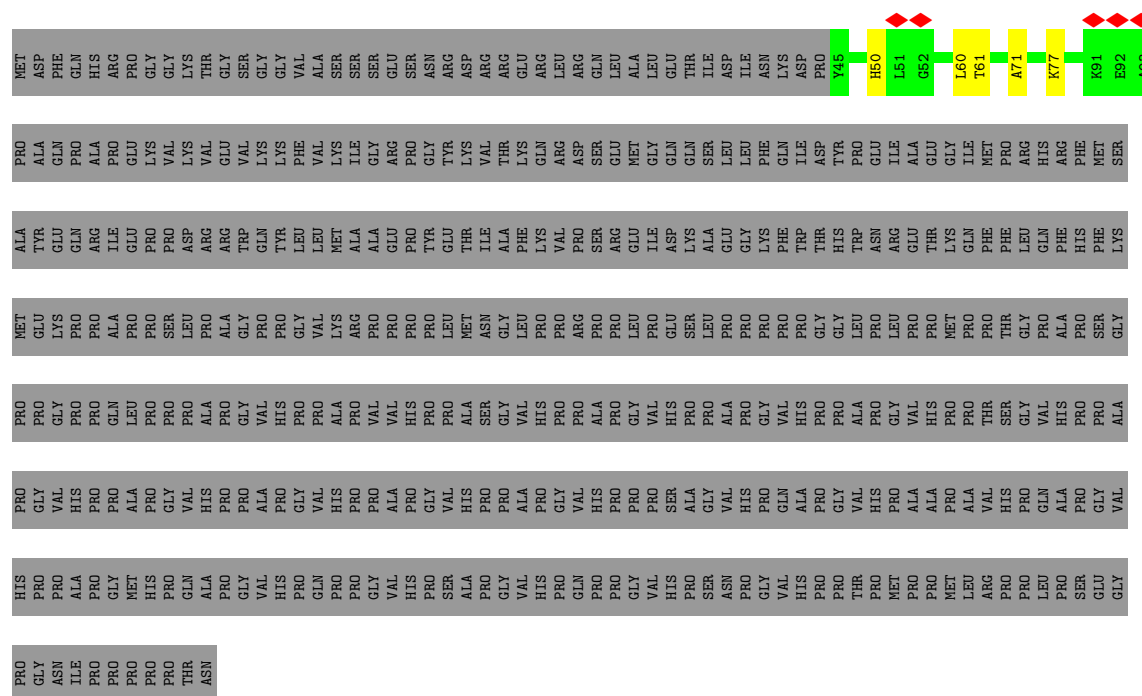


- Molecule 3: Splicing factor 3B subunit 6

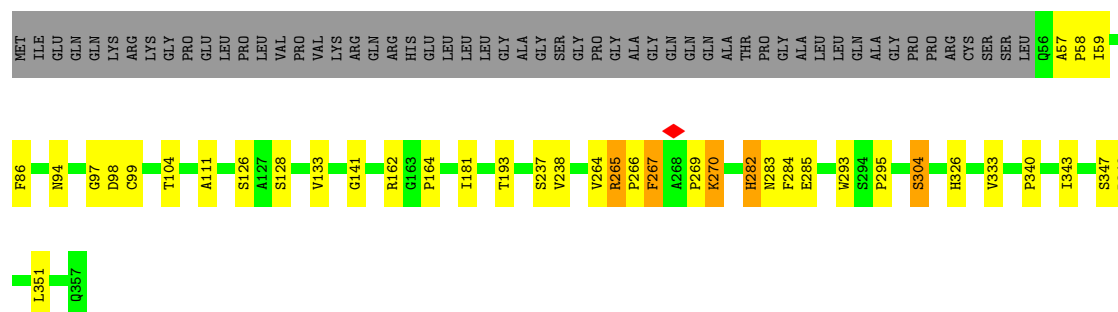


- Molecule 4: Splicing factor 3A subunit 2

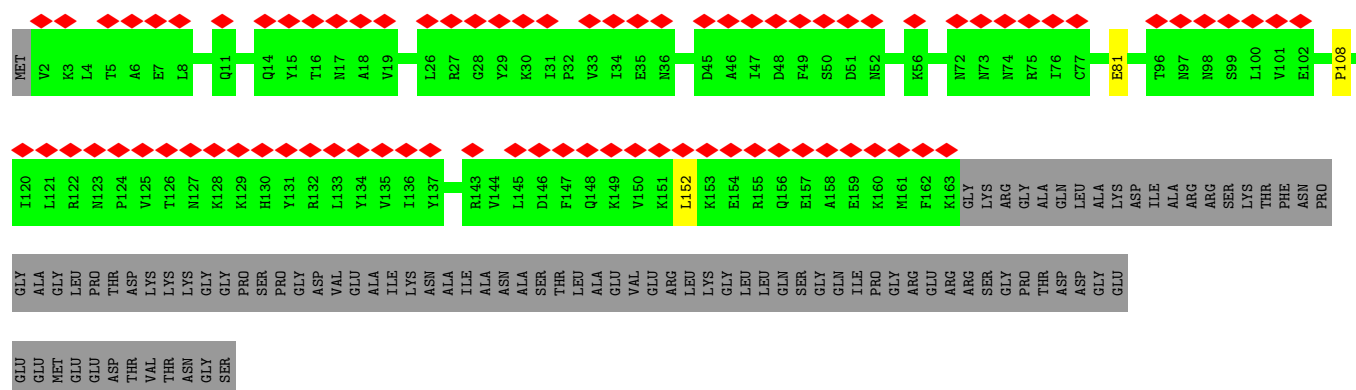




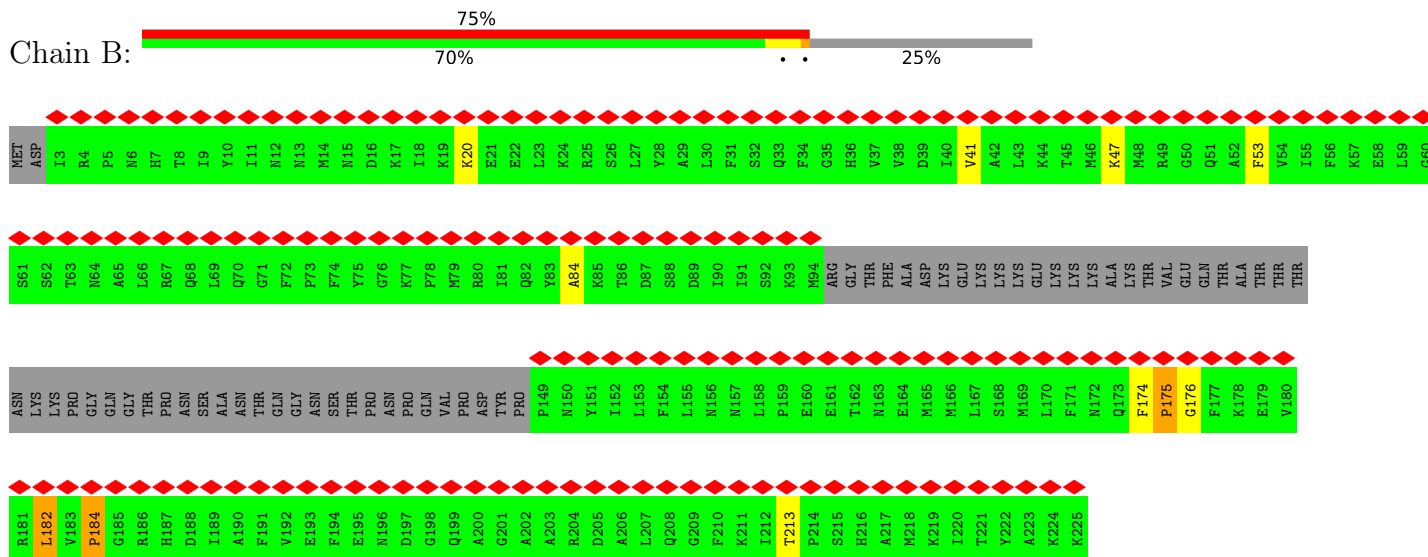
- Molecule 5: U5 small nuclear ribonucleoprotein 40 kDa protein



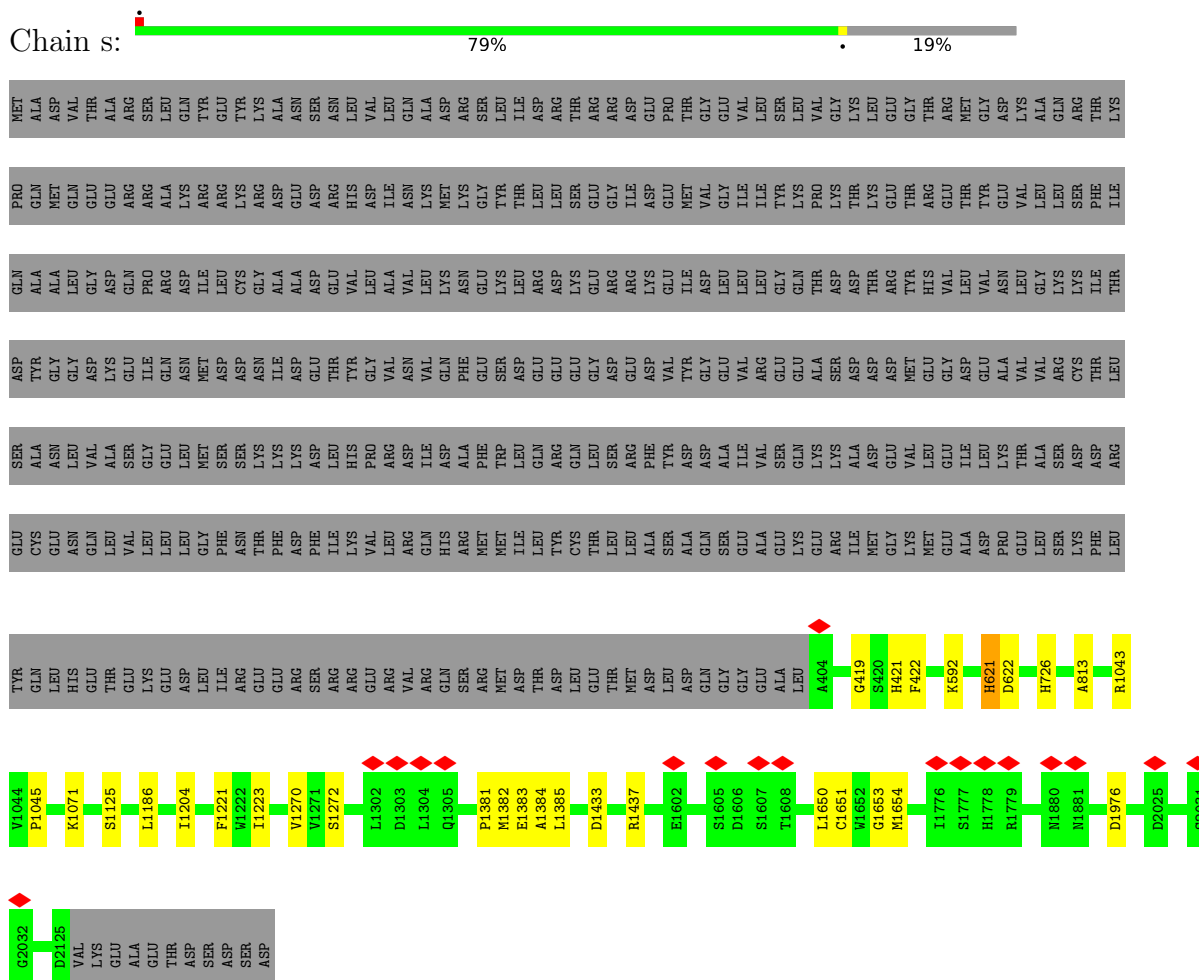
- Molecule 6: U2 small nuclear ribonucleoprotein A'



Chain B:

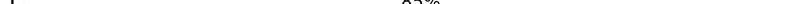


Chain s:



- Molecule 9: Protein BUD31 homolog

Sequence logo for the 12th position. The y-axis represents information content in bits, ranging from 0 to 1.5. The x-axis shows the amino acid frequencies for each position from 1 to 14. Position 12 is highlighted in yellow. The amino acids are MET, PRO, K3, A90, P122, L126, R140, GLY, CYS, SER, and GLY.

- Chain A1:  85% 9% 5%

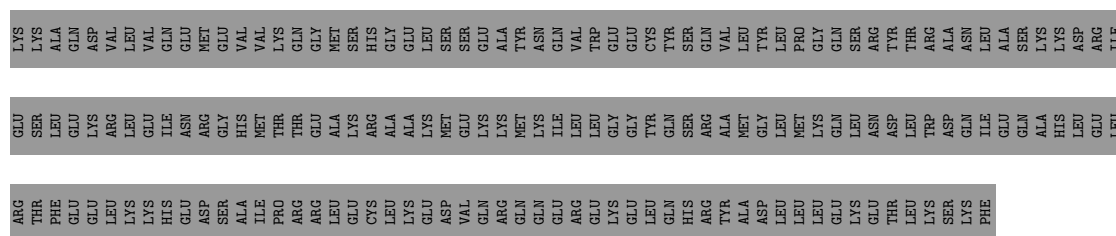
MET	SER	GLY	GLY	LEU	L6	K7	A8	L9	Q19	Y20	Q23	N29	C40	S48	C81	R99	G126	R127	G128	G132	A153	GLN	ASN	GLN
-----	-----	-----	-----	-----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	-----	-----	-----

- Chain 5: 43% 47% 9%

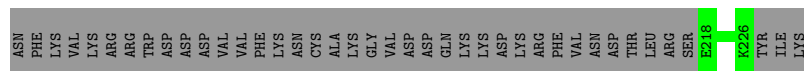
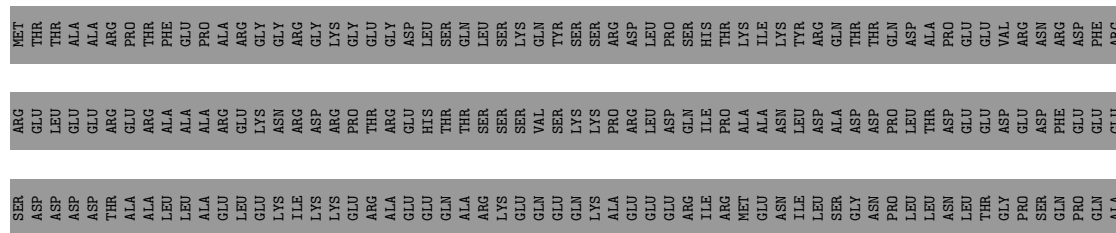
[illegible]

- Chain L: 12% 87%

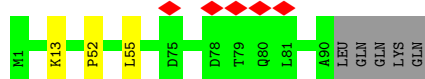
[illegible]



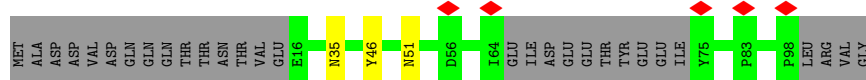
- Molecule 13: Spliceosome-associated protein CWC15 homolog



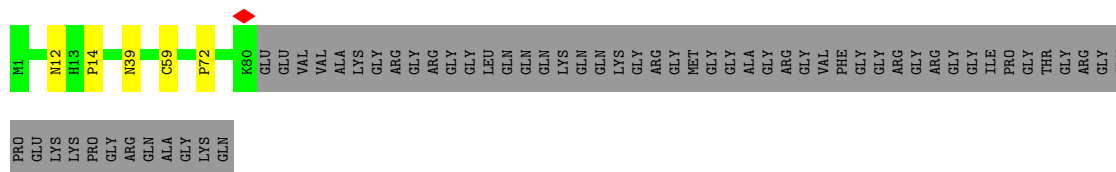
- Molecule 14: U6 snRNA-associated Sm-like protein LSm2



- Molecule 15: U6 snRNA-associated Sm-like protein LSm3

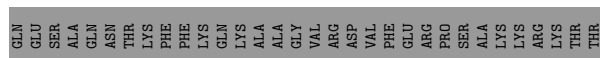


- Molecule 16: U6 snRNA-associated Sm-like protein LSm4

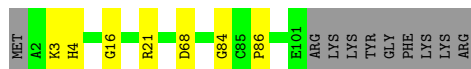


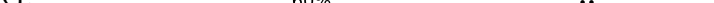
- Molecule 17: U6 snRNA-associated Sm-like protein LSm5

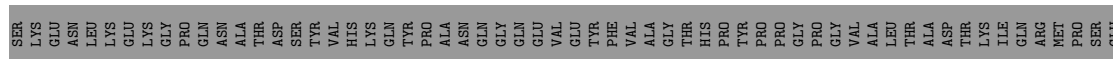
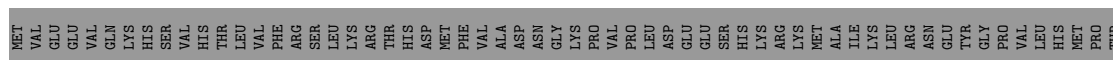




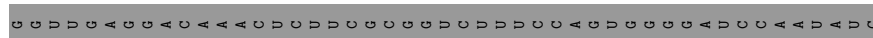
- Chain y:  85% 6% 9%



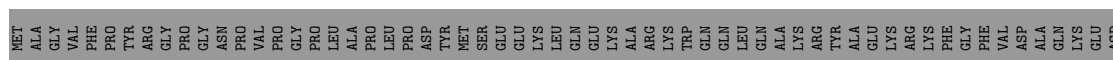
- Chain G:  60% .. 38%

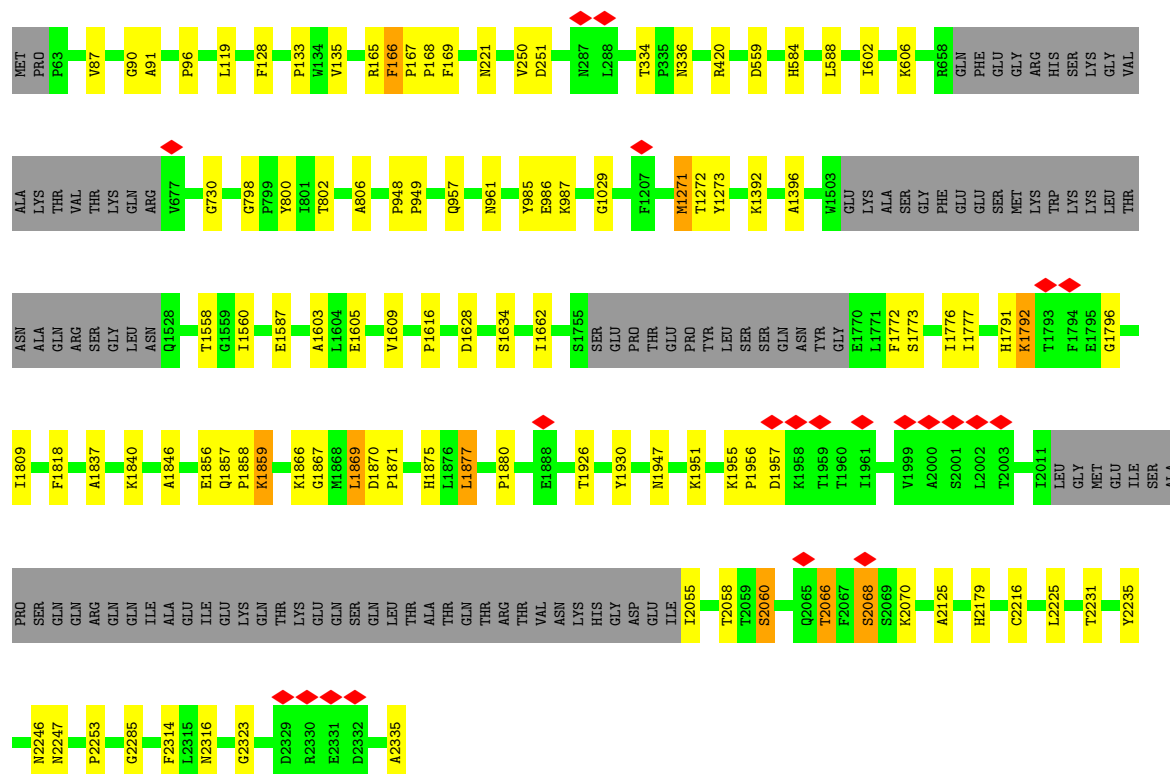


- Chain Z:  6% 9% 5% 80%

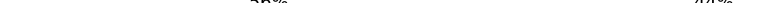


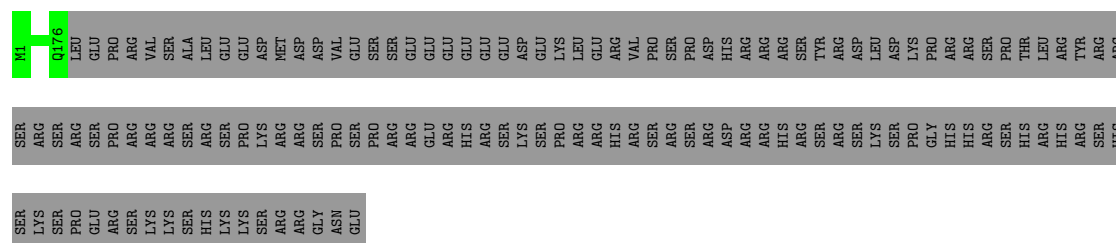
- Chain A: 89% 7%





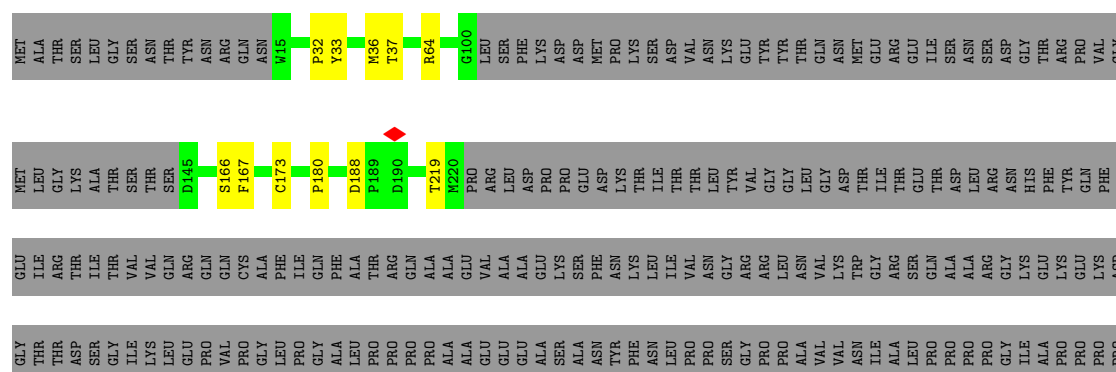
- Molecule 26: Pre-mRNA-splicing factor 38A

Chain I:  56% 44%

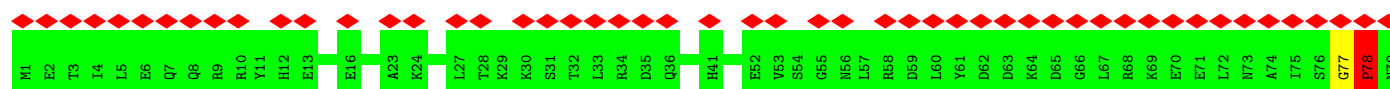
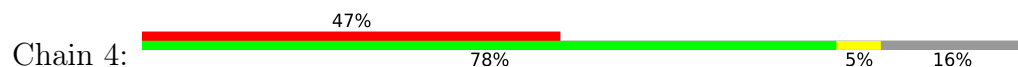


- Molecule 27: Pre-mRNA-splicing factor RBM22

Chain P: 36% 1% 61%

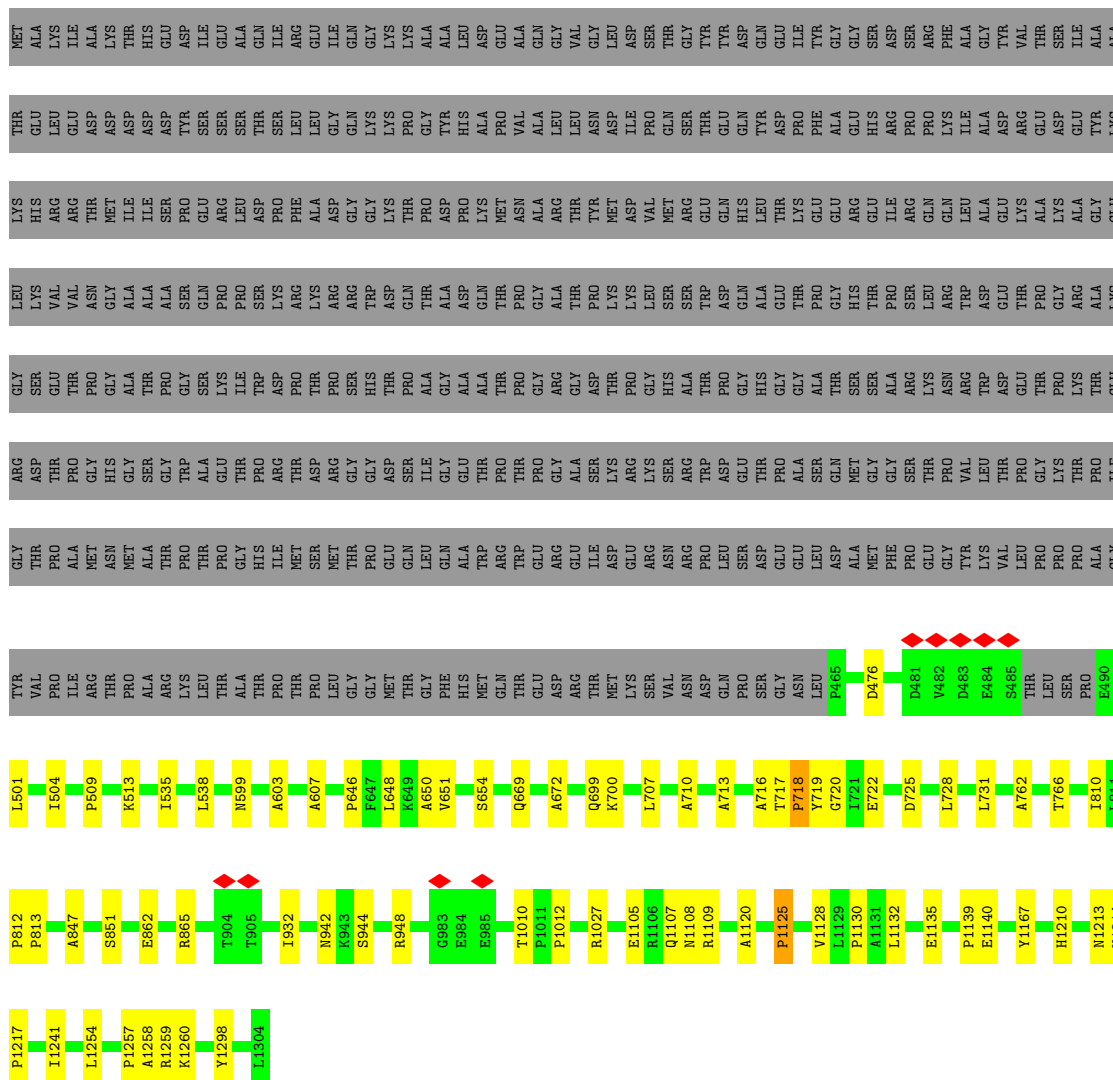


Chain p:



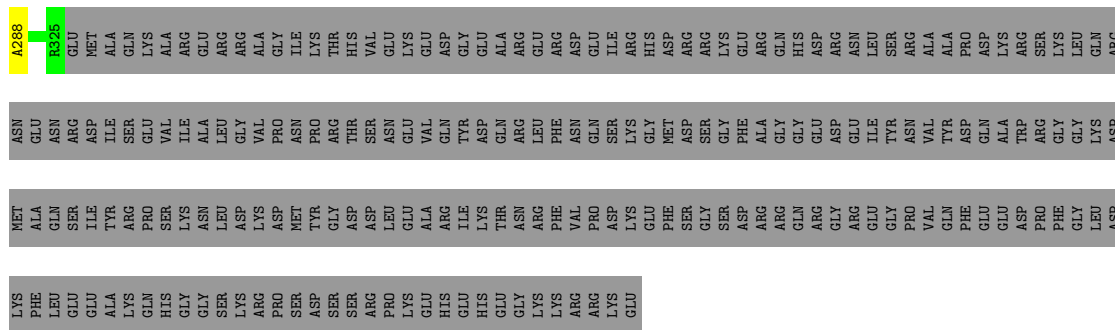


- Molecule 31: Splicing factor 3B subunit 1

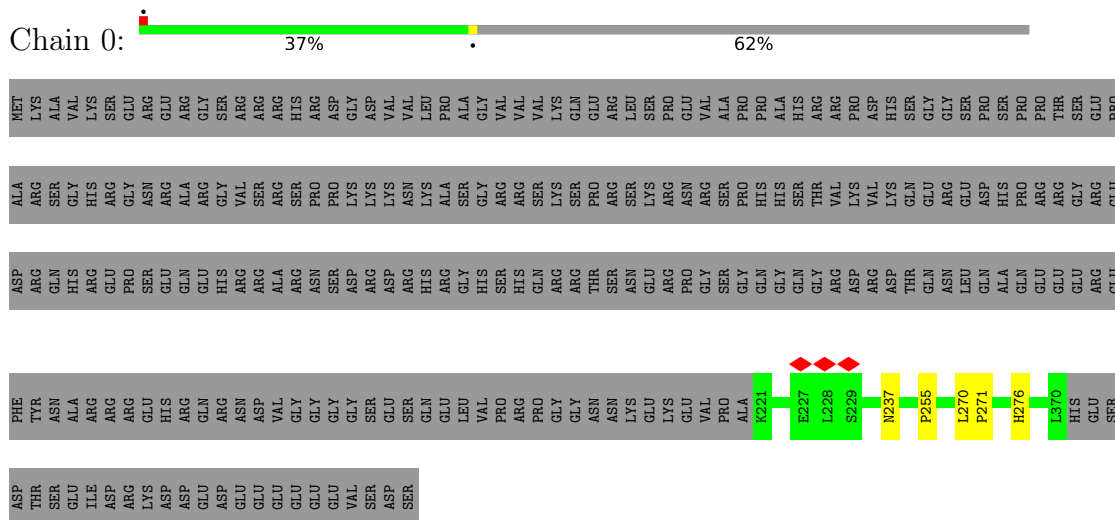


- Molecule 32: Splicing factor 3B subunit 2

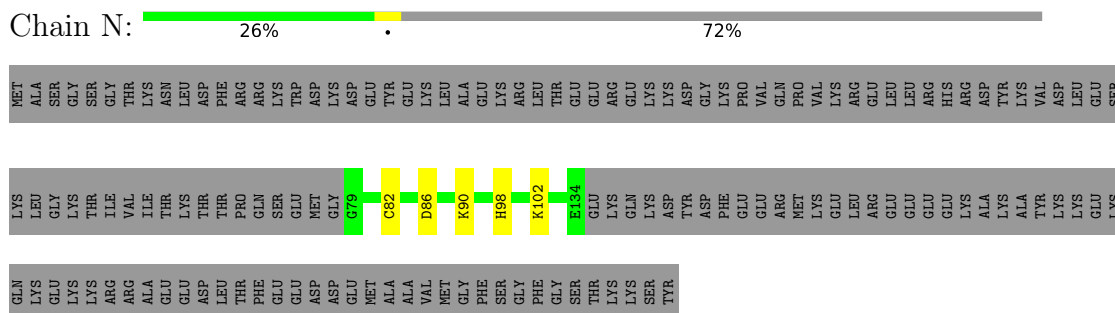




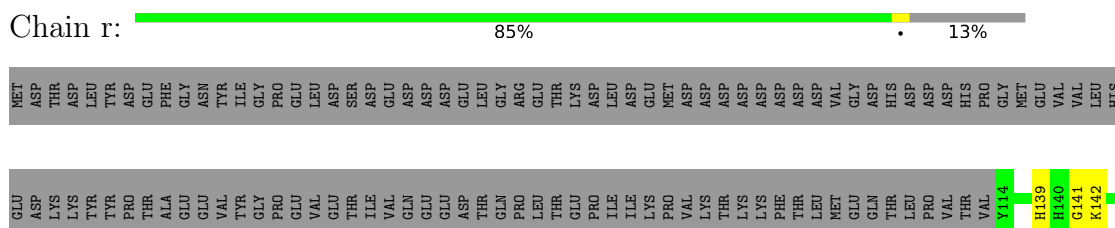
- Molecule 37: Smad nuclear-interacting protein 1



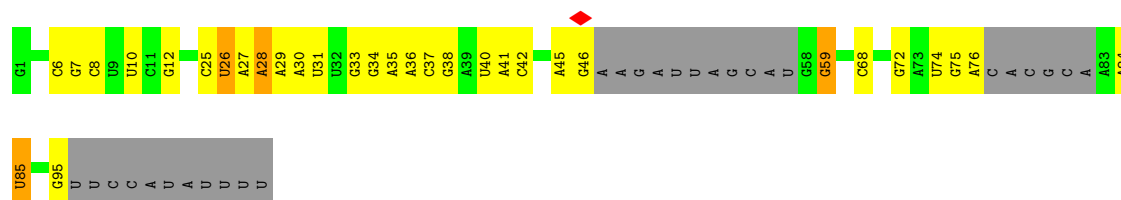
- Molecule 38: Zinc finger matrin-type protein 2



- Molecule 39: 116 kDa U5 small nuclear ribonucleoprotein component

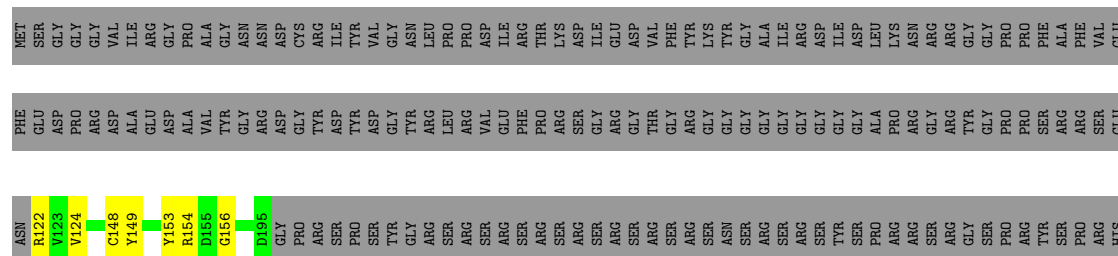






- Molecule 42: Serine/arginine-rich splicing factor 1

Chain A6: 27% 70%



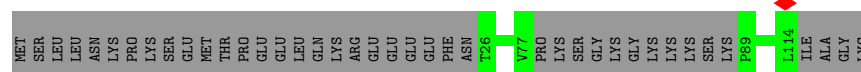
- Molecule 43: Small nuclear ribonucleoprotein Sm D2

Chain h: 9% 77% 19%



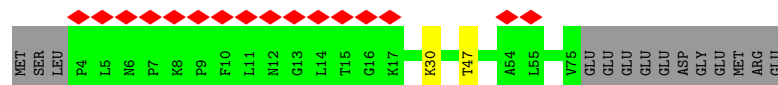
- Molecule 43: Small nuclear ribonucleoprotein Sm D2

Chain a: 66% 34%



- Molecule 44: Small nuclear ribonucleoprotein F

Chain i: 19% 81% 16%



- Molecule 44: Small nuclear ribonucleoprotein F

Chain b: 81% 15%

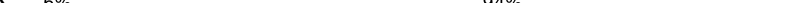
MET
K2
T16
L19
H26
S36
MET
N37
N49
R50
N63
M64
I65
V83
E84
P85
K86
K90
K91
V96
A1A
GLY
ARG
GLY
ARG
GLY
ARG
GLY
ARG
GLY
ARG
GLY
ARG
GLY
ARG
GLY
ARG
GLY
ARG
PRO
ARG
ARG

- Chain q: 97% .

```

graph LR
    M1[M1] --- A33_Q34[A33  
Q34]
    A33_Q34 --- Q73[Q73]

```

- Chain X:  6% 94%

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

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	84539	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2.25	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	0.055	Depositor
Minimum map value	-0.015	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0095	Depositor
Map size ($\text{\AA}$)	445.44, 445.44, 445.44	wwPDB
Map dimensions	384, 384, 384	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 ⓘ

5.1 Standard geometry ⓘ

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

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	A5	0.71	4/3759 (0.1%)	1.29	26/5280 (0.5%)
2	A2	0.96	0/395	1.24	1/549 (0.2%)
3	z	0.35	0/548	0.62	0/766
4	F	0.45	0/241	0.77	0/334
5	D	1.42	3/1515 (0.2%)	1.52	19/2113 (0.9%)
6	W	0.28	0/821	0.69	0/1149
7	B	1.05	0/857	1.23	6/1196 (0.5%)
8	s	0.20	0/8766	0.57	2/12286 (0.0%)
9	Q	0.21	0/700	0.58	0/979
10	A1	0.50	0/723	1.30	7/1001 (0.7%)
11	5	0.19	0/2672	0.34	0/4154
12	L	0.17	0/519	0.61	0/725
13	R	0.07	0/44	0.33	0/60
14	V	0.78	0/455	1.23	0/636
15	9	0.80	0/371	1.28	0/517
16	C	0.77	0/407	1.29	0/569
17	H	0.83	0/382	1.34	1/532 (0.2%)
18	J	0.94	0/343	1.40	4/475 (0.8%)
19	2	0.36	6/3430 (0.2%)	0.65	11/5329 (0.2%)
20	A3	0.87	0/302	1.18	2/416 (0.5%)
21	K	0.12	0/615	0.34	0/858
22	y	0.16	0/501	0.53	0/697
23	G	0.31	0/1616	0.50	2/2258 (0.1%)
24	Z	0.48	6/1114 (0.5%)	0.25	0/1730
25	A	0.27	1/11142 (0.0%)	0.56	1/15633 (0.0%)
26	I	0.20	0/888	0.49	0/1241
27	P	0.63	1/835 (0.1%)	1.18	4/1170 (0.3%)
28	p	0.93	0/301	1.70	2/420 (0.5%)
29	4	0.86	0/2119	1.58	11/2960 (0.4%)
30	A4	0.51	0/2037	0.78	2/2850 (0.1%)
31	u	0.33	0/4241	0.70	9/5935 (0.2%)
32	T	0.84	4/957 (0.4%)	1.10	6/1341 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	E	0.22	0/5980	0.47	2/8363 (0.0%)
34	w	0.99	0/394	1.14	1/549 (0.2%)
35	x	0.64	0/399	0.75	0/557
36	v	0.23	0/607	0.52	0/847
37	0	0.18	0/770	0.51	0/1079
38	N	0.32	0/276	0.56	0/383
39	r	0.20	0/4313	0.48	0/6044
40	Y	0.33	0/481	0.58	0/672
41	6	0.12	0/1870	0.27	0/2909
42	A6	0.32	0/369	0.70	0/513
43	a	0.17	0/394	0.51	0/548
43	h	0.38	0/485	0.71	0/677
44	b	0.20	0/367	0.49	0/509
44	i	0.40	0/362	0.71	0/502
45	f	0.16	0/319	0.42	0/442
45	m	0.40	0/416	0.65	0/581
46	e	0.18	0/392	0.62	0/546
46	l	0.47	0/417	0.78	0/581
47	d	0.22	0/346	0.58	0/481
47	k	0.45	0/366	0.72	0/509
48	c	0.17	0/388	0.51	0/540
48	j	0.42	0/403	0.76	0/561
49	g	0.18	0/471	0.48	0/657
49	n	0.39	0/404	0.66	0/564
50	q	0.23	0/359	0.55	0/498
51	X	0.12	0/182	0.36	0/254
All	All	0.46	25/75146 (0.0%)	0.77	119/106525 (0.1%)

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A5	252	PRO	N-CA	20.75	1.70	1.47
32	T	605	LYS	C-N	14.87	1.50	1.33
27	P	188	ASP	C-N	13.72	1.50	1.33
1	A5	251	ARG	C-N	13.51	1.45	1.33
1	A5	223	HIS	C-N	12.81	1.50	1.33
1	A5	365	PRO	C-N	11.01	1.50	1.33
25	A	1869	LEU	C-O	7.39	1.33	1.24
19	2	72	U	C1'-N1	7.26	1.59	1.48
19	2	69	U	C1'-N1	7.05	1.59	1.48
19	2	73	C	C1'-N1	6.57	1.58	1.48
24	Z	146	G	C1'-N9	-6.46	1.38	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	2	84	C	C1'-N1	6.46	1.58	1.48
32	T	619	MET	C-N	6.37	1.41	1.33
19	2	70	C	C1'-N1	6.31	1.57	1.48
19	2	71	C	C1'-N1	6.23	1.57	1.48
5	D	283	ASN	CA-C	-6.06	1.46	1.53
24	Z	147	U	C1'-N1	6.05	1.57	1.48
24	Z	145	U	C1'-N1	6.01	1.57	1.48
24	Z	154	U	C1'-N1	5.54	1.56	1.48
5	D	237	SER	C-N	5.51	1.41	1.33
32	T	620	PRO	N-CD	5.51	1.55	1.47
24	Z	144	A	C1'-N9	-5.37	1.39	1.48
32	T	643	PRO	N-CD	5.34	1.55	1.47
24	Z	141	A	C1'-N9	-5.26	1.40	1.48
5	D	284	PHE	CA-C	-5.25	1.45	1.52

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	P	188	ASP	CA-C-N	18.47	138.40	119.56
27	P	188	ASP	C-N-CA	18.47	138.40	119.56
1	A5	223	HIS	CA-C-N	18.38	138.69	119.76
1	A5	223	HIS	C-N-CA	18.38	138.69	119.76
32	T	605	LYS	CA-C-N	17.34	140.09	119.98
32	T	605	LYS	C-N-CA	17.34	140.09	119.98
1	A5	251	ARG	CA-C-N	16.32	140.64	120.89
1	A5	251	ARG	C-N-CA	16.32	140.64	120.89
1	A5	365	PRO	CA-C-N	16.25	137.85	119.32
1	A5	365	PRO	C-N-CA	16.25	137.85	119.32
30	A4	845	GLU	CA-C-O	-11.71	100.90	120.80
5	D	99	CYS	N-CA-C	-10.75	99.62	113.17
1	A5	252	PRO	CA-N-CD	-10.16	97.77	112.00
29	4	472	GLN	C-N-CD	-9.74	85.08	125.00
10	A1	29	ASN	N-CA-C	-9.70	100.87	112.89
1	A5	222	PRO	CA-N-CD	-9.15	99.19	112.00
23	G	382	PRO	CA-N-CD	-9.14	99.20	112.00
1	A5	363	PRO	CA-N-CD	-9.08	99.28	112.00
19	2	84	C	O3'-P-O5'	-8.75	90.87	104.00
19	2	72	U	O3'-P-O5'	-8.69	90.97	104.00
19	2	81	G	O3'-P-O5'	-8.66	91.02	104.00
19	2	82	G	O3'-P-O5'	-8.64	91.05	104.00
19	2	71	C	O3'-P-O5'	-8.62	91.08	104.00
19	2	79	G	O3'-P-O5'	-8.59	91.12	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	80	A	O3'-P-O5'	-8.57	91.15	104.00
19	2	68	G	O3'-P-O5'	-8.53	91.20	104.00
19	2	70	C	O3'-P-O5'	-8.52	91.21	104.00
19	2	69	U	O3'-P-O5'	-8.50	91.26	104.00
19	2	83	A	O3'-P-O5'	-8.45	91.33	104.00
8	s	1976	ASP	CB-CA-C	8.40	127.51	110.38
8	s	621	HIS	CB-CA-C	8.13	127.53	110.45
5	D	347	SER	CA-C-N	8.13	133.61	120.60
5	D	347	SER	C-N-CA	8.13	133.61	120.60
5	D	270	LYS	N-CA-C	-7.99	102.57	111.28
5	D	351	LEU	CA-C-N	-7.54	110.85	122.62
5	D	351	LEU	C-N-CA	-7.54	110.85	122.62
1	A5	193	ASP	N-CA-C	-7.52	103.18	113.18
29	4	77	GLY	CA-C-N	7.38	129.07	119.84
29	4	77	GLY	C-N-CA	7.38	129.07	119.84
7	B	175	PRO	N-CA-C	7.04	126.97	112.47
2	A2	56	ARG	N-CA-CB	-7.01	99.10	111.08
29	4	281	ARG	N-CA-C	6.94	119.44	111.11
10	A1	127	ARG	N-CA-C	-6.67	104.76	113.17
5	D	282	HIS	N-CA-C	-6.64	103.97	111.07
18	J	49	GLU	CA-C-N	6.51	133.97	121.54
18	J	49	GLU	C-N-CA	6.51	133.97	121.54
32	T	619	MET	CA-C-N	-6.48	113.62	120.03
32	T	619	MET	C-N-CA	-6.48	113.62	120.03
1	A5	228	TYR	N-CA-C	6.47	119.15	111.71
5	D	348	ASP	N-CA-C	-6.42	104.55	112.38
7	B	174	PHE	CA-C-N	6.23	127.63	119.84
7	B	174	PHE	C-N-CA	6.23	127.63	119.84
29	4	351	ARG	N-CA-C	6.09	118.63	110.35
1	A5	226	GLU	N-CA-C	5.99	119.35	110.48
1	A5	594	TRP	N-CA-C	5.96	119.86	112.59
7	B	182	LEU	CA-C-N	-5.93	116.86	123.02
7	B	182	LEU	C-N-CA	-5.93	116.86	123.02
31	u	1254	LEU	CA-C-N	5.91	130.59	121.19
31	u	1254	LEU	C-N-CA	5.91	130.59	121.19
30	A4	790	THR	N-CA-C	-5.84	106.77	114.31
5	D	304	SER	CA-C-N	5.84	129.18	120.31
5	D	304	SER	C-N-CA	5.84	129.18	120.31
5	D	141	GLY	N-CA-C	-5.80	107.31	115.32
27	P	219	THR	CA-C-N	5.79	132.12	121.70
27	P	219	THR	C-N-CA	5.79	132.12	121.70
29	4	291	LYS	CA-C-N	5.78	132.57	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	4	291	LYS	C-N-CA	5.78	132.57	121.54
10	A1	126	GLY	N-CA-C	-5.76	104.62	111.36
31	u	1254	LEU	O-C-N	5.75	128.01	122.03
33	E	405	SER	CA-C-N	5.71	126.97	119.84
33	E	405	SER	C-N-CA	5.71	126.97	119.84
1	A5	693	GLU	N-CA-C	-5.71	105.14	111.36
1	A5	597	HIS	CA-C-N	5.69	125.81	119.32
1	A5	597	HIS	C-N-CA	5.69	125.81	119.32
1	A5	491	SER	N-CA-C	-5.66	105.11	113.72
29	4	78	PRO	N-CA-C	5.60	124.01	112.47
20	A3	41	SER	CB-CA-C	-5.60	100.56	109.80
1	A5	131	LEU	N-CA-C	-5.59	104.88	110.97
34	w	81	GLY	N-CA-C	-5.53	108.22	115.47
1	A5	635	LEU	N-CA-C	5.50	116.96	111.07
20	A3	56	VAL	CA-C-O	-5.49	114.95	121.05
29	4	104	VAL	CA-C-O	-5.48	115.02	118.69
5	D	285	GLU	CA-C-N	-5.48	111.08	121.54
5	D	285	GLU	C-N-CA	-5.48	111.08	121.54
5	D	237	SER	CA-C-O	-5.47	115.21	121.40
5	D	128	SER	CA-C-N	5.46	128.60	120.31
5	D	128	SER	C-N-CA	5.46	128.60	120.31
18	J	49	GLU	O-C-N	5.44	129.82	122.59
32	T	642	PRO	CA-C-N	-5.41	113.05	119.05
32	T	642	PRO	C-N-CA	-5.41	113.05	119.05
10	A1	99	ARG	N-CA-C	5.40	117.25	111.36
25	A	1877	LEU	N-CA-C	-5.35	105.34	111.07
7	B	184	PRO	N-CA-C	-5.34	106.76	114.18
17	H	66	ILE	O-C-N	5.31	127.23	121.87
31	u	1125	PRO	CA-C-N	5.30	128.12	120.38
31	u	1125	PRO	C-N-CA	5.30	128.12	120.38
5	D	162	ARG	N-CA-C	-5.28	105.64	111.71
1	A5	87	THR	N-CA-C	-5.27	105.53	111.28
1	A5	121	TYR	N-CA-C	5.21	117.63	111.33
10	A1	40	CYS	N-CA-C	-5.21	105.66	113.89
23	G	384	HIS	O-C-N	5.20	124.68	120.83
1	A5	186	GLU	N-CA-C	-5.18	106.22	112.54
10	A1	48	SER	N-CA-C	-5.18	102.86	110.52
5	D	326	HIS	CA-C-N	5.17	127.64	120.29
5	D	326	HIS	C-N-CA	5.17	127.64	120.29
1	A5	329	ARG	N-CA-C	5.12	116.86	111.28
31	u	717	THR	CA-C-N	5.11	126.23	119.84
31	u	717	THR	C-N-CA	5.11	126.23	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A5	430	TRP	N-CA-C	5.11	117.58	111.71
18	J	49	GLU	CA-C-O	-5.09	113.23	120.51
10	A1	81	CYS	N-CA-C	5.09	119.76	113.50
1	A5	495	LEU	CA-C-N	5.08	125.01	119.78
1	A5	495	LEU	C-N-CA	5.08	125.01	119.78
28	p	162	PHE	CA-C-N	5.08	127.04	120.44
28	p	162	PHE	C-N-CA	5.08	127.04	120.44
29	4	312	ARG	CA-C-N	5.06	131.21	121.54
29	4	312	ARG	C-N-CA	5.06	131.21	121.54
31	u	1027	ARG	CA-C-N	5.04	128.82	121.31
31	u	1027	ARG	C-N-CA	5.04	128.82	121.31

There are no chirality outliers.

There are no planarity outliers.

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	A5	3723	0	1806	75	0
2	A2	393	0	183	4	0
3	z	544	0	264	9	0
4	F	242	0	118	25	0
5	D	1506	0	737	29	0
6	W	816	0	386	2	0
7	B	851	0	423	7	0
8	s	8688	0	4220	19	0
9	Q	695	0	327	2	0
10	A1	724	0	335	13	0
11	5	2397	0	1216	65	0
12	L	517	0	257	5	0
13	R	45	0	17	0	0
14	V	453	0	212	1	0
15	9	369	0	174	1	0
16	C	404	0	189	2	0
17	H	380	0	172	6	0
18	J	342	0	164	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	2	3077	0	1559	146	0
20	A3	304	0	137	7	0
21	K	614	0	284	9	0
22	y	498	0	241	10	0
23	G	1604	0	795	22	0
24	Z	998	0	504	54	0
25	A	11024	0	5384	80	0
26	I	883	0	414	0	0
27	P	825	0	409	25	0
28	p	301	0	134	0	0
29	4	2110	0	987	51	0
30	A4	2034	0	912	29	0
31	u	4207	0	2103	109	0
32	T	942	0	490	55	0
33	E	5926	0	2964	78	0
34	w	391	0	197	19	0
35	x	397	0	191	11	0
36	v	605	0	311	27	0
37	0	761	0	376	7	0
38	N	277	0	114	3	0
39	r	4265	0	2120	19	0
40	Y	478	0	226	25	0
41	6	1672	0	846	34	0
42	A6	368	0	175	23	0
43	a	393	0	176	0	0
43	h	482	0	220	6	0
44	b	364	0	181	2	0
44	i	359	0	179	1	0
45	f	319	0	144	6	0
45	m	413	0	193	7	0
46	e	390	0	188	3	0
46	l	415	0	198	21	0
47	d	344	0	168	0	0
47	k	364	0	176	12	0
48	c	388	0	167	0	0
48	j	403	0	173	6	0
49	g	469	0	214	9	0
49	n	402	0	184	24	0
50	q	360	0	159	2	0
51	X	182	0	85	0	0
52	A	36	0	6	0	0
53	r	32	0	12	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	r	1	0	0	0	0
55	A6	52	0	26	11	0
All	All	73818	0	35922	850	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 8.

All (850) 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:A:91:ALA:HB2	36:v:207:MET:CA	1.21	1.65
1:A5:258:SER:CB	30:A4:766:MET:HA	1.27	1.64
1:A5:258:SER:CB	30:A4:766:MET:CA	1.77	1.63
25:A:1772:PHE:CB	25:A:2246:ASN:CB	1.79	1.60
30:A4:731:ASP:CB	30:A4:759:ARG:CA	1.77	1.59
30:A4:731:ASP:CB	30:A4:759:ARG:CB	1.75	1.58
31:u:1257:PRO:HG3	32:T:481:THR:CB	1.20	1.58
25:A:91:ALA:CB	36:v:207:MET:CB	1.79	1.56
30:A4:731:ASP:CB	30:A4:759:ARG:C	1.78	1.56
1:A5:88:THR:CB	1:A5:253:TYR:CB	1.82	1.54
4:F:50:HIS:CB	31:u:1139:PRO:C	1.79	1.51
1:A5:258:SER:CB	30:A4:766:MET:CB	1.86	1.50
31:u:1214:TYR:CA	32:T:591:TYR:CB	1.87	1.48
25:A:91:ALA:HB3	36:v:207:MET:CB	1.32	1.46
19:2:181:G:H21	46:l:52:ASP:CB	1.30	1.45
25:A:1616:PRO:HA	25:A:2058:THR:CB	1.46	1.45
8:s:1125:SER:CB	25:A:2314:PHE:CB	1.96	1.44
1:A5:358:GLU:O	1:A5:365:PRO:CB	1.65	1.44
31:u:1257:PRO:CG	32:T:481:THR:CB	1.97	1.42
29:4:485:ASN:N	33:E:974:LYS:CB	1.82	1.41
1:A5:252:PRO:CA	1:A5:252:PRO:N	1.70	1.41
22:y:3:LYS:CB	24:Z:155:A:OP2	1.68	1.41
31:u:1214:TYR:HA	32:T:591:TYR:CB	0.93	1.41
22:y:3:LYS:CB	24:Z:155:A:P	2.08	1.40
4:F:50:HIS:CB	31:u:1140:GLU:N	1.84	1.37
5:D:104:THR:O	11:5:6:C:C5'	1.69	1.37
1:A5:88:THR:CA	1:A5:253:TYR:CB	2.01	1.36
29:4:470:ARG:CB	33:E:1019:ASN:CB	2.03	1.36
1:A5:88:THR:HA	1:A5:253:TYR:CB	1.54	1.35
19:2:181:G:N2	46:l:52:ASP:CB	1.87	1.34
27:P:173:CYS:CA	41:6:28:A:N6	1.88	1.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:2:181:G:N3	46:l:52:ASP:CB	1.88	1.33
10:A1:19:GLN:HA	42:A6:122:ARG:N	1.42	1.33
20:A3:32:GLN:CB	41:6:95:G:OP1	1.74	1.33
30:A4:731:ASP:CA	30:A4:759:ARG:CB	2.06	1.32
8:s:1382:MET:O	8:s:1653:GLY:N	1.60	1.31
31:u:1217:PRO:CG	32:T:591:TYR:O	1.77	1.31
25:A:91:ALA:CB	36:v:207:MET:HA	1.55	1.30
5:D:104:THR:O	11:5:6:C:H5'	1.26	1.30
10:A1:19:GLN:O	42:A6:122:ARG:HA	1.29	1.30
19:2:53:U:C2	19:2:61:C:N4	1.97	1.30
19:2:181:G:C2	46:l:52:ASP:CB	2.15	1.29
27:P:173:CYS:HA	41:6:28:A:N6	1.45	1.28
42:A6:148:CYS:O	55:A6:301:GTG:H3B	1.26	1.28
25:A:1926:THR:O	25:A:2253:PRO:HG3	1.27	1.27
34:w:14:THR:HA	34:w:59:VAL:O	1.32	1.26
30:A4:728:ALA:HB1	30:A4:763:ILE:CB	1.66	1.26
19:2:181:G:O2'	46:l:51:ARG:O	1.53	1.25
29:4:484:GLY:C	33:E:974:LYS:CB	2.08	1.25
39:r:139:HIS:O	53:r:1500:GTP:C5'	1.83	1.25
29:4:356:ARG:CB	49:n:75:PRO:HB3	1.66	1.25
42:A6:148:CYS:O	55:A6:301:GTG:H5B2	1.25	1.25
30:A4:731:ASP:CB	30:A4:759:ARG:O	1.75	1.24
33:E:805:ASN:CB	35:x:58:ASN:CB	2.14	1.24
39:r:139:HIS:O	53:r:1500:GTP:H5''	1.33	1.23
27:P:64:ARG:HA	41:6:26:U:O4	1.39	1.22
42:A6:149:TYR:CB	55:A6:301:GTG:O1G	1.88	1.22
5:D:104:THR:N	11:5:6:C:H4'	1.53	1.21
10:A1:19:GLN:O	42:A6:122:ARG:CA	1.87	1.20
31:u:1213:ASN:CA	32:T:590:LEU:HA	1.71	1.20
25:A:1772:PHE:CA	25:A:2246:ASN:CB	2.19	1.20
33:E:192:ALA:HB1	35:x:74:GLN:CB	1.69	1.20
19:2:44:U:N3	24:Z:144:A:N1	1.90	1.20
32:T:605:LYS:CB	32:T:606:PRO:HD2	1.56	1.18
1:A5:258:SER:C	30:A4:766:MET:CB	2.17	1.18
10:A1:29:ASN:CB	42:A6:124:VAL:CB	2.22	1.18
11:5:13:C:N3	11:5:65:G:N1	1.91	1.18
1:A5:358:GLU:C	1:A5:365:PRO:HB3	1.67	1.18
4:F:61:THR:CB	19:2:40:C:O5'	1.93	1.16
31:u:1217:PRO:HG2	32:T:591:TYR:O	1.39	1.16
30:A4:731:ASP:HA	30:A4:759:ARG:CB	1.73	1.15
4:F:50:HIS:CB	31:u:1139:PRO:CB	2.24	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:2:103:U:O4	45:m:38:MET:CB	1.93	1.15
27:P:173:CYS:CA	41:6:28:A:H61	1.53	1.14
40:Y:86:GLN:O	40:Y:90:THR:CB	1.95	1.14
25:A:730:GLY:CA	36:v:248:PRO:CG	2.23	1.13
40:Y:89:LEU:O	40:Y:98:ALA:HB1	1.46	1.12
31:u:1257:PRO:HB3	32:T:481:THR:O	1.47	1.12
25:A:730:GLY:HA3	36:v:248:PRO:HG2	1.17	1.11
27:P:173:CYS:C	41:6:28:A:H61	1.40	1.11
29:4:356:ARG:C	49:n:75:PRO:HG3	1.76	1.11
23:G:382:PRO:HB3	23:G:425:GLY:HA2	1.28	1.10
31:u:1213:ASN:CB	32:T:590:LEU:HA	1.81	1.10
31:u:654:SER:CB	40:Y:65:ASP:CB	2.30	1.10
34:w:17:VAL:HA	34:w:85:ARG:O	1.53	1.09
4:F:50:HIS:CB	31:u:1139:PRO:CA	2.30	1.09
34:w:25:SER:C	34:w:27:PRO:HD2	1.77	1.09
4:F:50:HIS:CB	31:u:1139:PRO:HG2	1.84	1.08
18:J:29:ASP:O	18:J:49:GLU:CB	2.00	1.08
1:A5:363:PRO:HD2	1:A5:364:ALA:H	1.09	1.08
19:2:100:U:H1'	47:k:65:ASN:CB	1.83	1.08
5:D:104:THR:H	11:5:6:C:C4'	1.67	1.08
19:2:34:U:OP1	31:u:509:PRO:CB	2.02	1.07
19:2:104:U:O3'	43:h:104:ASP:CB	2.03	1.06
25:A:1772:PHE:HA	25:A:2246:ASN:CB	1.81	1.06
29:4:483:SER:C	33:E:974:LYS:O	1.98	1.06
23:G:382:PRO:CB	23:G:425:GLY:HA2	1.84	1.05
40:Y:103:GLY:O	40:Y:107:PRO:CD	2.03	1.05
33:E:354:GLY:H	33:E:405:SER:CB	1.67	1.05
42:A6:149:TYR:CB	55:A6:301:GTG:O5E	2.04	1.05
4:F:50:HIS:CB	31:u:1139:PRO:CG	2.35	1.05
31:u:1217:PRO:HG3	32:T:591:TYR:O	1.55	1.05
31:u:1257:PRO:HG3	32:T:481:THR:CA	1.85	1.05
25:A:91:ALA:CB	36:v:207:MET:CA	2.03	1.05
33:E:114:ARG:CB	35:x:41:CYS:CB	2.34	1.05
11:5:13:C:O2	11:5:65:G:N2	1.91	1.04
40:Y:89:LEU:O	40:Y:98:ALA:CB	2.05	1.04
19:2:100:U:O2	47:k:65:ASN:N	1.90	1.04
29:4:470:ARG:CA	33:E:1019:ASN:CB	2.34	1.04
5:D:104:THR:O	11:5:6:C:H5''	1.54	1.03
3:z:55:GLU:CB	31:u:476:ASP:CB	2.35	1.03
25:A:730:GLY:CA	36:v:248:PRO:HG2	1.77	1.03
25:A:87:VAL:CB	36:v:207:MET:O	2.06	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:w:70:ALA:O	34:w:74:MET:CB	2.06	1.03
10:A1:19:GLN:CA	42:A6:122:ARG:N	2.20	1.03
25:A:166:PHE:CB	25:A:167:PRO:CD	2.37	1.03
29:4:483:SER:O	33:E:974:LYS:O	1.76	1.02
31:u:646:PRO:HA	40:Y:73:ASN:CB	1.89	1.02
5:D:104:THR:CB	11:5:6:C:O3'	2.07	1.02
42:A6:148:CYS:O	55:A6:301:GTG:C3E	2.07	1.02
25:A:1616:PRO:CA	25:A:2058:THR:CB	2.37	1.02
1:A5:258:SER:CA	30:A4:766:MET:CB	2.38	1.01
19:2:136:G:O3'	43:h:87:SER:N	1.93	1.01
29:4:473:PRO:HB2	33:E:978:LEU:CB	1.90	1.01
11:5:44:A:H8	24:Z:55:A:N1	1.58	1.01
31:u:1213:ASN:HA	32:T:590:LEU:HA	1.36	1.01
40:Y:103:GLY:O	40:Y:107:PRO:HD3	1.57	1.00
39:r:139:HIS:HA	53:r:1500:GTP:O3B	1.62	1.00
19:2:101:U:H1'	46:l:66:SER:N	1.77	0.99
25:A:1926:THR:O	25:A:2253:PRO:CG	2.08	0.99
31:u:1213:ASN:C	32:T:591:TYR:H	1.70	0.99
27:P:180:PRO:CG	41:6:26:U:O2'	2.11	0.99
30:A4:731:ASP:CB	30:A4:759:ARG:HA	1.93	0.98
24:Z:64:A:N6	41:6:41:A:N1	2.12	0.98
29:4:470:ARG:CB	33:E:1018:GLU:O	2.13	0.97
27:P:64:ARG:CA	41:6:26:U:O4	2.12	0.97
25:A:1877:LEU:O	25:A:1880:PRO:HD3	1.66	0.96
10:A1:20:TYR:O	42:A6:122:ARG:CB	2.13	0.96
31:u:646:PRO:CA	40:Y:73:ASN:CB	2.43	0.96
1:A5:359:LEU:HA	1:A5:365:PRO:HG3	1.48	0.96
22:y:3:LYS:C	24:Z:154:U:O3'	2.08	0.96
23:G:382:PRO:HD2	23:G:383:ARG:H	1.29	0.95
32:T:605:LYS:CB	32:T:606:PRO:CD	2.44	0.95
39:r:139:HIS:O	53:r:1500:GTP:H5'	1.63	0.95
24:Z:74:G:H1'	41:6:30:A:H61	1.32	0.95
31:u:1257:PRO:HG3	32:T:481:THR:C	1.92	0.95
5:D:104:THR:C	11:5:6:C:H5''	1.91	0.95
23:G:382:PRO:HB3	23:G:425:GLY:CA	1.97	0.95
33:E:189:TYR:CB	35:x:73:LEU:CB	2.45	0.95
23:G:382:PRO:CG	23:G:425:GLY:HA2	1.97	0.95
11:5:40:U:H5	21:K:383:PHE:CB	1.78	0.95
42:A6:149:TYR:CB	55:A6:301:GTG:PG	2.55	0.94
19:2:181:G:N3	46:l:52:ASP:CA	2.30	0.94
19:2:100:U:O2	47:k:64:GLY:N	2.00	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:730:GLY:CA	36:v:248:PRO:HG3	1.96	0.94
31:u:1257:PRO:CB	32:T:481:THR:O	2.16	0.93
29:4:484:GLY:N	33:E:974:LYS:CB	2.31	0.93
33:E:354:GLY:N	33:E:405:SER:CB	2.30	0.93
23:G:342:GLU:CB	23:G:343:PRO:CD	2.46	0.92
27:P:36:MET:N	36:v:198:ARG:O	2.02	0.92
31:u:1213:ASN:CB	32:T:590:LEU:CA	2.46	0.92
24:Z:74:G:N3	41:6:30:A:N6	2.19	0.91
29:4:472:GLN:N	29:4:473:PRO:HD2	1.85	0.91
29:4:484:GLY:CA	33:E:974:LYS:CB	2.47	0.91
29:4:485:ASN:H	33:E:974:LYS:CB	1.82	0.91
25:A:730:GLY:HA2	36:v:248:PRO:HG3	1.51	0.91
7:B:20:LYS:CB	19:2:170:C:OP1	2.18	0.91
10:A1:19:GLN:O	42:A6:122:ARG:CB	2.17	0.91
19:2:45:C:N3	24:Z:144:A:C2	2.38	0.91
22:y:3:LYS:CB	24:Z:154:U:O3'	2.17	0.91
11:5:13:C:C2	11:5:65:G:C2	2.59	0.91
31:u:646:PRO:O	40:Y:73:ASN:CB	2.18	0.91
11:5:13:C:N4	11:5:65:G:O6	2.02	0.91
11:5:109:C:P	49:g:49:ASN:O	2.28	0.91
10:A1:20:TYR:C	42:A6:122:ARG:CB	2.43	0.91
29:4:472:GLN:N	29:4:473:PRO:CD	2.34	0.91
8:s:1071:LYS:CB	25:A:2323:GLY:HA3	2.01	0.90
29:4:356:ARG:CB	49:n:75:PRO:CB	2.49	0.90
33:E:192:ALA:CB	35:x:74:GLN:CB	2.50	0.90
23:G:382:PRO:CB	23:G:425:GLY:CA	2.48	0.90
4:F:50:HIS:O	31:u:1140:GLU:CB	2.21	0.89
4:F:50:HIS:CB	31:u:1139:PRO:HB2	2.02	0.89
42:A6:148:CYS:O	55:A6:301:GTG:C2E	2.20	0.89
34:w:26:GLU:N	34:w:27:PRO:HD2	1.88	0.89
40:Y:86:GLN:O	40:Y:90:THR:N	2.06	0.89
42:A6:148:CYS:O	55:A6:301:GTG:H2B	1.72	0.88
29:4:353:GLY:C	49:n:78:THR:CB	2.47	0.88
1:A5:358:GLU:O	1:A5:365:PRO:HB3	0.71	0.88
25:A:166:PHE:CB	25:A:167:PRO:HD3	2.02	0.88
31:u:1257:PRO:HG2	32:T:481:THR:CB	2.02	0.88
42:A6:148:CYS:O	55:A6:301:GTG:C5E	2.18	0.88
11:5:44:A:C8	24:Z:55:A:N1	2.41	0.87
20:A3:32:GLN:CB	41:6:95:G:P	2.61	0.87
23:G:382:PRO:HG3	23:G:425:GLY:HA2	1.54	0.87
37:0:255:PRO:HG2	37:0:276:HIS:CB	2.05	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:u:1130:PRO:CB	32:T:528:ILE:CB	2.53	0.87
19:2:34:U:OP1	31:u:509:PRO:HB2	1.71	0.87
31:u:1214:TYR:HA	32:T:591:TYR:CA	2.06	0.86
19:2:43:U:C2	24:Z:146:G:N2	2.43	0.86
24:Z:152:C:OP2	31:u:1105:GLU:CB	2.24	0.86
29:4:469:GLU:O	33:E:981:CYS:HA	1.75	0.86
19:2:43:U:N3	24:Z:146:G:N2	2.23	0.86
27:P:173:CYS:C	41:6:28:A:N6	2.06	0.86
1:A5:363:PRO:HD2	1:A5:364:ALA:N	1.87	0.85
11:5:13:C:C2	11:5:65:G:N2	2.44	0.85
12:L:77:LEU:HA	36:v:288:ALA:CB	2.05	0.85
11:5:13:C:O2	11:5:65:G:C2	2.29	0.85
19:2:181:G:H1'	46:l:51:ARG:O	1.77	0.85
22:y:3:LYS:O	24:Z:154:U:O3'	1.93	0.85
31:u:1213:ASN:C	32:T:591:TYR:N	2.35	0.85
39:r:142:LYS:CB	53:r:1500:GTP:O1B	2.25	0.84
19:2:53:U:O2	19:2:61:C:N4	1.92	0.84
29:4:357:GLU:CA	49:n:75:PRO:HG2	2.07	0.84
31:u:1130:PRO:HB3	32:T:528:ILE:CB	2.07	0.84
4:F:61:THR:CB	19:2:40:C:P	2.66	0.84
11:5:40:U:C5	21:K:383:PHE:CB	2.60	0.84
19:2:85:A:C5'	49:n:9:LYS:HA	2.08	0.84
25:A:2055:ILE:CB	41:6:42:C:OP1	2.26	0.83
38:N:90:LYS:CB	41:6:40:U:O2'	2.25	0.83
19:2:105:G:P	43:h:104:ASP:CB	2.66	0.83
29:4:472:GLN:H	29:4:473:PRO:HD2	1.44	0.83
23:G:382:PRO:CG	23:G:425:GLY:CA	2.56	0.83
18:J:30:TYR:HA	18:J:49:GLU:HA	1.59	0.83
34:w:26:GLU:N	34:w:27:PRO:CD	2.41	0.83
29:4:473:PRO:CB	33:E:978:LEU:CB	2.57	0.83
10:A1:19:GLN:C	42:A6:122:ARG:CA	2.51	0.83
25:A:730:GLY:HA3	36:v:248:PRO:CG	1.96	0.83
11:5:13:C:N3	11:5:65:G:C2	2.47	0.82
29:4:357:GLU:N	49:n:75:PRO:CG	2.42	0.82
25:A:1858:PRO:O	25:A:1859:LYS:O	1.97	0.82
6:W:152:LEU:N	19:2:157:G:OP1	2.12	0.82
23:G:382:PRO:HG3	23:G:425:GLY:CA	2.09	0.82
34:w:28:LEU:O	34:w:32:LEU:CB	2.27	0.82
25:A:168:PRO:HG2	25:A:559:ASP:CB	2.09	0.82
27:P:173:CYS:HA	41:6:28:A:H62	1.44	0.82
29:4:356:ARG:C	49:n:75:PRO:CG	2.53	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:2:85:A:H5'	49:n:9:LYS:HA	1.62	0.82
27:P:173:CYS:CB	41:6:28:A:N6	2.43	0.82
48:j:58:LEU:O	48:j:76:ARG:HA	1.80	0.82
19:2:45:C:H42	24:Z:143:G:H1	1.28	0.81
19:2:101:U:C1'	46:l:66:SER:N	2.39	0.81
7:B:53:PHE:CB	19:2:165:A:H2	1.92	0.81
19:2:34:U:OP1	31:u:509:PRO:HB3	1.81	0.81
39:r:139:HIS:HA	53:r:1500:GTP:PB	2.20	0.81
31:u:1167:TYR:O	32:T:582:PRO:HG3	1.80	0.81
1:A5:255:ALA:HB2	30:A4:748:SER:HA	1.60	0.81
1:A5:259:ILE:N	30:A4:766:MET:CB	2.42	0.80
8:s:422:PHE:H	8:s:621:HIS:H	1.29	0.80
23:G:382:PRO:HD2	23:G:383:ARG:N	1.95	0.80
19:2:44:U:O2	24:Z:144:A:H2	1.64	0.80
19:2:45:C:N4	24:Z:143:G:H1	1.79	0.80
19:2:43:U:N3	24:Z:146:G:C2	2.50	0.80
25:A:90:GLY:HA3	36:v:209:PRO:HG3	1.61	0.79
5:D:104:THR:C	11:5:6:C:C5'	2.52	0.79
8:s:1382:MET:O	8:s:1653:GLY:CA	2.30	0.79
39:r:259:LYS:HA	53:r:1500:GTP:C6	2.17	0.79
1:A5:359:LEU:O	1:A5:365:PRO:HD3	1.82	0.79
1:A5:363:PRO:CD	1:A5:364:ALA:H	1.93	0.79
11:5:13:C:N3	11:5:65:G:C6	2.50	0.79
1:A5:256:PHE:CB	1:A5:260:LEU:CB	2.60	0.79
34:w:17:VAL:O	34:w:56:TYR:HA	1.83	0.79
19:2:181:G:N3	46:l:52:ASP:HA	1.98	0.79
5:D:265:ARG:CB	5:D:270:LYS:H	1.97	0.78
19:2:100:U:C1'	47:k:65:ASN:CB	2.61	0.78
5:D:104:THR:H	11:5:6:C:H4'	0.72	0.78
27:P:180:PRO:HG2	41:6:26:U:O2'	1.81	0.78
29:4:470:ARG:HA	33:E:1019:ASN:CB	2.13	0.78
18:J:29:ASP:O	18:J:49:GLU:CA	2.32	0.78
19:2:45:C:H2'	29:4:395:TRP:CB	2.14	0.78
40:Y:103:GLY:O	40:Y:107:PRO:CG	2.31	0.77
19:2:54:U:O2	19:2:59:A:N6	2.15	0.77
19:2:150:U:H3	19:2:181:G:H1	1.31	0.77
19:2:14:C:N3	41:6:85:U:O2	2.18	0.77
33:E:354:GLY:HA2	33:E:405:SER:CB	2.14	0.77
31:u:1167:TYR:C	32:T:582:PRO:HG3	2.09	0.76
27:P:64:ARG:C	41:6:26:U:O4	2.28	0.76
3:z:12:ARG:N	37:0:237:ASN:HA	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:4:357:GLU:N	49:n:75:PRO:HG2	1.99	0.76
19:2:105:G:OP2	43:h:104:ASP:CB	2.33	0.76
25:A:1791:HIS:O	25:A:1792:LYS:CB	2.32	0.76
1:A5:256:PHE:O	1:A5:261:CYS:CB	2.33	0.76
4:F:61:THR:CA	19:2:40:C:OP1	2.34	0.75
39:r:259:LYS:HA	53:r:1500:GTP:O6	1.85	0.75
4:F:61:THR:HA	19:2:40:C:OP1	1.86	0.75
25:A:1776:ILE:O	25:A:1858:PRO:O	2.05	0.75
19:2:44:U:O2	24:Z:144:A:C2	2.39	0.75
30:A4:728:ALA:CB	30:A4:763:ILE:CB	2.58	0.75
33:E:196:PRO:HB3	35:x:78:PRO:HB3	1.68	0.75
31:u:719:TYR:CB	33:E:216:GLY:O	2.35	0.75
27:P:37:THR:HA	36:v:200:VAL:O	1.87	0.75
10:A1:19:GLN:C	42:A6:122:ARG:N	2.45	0.74
19:2:181:G:O2'	46:l:51:ARG:C	2.29	0.74
29:4:483:SER:CA	33:E:974:LYS:O	2.34	0.74
33:E:354:GLY:CA	33:E:405:SER:CB	2.65	0.74
31:u:1213:ASN:O	32:T:591:TYR:N	2.11	0.74
41:6:59:G:O6	41:6:76:A:N1	2.21	0.74
5:D:57:ALA:HB1	5:D:58:PRO:HD2	1.69	0.74
31:u:1257:PRO:CG	32:T:481:THR:O	2.36	0.73
33:E:192:ALA:O	35:x:74:GLN:CB	2.36	0.73
8:s:421:HIS:H	8:s:622:ASP:H	1.36	0.73
46:l:48:VAL:O	46:l:55:VAL:HA	1.88	0.73
25:A:90:GLY:CA	36:v:209:PRO:HG3	2.18	0.73
10:A1:19:GLN:C	42:A6:122:ARG:CB	2.62	0.73
19:2:101:U:H1'	46:l:66:SER:H	1.50	0.73
23:G:342:GLU:CB	23:G:343:PRO:HD3	2.18	0.72
40:Y:103:GLY:O	40:Y:107:PRO:HG3	1.88	0.72
32:T:519:LYS:CB	32:T:520:PRO:HD2	2.20	0.72
29:4:357:GLU:HA	49:n:75:PRO:HG2	1.71	0.71
4:F:61:THR:CB	19:2:40:C:OP1	2.38	0.71
31:u:1210:HIS:CB	32:T:585:THR:CB	2.68	0.71
19:2:105:G:N1	49:n:20:LYS:CB	2.54	0.71
31:u:646:PRO:C	40:Y:73:ASN:CB	2.62	0.71
40:Y:86:GLN:O	40:Y:90:THR:CA	2.38	0.71
27:P:173:CYS:CB	41:6:28:A:H61	2.01	0.71
32:T:470:ALA:C	32:T:472:PRO:HD3	2.16	0.71
46:e:6:PRO:O	46:e:10:LEU:CB	2.39	0.71
19:2:181:G:C1'	46:l:51:ARG:O	2.39	0.71
19:2:181:G:C2'	46:l:51:ARG:O	2.38	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:293:TRP:O	5:D:295:PRO:HD3	1.90	0.71
31:u:1257:PRO:CG	32:T:481:THR:C	2.62	0.70
1:A5:361:GLN:O	1:A5:363:PRO:CD	2.40	0.70
1:A5:488:GLY:C	1:A5:490:GLU:H	2.00	0.70
11:5:13:C:N4	11:5:65:G:C6	2.58	0.70
19:2:45:C:C2	24:Z:144:A:C2	2.80	0.70
31:u:1214:TYR:C	32:T:591:TYR:CB	2.63	0.70
23:G:382:PRO:CD	23:G:383:ARG:H	2.04	0.70
21:K:272:ASP:CB	30:A4:679:SER:HA	2.22	0.70
19:2:53:U:N3	19:2:61:C:N4	2.39	0.69
42:A6:148:CYS:C	55:A6:301:GTG:H3B	2.15	0.69
27:P:180:PRO:CB	41:6:26:U:O2'	2.41	0.69
19:2:34:U:P	31:u:509:PRO:CB	2.81	0.69
25:A:166:PHE:CB	25:A:167:PRO:HD2	2.20	0.69
39:r:208:HIS:O	39:r:212:SER:N	2.26	0.69
25:A:584:HIS:O	25:A:588:LEU:N	2.26	0.69
41:6:34:G:OP2	41:6:34:G:N2	2.25	0.69
19:2:45:C:C4	24:Z:144:A:N1	2.62	0.68
11:5:39:C:H4'	21:K:383:PHE:CB	2.24	0.68
23:G:342:GLU:CB	23:G:343:PRO:HD2	2.23	0.68
27:P:33:TYR:HA	36:v:196:VAL:O	1.93	0.68
24:Z:152:C:P	31:u:1105:GLU:CB	2.82	0.67
19:2:45:C:N4	24:Z:144:A:C6	2.63	0.67
31:u:1217:PRO:HG2	32:T:591:TYR:C	2.19	0.67
33:E:406:PRO:HA	33:E:1122:LEU:O	1.94	0.67
19:2:34:U:P	31:u:509:PRO:HB2	2.35	0.66
34:w:25:SER:C	34:w:27:PRO:CD	2.61	0.66
24:Z:75:U:H2'	24:Z:76:A:H8	1.59	0.66
34:w:25:SER:CB	34:w:27:PRO:HD2	2.26	0.66
31:u:607:ALA:HB2	40:Y:87:ILE:O	1.95	0.66
11:5:13:C:C2	11:5:65:G:N1	2.63	0.66
29:4:483:SER:HA	33:E:974:LYS:O	1.96	0.66
3:z:98:PHE:C	3:z:100:LYS:H	2.04	0.66
30:A4:728:ALA:HB1	30:A4:763:ILE:CA	2.25	0.65
1:A5:361:GLN:O	1:A5:363:PRO:HD2	1.96	0.65
19:2:101:U:C1'	46:l:66:SER:H	2.06	0.65
25:A:90:GLY:HA3	36:v:209:PRO:CG	2.25	0.65
19:2:136:G:C3'	43:h:87:SER:N	2.55	0.65
7:B:47:LYS:O	19:2:163:G:O2'	2.07	0.64
19:2:34:U:P	31:u:509:PRO:HB3	2.38	0.64
25:A:1603:ALA:HB1	25:A:2285:GLY:HA3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:2:35:A:OP2	31:u:513:LYS:CB	2.45	0.64
31:u:607:ALA:CB	40:Y:87:ILE:O	2.45	0.64
5:D:86:PHE:HA	5:D:111:ALA:HB1	1.79	0.64
31:u:599:ASN:O	31:u:603:ALA:HB2	1.98	0.64
7:B:53:PHE:CB	19:2:165:A:C2	2.78	0.64
31:u:847:ALA:O	31:u:851:SER:CB	2.46	0.64
31:u:1107:GLN:C	31:u:1109:ARG:H	2.06	0.64
34:w:15:VAL:O	34:w:58:PHE:HA	1.98	0.64
49:g:86:LYS:O	49:g:90:LYS:CB	2.46	0.63
31:u:1257:PRO:HG3	32:T:481:THR:O	1.98	0.63
25:A:1587:GLU:CB	25:A:2060:SER:CB	2.76	0.63
11:5:13:C:C4	11:5:65:G:N1	2.67	0.63
29:4:472:GLN:H	29:4:473:PRO:CD	2.05	0.63
29:4:483:SER:C	33:E:974:LYS:C	2.66	0.63
39:r:139:HIS:C	53:r:1500:GTP:H5''	2.21	0.63
4:F:61:THR:CB	19:2:40:C:C5'	2.76	0.63
19:2:103:U:OP1	45:m:75:GLU:HA	1.99	0.63
18:J:48:THR:CB	18:J:58:ASN:HA	2.28	0.62
29:4:356:ARG:O	49:n:75:PRO:HG3	1.98	0.62
4:F:50:HIS:CB	31:u:1140:GLU:CA	2.75	0.62
24:Z:77:G:H2'	24:Z:78:A:H8	1.64	0.62
1:A5:363:PRO:CD	1:A5:364:ALA:N	2.56	0.62
19:2:85:A:H5''	49:n:9:LYS:HA	1.82	0.62
23:G:382:PRO:CD	23:G:383:ARG:N	2.61	0.62
37:0:255:PRO:HG2	37:0:276:HIS:CA	2.29	0.62
31:u:713:ALA:HA	31:u:716:ALA:HB3	1.82	0.62
23:G:382:PRO:CG	23:G:425:GLY:HA3	2.29	0.62
25:A:1870:ASP:CB	25:A:1871:PRO:HD3	2.30	0.62
11:5:92:U:OP1	49:g:63:ASN:CB	2.48	0.62
19:2:103:U:C5	45:m:37:HIS:O	2.53	0.62
40:Y:106:TRP:N	40:Y:107:PRO:HD2	2.14	0.62
31:u:812:PRO:HB2	31:u:813:PRO:HD3	1.81	0.62
37:0:255:PRO:HG2	37:0:276:HIS:HA	1.82	0.61
25:A:1605:GLU:O	25:A:1634:SER:N	2.33	0.61
31:u:1210:HIS:CB	32:T:585:THR:H	2.12	0.61
1:A5:365:PRO:HB2	1:A5:366:PRO:HD2	1.81	0.61
4:F:60:LEU:O	19:2:40:C:OP1	2.19	0.61
32:T:612:GLU:O	32:T:615:ILE:N	2.33	0.61
33:E:428:GLY:HA3	33:E:433:SER:HA	1.83	0.61
31:u:648:LEU:O	31:u:651:VAL:N	2.33	0.61
44:b:7:PRO:HB3	44:b:38:GLY:HA2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:135:VAL:N	25:A:420:ARG:O	2.33	0.61
29:4:473:PRO:HG3	33:E:979:ARG:C	2.25	0.61
11:5:13:C:C4	11:5:65:G:C6	2.88	0.61
39:r:311:SER:O	39:r:315:SER:N	2.33	0.61
34:w:14:THR:CA	34:w:59:VAL:O	2.27	0.61
17:H:53:ASP:HA	17:H:68:LYS:O	2.01	0.60
31:u:1214:TYR:CB	32:T:591:TYR:CB	2.75	0.60
1:A5:490:GLU:C	1:A5:492:SER:H	2.07	0.60
19:2:102:U:O3'	45:m:75:GLU:CB	2.49	0.60
40:Y:89:LEU:O	40:Y:98:ALA:HB2	1.99	0.60
39:r:139:HIS:HA	53:r:1500:GTP:O3A	1.99	0.60
44:i:30:LYS:O	44:i:47:THR:HA	2.00	0.60
19:2:100:U:O2	47:k:64:GLY:CA	2.49	0.60
3:z:55:GLU:CB	31:u:476:ASP:CA	2.79	0.60
33:E:192:ALA:C	35:x:74:GLN:CB	2.74	0.60
37:0:270:LEU:CB	37:0:271:PRO:HD3	2.32	0.60
4:F:50:HIS:CB	31:u:1140:GLU:H	2.08	0.60
19:2:44:U:C2	24:Z:144:A:C2	2.90	0.59
19:2:34:U:OP1	31:u:509:PRO:C	2.45	0.59
19:2:44:U:C2	24:Z:144:A:N1	2.67	0.59
24:Z:67:C:H2'	24:Z:68:U:C6	2.37	0.59
39:r:139:HIS:CA	53:r:1500:GTP:O3B	2.45	0.59
3:z:97:ALA:C	3:z:99:GLN:H	2.10	0.59
29:4:470:ARG:C	33:E:1019:ASN:CB	2.75	0.59
15:9:46:TYR:HA	15:9:51:ASN:O	2.03	0.59
24:Z:74:G:H3'	24:Z:75:U:H5'	1.83	0.59
40:Y:104:GLU:C	40:Y:107:PRO:HD2	2.28	0.59
22:y:84:GLY:O	22:y:86:PRO:HD3	2.02	0.59
30:A4:728:ALA:CB	30:A4:763:ILE:CA	2.81	0.59
19:2:103:U:H5	45:m:37:HIS:O	1.86	0.59
29:4:485:ASN:CA	33:E:974:LYS:CB	2.80	0.59
18:J:48:THR:CB	18:J:57:LYS:O	2.51	0.58
27:P:180:PRO:HB2	41:6:26:U:O2'	2.02	0.58
8:s:1383:GLU:CB	8:s:1654:MET:O	2.51	0.58
19:2:45:C:C4	24:Z:144:A:C2	2.90	0.58
1:A5:488:GLY:O	1:A5:490:GLU:N	2.27	0.58
25:A:1777:ILE:HA	25:A:1858:PRO:O	2.03	0.58
25:A:91:ALA:HB2	36:v:207:MET:HA	0.59	0.58
1:A5:488:GLY:C	1:A5:490:GLU:N	2.62	0.58
5:D:104:THR:CA	11:5:6:C:H4'	2.29	0.58
11:5:9:G:H2'	11:5:9:G:OP2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:2:60:U:C6	19:2:60:U:C5'	2.86	0.58
12:L:77:LEU:HA	36:v:288:ALA:HB2	1.85	0.58
12:L:86:ALA:HB3	12:L:87:PRO:HD3	1.85	0.58
25:A:1930:TYR:CB	25:A:2247:ASN:CB	2.82	0.58
7:B:41:VAL:HA	19:2:167:U:O4	2.04	0.58
16:C:14:PRO:O	16:C:72:PRO:HD3	2.03	0.58
31:u:646:PRO:CB	40:Y:73:ASN:CB	2.81	0.57
37:0:270:LEU:CB	37:0:271:PRO:CD	2.83	0.57
36:v:188:PHE:O	36:v:192:ALA:HB2	2.03	0.57
3:z:98:PHE:O	3:z:100:LYS:N	2.38	0.57
24:Z:55:A:H2'	24:Z:56:A:H8	1.68	0.57
19:2:71:C:H2'	19:2:72:U:H6	1.70	0.56
34:w:25:SER:CA	34:w:27:PRO:HD2	2.34	0.56
49:g:19:LEU:HA	49:g:65:ILE:HA	1.87	0.56
11:5:109:C:H2'	11:5:110:A:H8	1.70	0.56
19:2:43:U:C2	24:Z:146:G:C2	2.93	0.56
19:2:71:C:C2	19:2:72:U:C5	2.94	0.56
19:2:72:U:H2'	19:2:73:C:H6	1.71	0.56
19:2:85:A:H4'	49:n:8:MET:O	2.05	0.56
19:2:181:G:H1'	46:l:52:ASP:HA	1.88	0.56
24:Z:54:G:O2'	24:Z:55:A:H5''	2.03	0.56
25:A:1926:THR:O	25:A:2253:PRO:CB	2.54	0.56
19:2:33:G:O3'	31:u:509:PRO:HB3	2.06	0.56
1:A5:382:LEU:C	1:A5:384:PRO:HD3	2.31	0.56
19:2:70:C:H2'	19:2:71:C:H6	1.71	0.56
19:2:72:U:C2	19:2:73:C:C5	2.94	0.56
22:y:16:GLY:HA2	33:E:156:SER:CB	2.36	0.56
1:A5:142:ALA:HB3	1:A5:143:PRO:HD3	1.87	0.56
1:A5:258:SER:O	30:A4:766:MET:N	2.31	0.56
8:s:1043:ARG:O	25:A:2316:ASN:O	2.24	0.56
19:2:68:G:H2'	19:2:69:U:H6	1.70	0.56
19:2:70:C:C2	19:2:71:C:C5	2.94	0.56
24:Z:75:U:H2'	24:Z:76:A:C8	2.39	0.56
11:5:109:C:OP1	49:g:49:ASN:O	2.24	0.55
19:2:83:A:H2'	19:2:84:C:H6	1.70	0.55
24:Z:152:C:O5'	31:u:1105:GLU:CB	2.55	0.55
25:A:1271:MET:O	25:A:1273:TYR:N	2.39	0.55
35:x:6:THR:O	35:x:8:HIS:N	2.39	0.55
19:2:100:U:C2	47:k:64:GLY:N	2.74	0.55
33:E:442:LEU:CB	33:E:771:GLY:HA3	2.36	0.55
19:2:69:U:C2	19:2:70:C:C5	2.94	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:2:105:G:C2	49:n:20:LYS:CB	2.89	0.55
27:P:180:PRO:HG3	41:6:26:U:O2'	2.02	0.55
5:D:267:PHE:O	5:D:269:PRO:HD3	2.06	0.55
31:u:944:SER:HA	31:u:948:ARG:CB	2.36	0.55
19:2:83:A:C4	19:2:84:C:C5	2.95	0.55
25:A:1628:ASP:N	25:A:1662:ILE:O	2.38	0.55
1:A5:365:PRO:HB2	1:A5:366:PRO:CD	2.37	0.55
11:5:109:C:H2'	11:5:110:A:C8	2.42	0.55
19:2:68:G:C4	19:2:69:U:C5	2.94	0.55
1:A5:191:GLU:C	1:A5:193:ASP:H	2.15	0.54
22:y:3:LYS:CA	24:Z:154:U:O3'	2.55	0.54
19:2:69:U:H2'	19:2:70:C:H6	1.71	0.54
24:Z:66:C:O2'	24:Z:67:C:H5'	2.07	0.54
25:A:1870:ASP:CB	25:A:1871:PRO:CD	2.86	0.54
19:2:85:A:H5'	49:n:9:LYS:CA	2.35	0.54
33:E:3:LEU:HA	33:E:1131:PRO:HA	1.89	0.54
4:F:61:THR:CB	19:2:40:C:H4'	2.38	0.54
24:Z:77:G:H2'	24:Z:78:A:C8	2.43	0.54
30:A4:751:ALA:O	30:A4:755:ALA:HB2	2.07	0.54
31:u:1130:PRO:HB2	32:T:528:ILE:CB	2.38	0.54
37:0:255:PRO:CG	37:0:276:HIS:HA	2.38	0.54
19:2:101:U:O5'	46:l:66:SER:CB	2.53	0.53
23:G:382:PRO:HB3	23:G:425:GLY:N	2.23	0.53
31:u:599:ASN:O	31:u:603:ALA:CB	2.57	0.53
31:u:1010:THR:O	31:u:1012:PRO:HD3	2.08	0.53
19:2:151:C:H2'	19:2:152:G:H8	1.74	0.53
5:D:265:ARG:CB	5:D:270:LYS:N	2.69	0.53
23:G:381:HIS:CB	23:G:382:PRO:HD3	2.39	0.53
19:2:60:U:H6	19:2:60:U:O5'	1.91	0.53
25:A:90:GLY:HA3	36:v:209:PRO:HD3	1.91	0.53
29:4:354:GLU:N	49:n:78:THR:CB	2.72	0.53
29:4:485:ASN:CB	33:E:974:LYS:CB	2.86	0.53
27:P:173:CYS:HA	41:6:28:A:C6	2.34	0.53
33:E:336:ALA:HA	33:E:351:SER:HA	1.91	0.53
42:A6:153:TYR:O	42:A6:154:ARG:CB	2.56	0.53
19:2:35:A:P	31:u:513:LYS:CB	2.97	0.53
5:D:164:PRO:O	5:D:181:ILE:CB	2.57	0.53
31:u:1210:HIS:CB	32:T:585:THR:N	2.71	0.52
1:A5:362:LEU:CB	1:A5:363:PRO:HD3	2.38	0.52
1:A5:258:SER:CB	30:A4:766:MET:N	2.64	0.52
1:A5:363:PRO:HB3	1:A5:752:LEU:CB	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:A4:728:ALA:HB2	30:A4:763:ILE:HA	1.92	0.52
11:5:98:C:H2'	11:5:99:C:C6	2.44	0.52
17:H:36:ILE:HA	17:H:55:THR:O	2.10	0.52
20:A3:30:PHE:HA	20:A3:35:ASN:O	2.10	0.52
2:A2:45:ASN:O	17:H:14:PRO:HG2	2.10	0.52
33:E:637:PRO:HA	33:E:669:LEU:HA	1.92	0.52
40:Y:106:TRP:N	40:Y:107:PRO:CD	2.72	0.52
42:A6:149:TYR:CB	55:A6:301:GTG:C5E	2.87	0.52
19:2:120:A:N1	19:2:137:U:O4	2.43	0.52
1:A5:141:ALA:O	1:A5:144:SER:N	2.43	0.52
5:D:104:THR:CB	11:5:6:C:H5''	2.39	0.52
19:2:101:U:H1'	46:l:65:GLY:C	2.34	0.51
25:A:1558:THR:O	25:A:1560:ILE:N	2.43	0.51
39:r:195:GLY:O	46:e:8:LYS:HA	2.10	0.51
8:s:592:LYS:CB	25:A:2335:ALA:H	2.23	0.51
19:2:43:U:C4	24:Z:146:G:N2	2.78	0.51
32:T:519:LYS:CB	32:T:520:PRO:CD	2.89	0.51
11:5:90:U:O4	45:f:39:ASN:CB	2.58	0.51
25:A:2125:ALA:HA	25:A:2179:HIS:HA	1.93	0.51
31:u:669:GLN:O	31:u:672:ALA:N	2.43	0.51
6:W:81:GLU:HA	6:W:108:PRO:HB3	1.92	0.51
19:2:38:A:O2'	19:2:39:U:O4'	2.14	0.51
29:4:470:ARG:C	33:E:980:LYS:O	2.54	0.51
25:A:1392:LYS:O	25:A:1396:ALA:N	2.41	0.51
1:A5:51:GLU:O	1:A5:54:ALA:HB3	2.10	0.51
30:A4:728:ALA:CB	30:A4:763:ILE:HA	2.40	0.51
33:E:916:ASN:CB	33:E:917:PRO:HD3	2.41	0.51
11:5:44:A:H8	24:Z:55:A:C2	2.26	0.51
25:A:1837:ALA:O	25:A:1840:LYS:N	2.44	0.51
1:A5:358:GLU:O	1:A5:365:PRO:CG	2.54	0.50
22:y:4:HIS:CB	24:Z:156:U:H4'	2.42	0.50
25:A:91:ALA:HB1	36:v:207:MET:CB	2.21	0.50
34:w:16:TYR:HA	34:w:57:GLY:O	2.10	0.50
34:w:34:LEU:HA	34:w:37:GLY:O	2.11	0.50
11:5:99:C:H2'	11:5:100:U:C6	2.47	0.50
45:f:16:ARG:HA	45:f:30:THR:HA	1.92	0.50
1:A5:490:GLU:C	1:A5:492:SER:N	2.70	0.50
11:5:90:U:O2	45:f:74:GLY:CA	2.59	0.50
25:A:133:PRO:O	25:A:420:ARG:HA	2.11	0.50
25:A:2068:SER:C	25:A:2070:LYS:H	2.19	0.50
5:D:104:THR:CB	11:5:7:U:P	3.00	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:2:100:U:O2	47:k:64:GLY:C	2.54	0.50
29:4:470:ARG:CB	33:E:1018:GLU:C	2.84	0.50
48:j:32:GLN:N	48:j:88:GLN:O	2.44	0.50
11:5:90:U:O2	45:f:74:GLY:N	2.45	0.50
24:Z:61:A:H2'	24:Z:62:A:O4'	2.11	0.50
29:4:353:GLY:O	49:n:78:THR:CB	2.60	0.50
29:4:470:ARG:O	33:E:980:LYS:O	2.29	0.50
8:s:1045:PRO:HB3	25:A:2314:PHE:CA	2.41	0.50
25:A:90:GLY:HA3	36:v:209:PRO:CD	2.41	0.50
33:E:1012:VAL:HA	33:E:1023:ILE:HA	1.94	0.50
8:s:1385:LEU:CB	8:s:1651:CYS:HA	2.41	0.50
11:5:11:U:OP1	25:A:221:ASN:O	2.30	0.50
18:J:29:ASP:O	18:J:49:GLU:HA	2.12	0.50
31:u:1132:LEU:O	31:u:1135:GLU:N	2.45	0.50
32:T:611:ASP:O	32:T:614:ARG:CB	2.60	0.50
9:Q:122:PRO:O	9:Q:126:LEU:N	2.45	0.49
24:Z:56:A:O2'	24:Z:57:C:H5'	2.12	0.49
11:5:97:G:H2'	11:5:98:C:H6	1.77	0.49
25:A:1777:ILE:HA	25:A:1859:LYS:O	2.11	0.49
31:u:1130:PRO:HB3	32:T:528:ILE:CA	2.43	0.49
27:P:32:PRO:O	36:v:195:ARG:HA	2.13	0.49
19:2:100:U:H1'	47:k:65:ASN:CA	2.42	0.49
24:Z:53:C:O2'	24:Z:54:G:H5'	2.12	0.49
33:E:189:TYR:CB	35:x:73:LEU:HA	2.42	0.49
46:l:23:ASN:N	46:l:67:LYS:O	2.46	0.49
2:A2:34:SER:O	2:A2:51:THR:HA	2.13	0.49
8:s:1382:MET:CB	8:s:1650:LEU:HA	2.43	0.49
1:A5:177:LEU:HA	1:A5:181:GLY:H	1.77	0.49
29:4:470:ARG:CB	33:E:1019:ASN:CA	2.85	0.49
31:u:1241:ILE:O	33:E:1169:PRO:HG2	2.13	0.49
33:E:380:GLU:O	33:E:383:ASP:N	2.46	0.49
29:4:473:PRO:HB3	33:E:978:LEU:CB	2.39	0.49
33:E:189:TYR:CB	35:x:73:LEU:CA	2.90	0.49
40:Y:49:LYS:N	40:Y:50:PRO:HD2	2.27	0.49
11:5:97:G:H2'	11:5:98:C:C6	2.48	0.48
32:T:471:ARG:N	32:T:472:PRO:HD3	2.25	0.48
31:u:1213:ASN:C	32:T:590:LEU:HA	2.33	0.48
12:L:86:ALA:HB3	12:L:87:PRO:CD	2.44	0.48
25:A:2068:SER:C	25:A:2070:LYS:N	2.70	0.48
38:N:98:HIS:O	38:N:102:LYS:N	2.46	0.48
39:r:718:PHE:O	39:r:723:ASP:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:2:33:G:O3'	31:u:509:PRO:CB	2.62	0.48
25:A:1846:ALA:HB2	25:A:1875:HIS:CB	2.43	0.48
29:4:357:GLU:HA	49:n:75:PRO:CG	2.40	0.48
1:A5:365:PRO:CB	1:A5:366:PRO:CD	2.91	0.48
24:Z:65:G:O2'	24:Z:66:C:H5'	2.14	0.48
25:A:1858:PRO:O	25:A:1859:LYS:C	2.57	0.48
32:T:652:GLY:N	32:T:655:SER:O	2.46	0.48
33:E:207:THR:HA	33:E:227:PRO:HA	1.96	0.48
19:2:120:A:N1	19:2:137:U:C4	2.82	0.48
11:5:68:C:O2	11:5:68:C:H3'	2.13	0.48
1:A5:251:ARG:O	30:A4:748:SER:CB	2.61	0.48
33:E:732:THR:CB	33:E:771:GLY:O	2.62	0.48
48:j:63:GLU:O	48:j:71:ARG:HA	2.14	0.48
22:y:21:ARG:HA	22:y:68:ASP:HA	1.94	0.47
25:A:119:LEU:N	25:A:128:PHE:O	2.44	0.47
29:4:409:GLU:HA	29:4:413:ASN:HA	1.96	0.47
11:5:98:C:H2'	11:5:99:C:H6	1.79	0.47
14:V:13:LYS:HA	23:G:181:LYS:CB	2.45	0.47
31:u:535:ILE:O	31:u:538:LEU:N	2.47	0.47
27:P:167:PHE:CB	41:6:28:A:N7	2.78	0.47
8:s:726:HIS:HA	8:s:813:ALA:HB2	1.96	0.47
24:Z:70:G:C6	24:Z:71:C:H1'	2.50	0.47
29:4:354:GLU:HA	49:n:78:THR:CB	2.45	0.47
31:u:1107:GLN:C	31:u:1109:ARG:N	2.73	0.47
27:P:166:SER:CB	41:6:30:A:O4'	2.63	0.47
19:2:83:A:H2'	19:2:84:C:C6	2.49	0.47
19:2:124:G:H2'	19:2:125:G:C8	2.49	0.47
45:m:69:LEU:O	46:l:73:LEU:N	2.40	0.47
31:u:862:GLU:O	31:u:865:ARG:N	2.48	0.46
11:5:37:G:H21	21:K:386:SER:HA	1.80	0.46
31:u:728:LEU:O	31:u:731:LEU:N	2.48	0.46
11:5:110:A:H2'	11:5:111:A:C8	2.50	0.46
19:2:39:U:C4	24:Z:149:A:N6	2.83	0.46
19:2:101:U:O4	47:k:38:MET:CB	2.64	0.46
25:A:1955:LYS:O	25:A:1956:PRO:C	2.58	0.46
48:j:44:GLU:O	48:j:61:ALA:HA	2.15	0.46
19:2:69:U:H2'	19:2:70:C:C6	2.49	0.46
19:2:100:U:H1'	47:k:65:ASN:N	2.31	0.46
32:T:630:PRO:HA	32:T:631:PRO:HD3	1.77	0.46
19:2:60:U:C6	19:2:60:U:H5''	2.50	0.46
19:2:68:G:H2'	19:2:69:U:C6	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:2:70:C:H2'	19:2:71:C:C6	2.49	0.46
48:j:36:TYR:N	48:j:83:ASN:O	2.45	0.46
1:A5:131:LEU:O	1:A5:132:SER:C	2.59	0.46
1:A5:240:LYS:C	1:A5:242:ASP:H	2.24	0.46
4:F:61:THR:HA	19:2:40:C:P	2.55	0.46
8:s:419:GLY:HA2	8:s:621:HIS:HA	1.98	0.46
20:A3:17:THR:HA	20:A3:66:ASN:O	2.16	0.46
33:E:37:ILE:HA	33:E:57:GLU:HA	1.98	0.46
11:5:93:U:C5	44:b:39:TYR:CB	2.99	0.46
33:E:796:ASN:HA	33:E:871:PRO:HD3	1.97	0.46
5:D:282:HIS:HA	5:D:304:SER:HA	1.98	0.46
7:B:182:LEU:O	7:B:184:PRO:HD3	2.15	0.46
33:E:62:ILE:HA	33:E:82:SER:HA	1.97	0.46
1:A5:50:LEU:O	1:A5:54:ALA:HB2	2.16	0.46
3:z:97:ALA:C	3:z:99:GLN:N	2.73	0.46
4:F:50:HIS:C	31:u:1140:GLU:CB	2.88	0.46
5:D:104:THR:O	11:5:6:C:C4'	2.54	0.46
31:u:1125:PRO:O	31:u:1128:VAL:N	2.49	0.46
31:u:1130:PRO:HB3	32:T:528:ILE:HA	1.98	0.46
33:E:43:PRO:HA	33:E:50:VAL:HA	1.97	0.46
1:A5:61:LEU:N	1:A5:62:PRO:CD	2.79	0.45
25:A:2231:THR:O	25:A:2235:TYR:N	2.45	0.45
31:u:501:LEU:O	31:u:504:ILE:N	2.48	0.45
19:2:81:G:H2'	19:2:82:G:H8	1.81	0.45
25:A:1856:GLU:O	25:A:1857:GLN:C	2.58	0.45
29:4:473:PRO:CD	33:E:980:LYS:HA	2.46	0.45
33:E:785:PRO:HA	33:E:801:GLU:HA	1.98	0.45
1:A5:182:LYS:HA	1:A5:244:TRP:CB	2.46	0.45
8:s:1223:ILE:HA	8:s:1270:VAL:HA	1.99	0.45
25:A:334:THR:O	25:A:336:ASN:N	2.49	0.45
1:A5:495:LEU:HA	1:A5:496:PRO:HD3	1.85	0.45
5:D:104:THR:CA	11:5:6:C:H5''	2.44	0.45
19:2:85:A:H5'	49:n:9:LYS:CB	2.47	0.45
19:2:120:A:C6	19:2:137:U:O4	2.69	0.45
41:6:59:G:O6	41:6:76:A:C6	2.70	0.45
1:A5:273:PRO:HA	1:A5:274:PRO:HD3	1.88	0.45
19:2:60:U:O2	19:2:60:U:H2'	2.16	0.45
25:A:602:ILE:O	25:A:606:LYS:N	2.47	0.45
33:E:1045:ALA:HA	33:E:1055:VAL:HA	1.99	0.45
1:A5:97:ASN:O	1:A5:98:TYR:C	2.60	0.45
18:J:33:VAL:O	18:J:45:LEU:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:s:1186:LEU:HA	8:s:1204:ILE:HA	1.99	0.45
19:2:72:U:H2'	19:2:73:C:C6	2.50	0.45
19:2:80:A:H2'	19:2:81:G:H8	1.81	0.45
25:A:798:GLY:O	25:A:800:TYR:N	2.50	0.45
17:H:26:ILE:O	17:H:37:VAL:HA	2.17	0.45
38:N:82:CYS:O	38:N:86:ASP:N	2.49	0.45
39:r:141:GLY:H	53:r:1500:GTP:H5'	1.82	0.45
1:A5:124:ALA:O	1:A5:127:LEU:N	2.50	0.45
1:A5:258:SER:C	30:A4:766:MET:H	2.24	0.45
1:A5:507:ALA:HB1	1:A5:512:ALA:HB2	1.99	0.45
5:D:126:SER:O	5:D:133:VAL:HA	2.17	0.45
19:2:79:G:H2'	19:2:80:A:H8	1.81	0.45
19:2:84:C:H2'	19:2:85:A:H8	1.82	0.45
31:u:810:ILE:O	31:u:813:PRO:HD2	2.17	0.45
33:E:970:TYR:HA	33:E:979:ARG:HA	1.99	0.45
18:J:35:ALA:HB3	18:J:44:ALA:CB	2.47	0.44
19:2:39:U:O4	24:Z:149:A:N6	2.49	0.44
19:2:100:U:O3'	47:k:65:ASN:CB	2.64	0.44
27:P:180:PRO:CB	41:6:26:U:HO2'	2.28	0.44
1:A5:27:THR:O	1:A5:28:GLU:C	2.61	0.44
1:A5:157:GLN:O	1:A5:158:GLU:C	2.60	0.44
19:2:40:C:C5	24:Z:149:A:N6	2.85	0.44
19:2:45:C:N4	24:Z:144:A:N1	2.64	0.44
31:u:762:ALA:O	31:u:766:THR:CB	2.65	0.44
33:E:642:ILE:HA	33:E:665:LEU:HA	2.00	0.44
19:2:71:C:H2'	19:2:72:U:C6	2.50	0.44
19:2:166:G:N2	19:2:166:G:OP2	2.50	0.44
34:w:67:ALA:HA	34:w:70:ALA:HB3	2.00	0.44
19:2:34:U:OP1	31:u:509:PRO:CA	2.63	0.44
27:P:173:CYS:CB	41:6:28:A:H62	2.28	0.44
19:2:82:G:H2'	19:2:83:A:H8	1.82	0.44
25:A:986:GLU:HA	25:A:1029:GLY:HA3	1.98	0.44
23:G:381:HIS:CB	23:G:382:PRO:CD	2.94	0.44
23:G:381:HIS:CB	23:G:387:PHE:CB	2.95	0.44
32:T:611:ASP:O	32:T:614:ARG:N	2.50	0.44
45:f:18:ARG:N	45:f:81:THR:O	2.39	0.44
16:C:39:ASN:HA	16:C:59:CYS:O	2.16	0.44
33:E:255:TYR:HA	33:E:270:PRO:HA	2.00	0.44
19:2:60:U:C5	19:2:60:U:OP2	2.70	0.44
39:r:686:THR:N	39:r:793:ASP:O	2.46	0.44
48:j:57:VAL:HA	48:j:77:ILE:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A5:223:HIS:HA	1:A5:224:PRO:HD3	1.66	0.44
4:F:50:HIS:CA	31:u:1139:PRO:HG2	2.43	0.44
39:r:895:ALA:O	39:r:897:SER:N	2.51	0.44
11:5:73:C:H2'	11:5:74:U:H6	1.83	0.43
39:r:139:HIS:CA	53:r:1500:GTP:O3A	2.65	0.43
1:A5:256:PHE:O	1:A5:261:CYS:CA	2.66	0.43
3:z:46:ARG:N	3:z:63:VAL:O	2.50	0.43
1:A5:26:GLU:O	1:A5:29:ASP:N	2.51	0.43
7:B:84:ALA:HB1	19:2:165:A:H61	1.83	0.43
19:2:144:C:H2'	19:2:145:A:H2'	2.00	0.43
43:h:30:SER:O	43:h:34:GLN:N	2.45	0.43
11:5:66:A:H2'	11:5:67:A:C4'	2.49	0.43
11:5:107:G:H3'	11:5:108:G:H8	1.82	0.43
29:4:473:PRO:CG	33:E:980:LYS:HA	2.48	0.43
33:E:931:VAL:N	33:E:936:LYS:O	2.50	0.43
1:A5:93:LEU:C	1:A5:95:ALA:N	2.76	0.43
11:5:74:U:H2'	11:5:75:G:C8	2.52	0.43
17:H:60:THR:N	17:H:61:PRO:HD2	2.33	0.43
25:A:90:GLY:HA2	36:v:209:PRO:HG3	1.97	0.43
45:f:15:TYR:O	45:f:31:PHE:N	2.42	0.43
1:A5:473:PHE:O	1:A5:474:SER:C	2.61	0.43
25:A:948:PRO:HG2	25:A:949:PRO:HD3	2.01	0.43
25:A:957:GLN:O	25:A:961:ASN:N	2.45	0.43
32:T:643:PRO:HG2	34:w:66:ASP:HA	2.01	0.43
33:E:440:HIS:HA	33:E:774:PHE:HA	2.01	0.43
11:5:109:C:OP2	49:g:49:ASN:O	2.37	0.43
18:J:50:GLU:HA	18:J:55:GLN:C	2.44	0.43
24:Z:61:A:H2'	24:Z:62:A:C8	2.54	0.43
5:D:333:VAL:HA	5:D:343:ILE:O	2.19	0.43
25:A:1809:ILE:O	25:A:1818:PHE:N	2.44	0.43
25:A:1947:ASN:O	25:A:1951:LYS:CB	2.67	0.43
31:u:1167:TYR:CB	32:T:582:PRO:CD	2.97	0.43
3:z:114:LYS:HA	3:z:119:ILE:O	2.19	0.43
11:5:37:G:N2	21:K:386:SER:HA	2.34	0.43
1:A5:88:THR:O	1:A5:91:GLY:N	2.46	0.42
31:u:1120:ALA:HB1	31:u:1125:PRO:HB3	2.01	0.42
31:u:1210:HIS:CB	32:T:585:THR:CA	2.97	0.42
49:g:16:THR:HA	49:g:26:HIS:HA	2.00	0.42
11:5:108:G:O3'	49:g:50:ARG:HA	2.19	0.42
19:2:151:C:H2'	19:2:152:G:C8	2.53	0.42
20:A3:43:GLU:O	20:A3:53:GLU:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:u:707:LEU:O	31:u:710:ALA:HB3	2.19	0.42
33:E:888:ALA:HA	33:E:909:VAL:HA	2.01	0.42
1:A5:183:GLU:C	1:A5:185:TYR:H	2.25	0.42
4:F:50:HIS:C	31:u:1140:GLU:HA	2.45	0.42
11:5:89:U:H1'	46:e:66:SER:CB	2.49	0.42
33:E:1052:ASN:HA	33:E:1096:HIS:HA	2.01	0.42
1:A5:338:SER:O	1:A5:339:TYR:C	2.63	0.42
5:D:94:ASN:O	5:D:98:ASP:CB	2.68	0.42
31:u:1298:TYR:CB	33:E:916:ASN:O	2.67	0.42
18:J:31:ARG:O	18:J:47:GLN:CB	2.67	0.42
25:A:2216:CYS:HA	25:A:2225:LEU:HA	2.01	0.42
32:T:614:ARG:O	32:T:618:GLY:N	2.51	0.42
40:Y:49:LYS:N	40:Y:50:PRO:CD	2.83	0.42
10:A1:128:GLY:HA3	10:A1:132:GLY:O	2.19	0.42
20:A3:42:HIS:HA	20:A3:54:GLN:O	2.20	0.42
31:u:722:GLU:O	31:u:725:ASP:CB	2.67	0.42
31:u:1258:ALA:C	31:u:1260:LYS:H	2.27	0.42
33:E:92:TYR:HA	33:E:99:PHE:HA	2.00	0.42
8:s:1433:ASP:O	8:s:1437:ARG:CB	2.68	0.42
21:K:304:ILE:O	21:K:308:ARG:N	2.52	0.42
25:A:802:THR:O	25:A:806:ALA:N	2.48	0.42
32:T:494:THR:O	33:E:1083:ASN:CB	2.68	0.42
33:E:436:ARG:HA	33:E:778:ALA:HA	2.02	0.42
33:E:456:PRO:HA	33:E:478:PHE:HA	2.02	0.42
49:n:14:THR:HA	49:n:28:THR:HA	2.02	0.42
1:A5:141:ALA:O	1:A5:142:ALA:C	2.63	0.42
1:A5:258:SER:CA	30:A4:766:MET:CA	2.77	0.42
5:D:264:VAL:O	5:D:269:PRO:HB3	2.20	0.42
19:2:100:U:H3	47:k:64:GLY:H	1.67	0.42
33:E:1059:PRO:HA	33:E:1060:PRO:HD3	1.95	0.42
21:K:345:GLY:HA3	50:q:34:GLN:HA	2.02	0.41
45:m:26:ILE:O	45:m:47:GLU:HA	2.20	0.41
1:A5:55:GLY:O	1:A5:58:GLU:N	2.52	0.41
4:F:61:THR:CA	19:2:40:C:P	3.08	0.41
33:E:209:THR:HA	33:E:225:SER:HA	2.02	0.41
1:A5:240:LYS:C	1:A5:242:ASP:N	2.79	0.41
4:F:50:HIS:C	31:u:1140:GLU:CA	2.93	0.41
11:5:73:C:H2'	11:5:74:U:C6	2.55	0.41
19:2:60:U:C6	19:2:60:U:O5'	2.72	0.41
31:u:607:ALA:HB1	40:Y:87:ILE:O	2.17	0.41
41:6:59:G:C6	41:6:76:A:N1	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:u:1167:TYR:CB	32:T:582:PRO:HD2	2.50	0.41
1:A5:55:GLY:O	1:A5:56:VAL:C	2.63	0.41
11:5:75:G:H2'	11:5:76:A:C8	2.55	0.41
29:4:353:GLY:HA3	49:n:78:THR:N	2.35	0.41
34:w:67:ALA:O	34:w:70:ALA:HB3	2.20	0.41
1:A5:199:THR:O	1:A5:200:GLU:C	2.62	0.41
31:u:699:GLN:O	31:u:700:LYS:C	2.63	0.41
8:s:1221:PHE:HA	8:s:1272:SER:HA	2.02	0.41
17:H:13:LEU:HA	17:H:14:PRO:HD3	1.95	0.41
18:J:35:ALA:HB3	18:J:44:ALA:HB3	2.03	0.41
30:A4:735:MET:CB	30:A4:754:HIS:CB	2.99	0.41
8:s:1045:PRO:HB3	25:A:2314:PHE:CB	2.51	0.41
11:5:5:U:H2'	11:5:6:C:C6	2.56	0.41
29:4:483:SER:O	33:E:974:LYS:C	2.56	0.41
19:2:33:G:O6	24:Z:156:U:O4	2.39	0.41
1:A5:80:PRO:C	1:A5:82:LYS:H	2.29	0.40
4:F:71:ALA:HB2	12:L:14:THR:CB	2.51	0.40
11:5:91:U:O4	49:g:37:ASN:CB	2.69	0.40
11:5:100:U:H2'	11:5:101:U:C6	2.56	0.40
19:2:45:C:C2'	29:4:395:TRP:CB	2.93	0.40
20:A3:39:ASP:HA	20:A3:58:GLY:O	2.20	0.40
24:Z:70:G:O6	41:6:35:A:N7	2.54	0.40
31:u:650:ALA:HA	40:Y:69:GLU:HA	1.85	0.40
5:D:266:PRO:O	5:D:267:PHE:CB	2.69	0.40
9:Q:90:ALA:HB1	11:5:67:A:OP1	2.21	0.40
19:2:152:G:H2'	19:2:153:A:H8	1.87	0.40
21:K:347:PHE:CB	50:q:33:ALA:O	2.69	0.40
23:G:290:ALA:O	23:G:308:ARG:N	2.54	0.40
2:A2:57:ASP:O	2:A2:62:TYR:HA	2.20	0.40
5:D:265:ARG:HA	5:D:266:PRO:HD2	1.70	0.40
10:A1:7:LYS:O	10:A1:9:LEU:N	2.54	0.40
33:E:743:SER:O	33:E:755:VAL:N	2.52	0.40
34:w:17:VAL:CA	34:w:85:ARG:O	2.45	0.40
1:A5:258:SER:C	30:A4:766:MET:N	2.79	0.40
5:D:265:ARG:O	5:D:269:PRO:HA	2.21	0.40
25:A:1609:VAL:H	25:A:2066:THR:H	1.67	0.40
1:A5:80:PRO:C	1:A5:82:LYS:N	2.79	0.40
1:A5:728:CYS:C	1:A5:730:THR:H	2.30	0.40
2:A2:25:VAL:HA	2:A2:83:LEU:O	2.22	0.40
31:u:1214:TYR:O	32:T:591:TYR:CB	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	A5	726/790 (92%)	655 (90%)	61 (8%)	10 (1%)	9	40
2	A2	77/103 (75%)	71 (92%)	3 (4%)	3 (4%)	2	19
3	z	106/125 (85%)	92 (87%)	12 (11%)	2 (2%)	6	32
4	F	47/464 (10%)	46 (98%)	0	1 (2%)	5	30
5	D	300/357 (84%)	276 (92%)	17 (6%)	7 (2%)	5	28
6	W	160/255 (63%)	147 (92%)	13 (8%)	0	100	100
7	B	165/225 (73%)	158 (96%)	4 (2%)	3 (2%)	6	34
8	s	1720/2136 (80%)	1660 (96%)	58 (3%)	2 (0%)	48	83
9	Q	136/144 (94%)	114 (84%)	22 (16%)	0	100	100
10	A1	146/156 (94%)	137 (94%)	7 (5%)	2 (1%)	9	40
12	L	101/802 (13%)	97 (96%)	4 (4%)	0	100	100
13	R	7/229 (3%)	7 (100%)	0	0	100	100
14	V	88/95 (93%)	79 (90%)	7 (8%)	2 (2%)	5	28
15	9	69/102 (68%)	66 (96%)	2 (3%)	1 (1%)	9	40
16	C	78/139 (56%)	73 (94%)	4 (5%)	1 (1%)	9	42
17	H	74/91 (81%)	64 (86%)	8 (11%)	2 (3%)	4	25
18	J	67/80 (84%)	57 (85%)	9 (13%)	1 (2%)	8	40
20	A3	58/96 (60%)	53 (91%)	4 (7%)	1 (2%)	7	36
21	K	121/439 (28%)	98 (81%)	23 (19%)	0	100	100
22	y	98/110 (89%)	96 (98%)	2 (2%)	0	100	100
23	G	318/514 (62%)	292 (92%)	22 (7%)	4 (1%)	9	42
25	A	2164/2335 (93%)	1904 (88%)	239 (11%)	21 (1%)	12	49
26	I	174/312 (56%)	152 (87%)	22 (13%)	0	100	100
27	P	158/420 (38%)	128 (81%)	30 (19%)	0	100	100
28	p	58/793 (7%)	53 (91%)	3 (5%)	2 (3%)	3	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	4	415/501 (83%)	369 (89%)	35 (8%)	11 (3%)	4	25
30	A4	399/1098 (36%)	387 (97%)	10 (2%)	2 (0%)	24	63
31	u	832/1304 (64%)	728 (88%)	98 (12%)	6 (1%)	18	56
32	T	175/895 (20%)	159 (91%)	15 (9%)	1 (1%)	21	59
33	E	1165/1217 (96%)	1143 (98%)	19 (2%)	3 (0%)	36	72
34	w	76/424 (18%)	69 (91%)	6 (8%)	1 (1%)	9	42
35	x	77/86 (90%)	68 (88%)	8 (10%)	1 (1%)	9	42
36	v	111/536 (21%)	98 (88%)	13 (12%)	0	100	100
37	0	148/396 (37%)	146 (99%)	2 (1%)	0	100	100
38	N	54/199 (27%)	53 (98%)	1 (2%)	0	100	100
39	r	842/972 (87%)	781 (93%)	61 (7%)	0	100	100
40	Y	93/904 (10%)	90 (97%)	2 (2%)	1 (1%)	11	46
42	A6	72/248 (29%)	61 (85%)	10 (14%)	1 (1%)	9	40
43	a	74/118 (63%)	71 (96%)	3 (4%)	0	100	100
43	h	91/118 (77%)	86 (94%)	5 (6%)	0	100	100
44	b	71/86 (83%)	70 (99%)	1 (1%)	0	100	100
44	i	70/86 (81%)	69 (99%)	1 (1%)	0	100	100
45	f	60/240 (25%)	57 (95%)	3 (5%)	0	100	100
45	m	80/240 (33%)	74 (92%)	6 (8%)	0	100	100
46	e	76/126 (60%)	73 (96%)	3 (4%)	0	100	100
46	l	81/126 (64%)	76 (94%)	5 (6%)	0	100	100
47	d	67/76 (88%)	63 (94%)	4 (6%)	0	100	100
47	k	71/76 (93%)	69 (97%)	2 (3%)	0	100	100
48	c	76/92 (83%)	70 (92%)	6 (8%)	0	100	100
48	j	79/92 (86%)	77 (98%)	2 (2%)	0	100	100
49	g	89/119 (75%)	83 (93%)	6 (7%)	0	100	100
49	n	78/119 (66%)	75 (96%)	3 (4%)	0	100	100
50	q	71/73 (97%)	65 (92%)	6 (8%)	0	100	100
51	X	34/641 (5%)	34 (100%)	0	0	100	100
All	All	12843/22520 (57%)	11839 (92%)	912 (7%)	92 (1%)	20	56

All (92) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A5	188	LYS
1	A5	222	PRO
1	A5	361	GLN
1	A5	362	LEU
3	z	99	GLN
5	D	193	THR
5	D	265	ARG
7	B	175	PRO
14	V	55	LEU
17	H	70	ASP
18	J	50	GLU
23	G	342	GLU
23	G	381	HIS
23	G	382	PRO
25	A	166	PHE
25	A	1272	THR
25	A	1792	LYS
25	A	1796	GLY
25	A	1859	LYS
25	A	2060	SER
28	p	192	ASN
29	4	78	PRO
29	4	463	LYS
29	4	473	PRO
31	u	718	PRO
31	u	942	ASN
33	E	406	PRO
35	x	7	ILE
2	A2	62	TYR
4	F	77	LYS
7	B	176	GLY
8	s	1384	ALA
10	A1	8	ALA
10	A1	23	GLN
16	C	12	ASN
17	H	67	THR
25	A	165	ARG
25	A	1866	LYS
29	4	227	PRO
29	4	292	SER
29	4	479	TYR
30	A4	812	SER
31	u	720	GLY

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Mol	Chain	Res	Type
31	u	1259	ARG
32	T	604	LYS
33	E	916	ASN
25	A	1867	GLY
25	A	1957	ASP
28	p	218	ILE
29	4	308	LYS
30	A4	741	PHE
33	E	404	LEU
1	A5	97	ASN
1	A5	249	ILE
3	z	98	PHE
5	D	267	PHE
14	V	52	PRO
23	G	343	PRO
25	A	169	PHE
25	A	251	ASP
25	A	1773	SER
25	A	1869	LEU
25	A	2068	SER
40	Y	93	LEU
1	A5	363	PRO
1	A5	489	ASP
1	A5	688	LEU
2	A2	66	GLU
2	A2	88	ASP
15	9	35	ASN
25	A	985	TYR
25	A	987	LYS
25	A	2066	THR
29	4	99	PRO
29	4	482	SER
29	4	483	SER
31	u	1108	ASN
1	A5	181	GLY
7	B	213	THR
25	A	96	PRO
25	A	1271	MET
5	D	59	ILE
5	D	97	GLY
20	A3	34	ILE
29	4	472	GLN

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Mol	Chain	Res	Type
8	s	1381	PRO
5	D	238	VAL
5	D	340	PRO
25	A	250	VAL
34	w	27	PRO
42	A6	156	GLY
31	u	932	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A5	39/724 (5%)	39 (100%)	0	100	100
2	A2	3/91 (3%)	3 (100%)	0	100	100
3	z	5/109 (5%)	5 (100%)	0	100	100
5	D	10/300 (3%)	10 (100%)	0	100	100
6	W	6/218 (3%)	6 (100%)	0	100	100
7	B	8/195 (4%)	8 (100%)	0	100	100
8	s	79/1908 (4%)	79 (100%)	0	100	100
9	Q	6/130 (5%)	6 (100%)	0	100	100
12	L	3/709 (0%)	3 (100%)	0	100	100
14	V	3/88 (3%)	3 (100%)	0	100	100
15	9	4/94 (4%)	4 (100%)	0	100	100
16	C	4/111 (4%)	4 (100%)	0	100	100
17	H	3/80 (4%)	3 (100%)	0	100	100
18	J	2/70 (3%)	2 (100%)	0	100	100
21	K	2/395 (0%)	2 (100%)	0	100	100
22	y	4/95 (4%)	4 (100%)	0	100	100
23	G	13/441 (3%)	13 (100%)	0	100	100
25	A	123/2108 (6%)	123 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	I	6/293 (2%)	6 (100%)	0	100	100
27	P	12/361 (3%)	12 (100%)	0	100	100
28	p	1/709 (0%)	1 (100%)	0	100	100
29	4	12/446 (3%)	11 (92%)	1 (8%)	10	30
30	A4	6/956 (1%)	6 (100%)	0	100	100
31	u	36/1104 (3%)	35 (97%)	1 (3%)	38	60
32	T	19/776 (2%)	19 (100%)	0	100	100
33	E	60/1051 (6%)	59 (98%)	1 (2%)	53	69
34	w	4/336 (1%)	4 (100%)	0	100	100
35	x	3/77 (4%)	3 (100%)	0	100	100
36	v	6/459 (1%)	6 (100%)	0	100	100
37	0	10/349 (3%)	10 (100%)	0	100	100
39	r	49/866 (6%)	49 (100%)	0	100	100
40	Y	4/831 (0%)	4 (100%)	0	100	100
42	A6	2/203 (1%)	2 (100%)	0	100	100
43	a	3/110 (3%)	3 (100%)	0	100	100
43	h	5/110 (4%)	5 (100%)	0	100	100
44	b	4/74 (5%)	4 (100%)	0	100	100
44	i	4/74 (5%)	4 (100%)	0	100	100
45	f	2/177 (1%)	2 (100%)	0	100	100
45	m	4/177 (2%)	4 (100%)	0	100	100
46	e	3/101 (3%)	3 (100%)	0	100	100
46	l	3/101 (3%)	3 (100%)	0	100	100
47	d	3/66 (4%)	3 (100%)	0	100	100
47	k	3/66 (4%)	3 (100%)	0	100	100
48	c	1/84 (1%)	1 (100%)	0	100	100
48	j	1/84 (1%)	1 (100%)	0	100	100
49	g	4/101 (4%)	4 (100%)	0	100	100
49	n	3/101 (3%)	3 (100%)	0	100	100
51	X	1/554 (0%)	1 (100%)	0	100	100
All	All	591/18663 (3%)	588 (100%)	3 (0%)	78	83

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

Mol	Chain	Res	Type
29	4	78	PRO
31	u	718	PRO
33	E	406	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	5	113/116 (97%)	40 (35%)	2 (1%)
19	2	139/188 (73%)	29 (20%)	1 (0%)
24	Z	45/230 (19%)	12 (26%)	0
41	6	75/106 (70%)	24 (32%)	0
All	All	372/640 (58%)	105 (28%)	3 (0%)

All (105) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	5	8	G
11	5	9	G
11	5	10	U
11	5	15	C
11	5	19	A
11	5	20	G
11	5	21	A
11	5	22	U
11	5	23	C
11	5	24	G
11	5	25	C
11	5	26	A
11	5	27	U
11	5	28	A
11	5	35	U
11	5	36	C
11	5	38	C
11	5	39	C
11	5	40	U
11	5	45	C
11	5	48	A

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Mol	Chain	Res	Type
11	5	57	G
11	5	61	A
11	5	66	A
11	5	67	A
11	5	68	C
11	5	69	A
11	5	72	U
11	5	79	C
11	5	80	U
11	5	81	U
11	5	82	A
11	5	83	A
11	5	88	A
11	5	90	U
11	5	92	U
11	5	93	U
11	5	95	G
11	5	96	A
11	5	109	C
19	2	15	U
19	2	33	G
19	2	40	C
19	2	44	U
19	2	49	U
19	2	58	U
19	2	60	U
19	2	61	C
19	2	101	U
19	2	102	U
19	2	103	U
19	2	111	G
19	2	116	A
19	2	117	U
19	2	121	A
19	2	122	U
19	2	123	A
19	2	124	G
19	2	128	C
19	2	129	U
19	2	130	U
19	2	131	G
19	2	136	G

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Mol	Chain	Res	Type
19	2	138	C
19	2	146	C
19	2	147	G
19	2	157	G
19	2	164	C
19	2	177	A
24	Z	51	U
24	Z	53	C
24	Z	54	G
24	Z	55	A
24	Z	61	A
24	Z	63	G
24	Z	71	C
24	Z	75	U
24	Z	147	U
24	Z	149	A
24	Z	151	A
24	Z	155	A
41	6	6	C
41	6	7	G
41	6	8	C
41	6	10	U
41	6	12	G
41	6	25	C
41	6	26	U
41	6	27	A
41	6	28	A
41	6	29	A
41	6	31	U
41	6	33	G
41	6	36	A
41	6	37	C
41	6	38	G
41	6	45	A
41	6	46	G
41	6	59	G
41	6	68	C
41	6	72	G
41	6	74	U
41	6	75	G
41	6	84	A
41	6	85	U

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	5	26	A
11	5	78	U
19	2	60	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	GTG	A6	301	-	57,57,57	2.28	18 (31%)	85,90,90	2.70	23 (27%)
52	IHP	A	3001	-	36,36,36	1.58	6 (16%)	60,60,60	0.93	2 (3%)
53	GTP	r	1500	54	33,34,34	1.18	4 (12%)	50,54,54	1.98	9 (18%)

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	GTG	A6	301	-	-	13/32/64/64	0/6/6/6
52	IHP	A	3001	-	-	3/30/54/54	0/1/1/1
53	GTP	r	1500	54	-	7/22/38/38	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	A6	301	GTG	PG-O3B	-7.59	1.51	1.59
55	A6	301	GTG	O4E-C1E	5.99	1.55	1.42
55	A6	301	GTG	O4E-C4E	5.92	1.58	1.45
55	A6	301	GTG	PA-O3A	-4.54	1.54	1.59
55	A6	301	GTG	C5E-C4E	-4.34	1.38	1.51
55	A6	301	GTG	PG-O5E	4.23	1.76	1.59
52	A	3001	IHP	P2-O12	3.75	1.66	1.59
52	A	3001	IHP	P3-O13	3.36	1.65	1.59
52	A	3001	IHP	P1-O11	3.34	1.65	1.59
53	r	1500	GTP	C6-N1	-3.33	1.32	1.38
52	A	3001	IHP	P6-O16	3.26	1.65	1.59
52	A	3001	IHP	P5-O15	3.25	1.65	1.59
52	A	3001	IHP	P4-O14	3.24	1.65	1.59
55	A6	301	GTG	O3E-C3E	-3.14	1.35	1.43
55	A6	301	GTG	PB-O3B	3.12	1.62	1.59
55	A6	301	GTG	C1E-N9B	3.05	1.56	1.47
55	A6	301	GTG	C3E-C4E	2.97	1.60	1.53
53	r	1500	GTP	C5-N7	-2.75	1.33	1.39
55	A6	301	GTG	O5E-C5E	-2.75	1.34	1.44
55	A6	301	GTG	PA-O5D	2.62	1.69	1.59
55	A6	301	GTG	C8B-N9B	-2.41	1.32	1.37
53	r	1500	GTP	C4-N9	-2.33	1.32	1.38
55	A6	301	GTG	PB-O1B	-2.26	1.43	1.50
53	r	1500	GTP	C5-C4	2.18	1.44	1.38
55	A6	301	GTG	C8B-N7B	-2.17	1.26	1.32
55	A6	301	GTG	C4B-N3B	2.11	1.39	1.34
55	A6	301	GTG	C4A-N3A	2.08	1.39	1.34
55	A6	301	GTG	C2E-C1E	-2.05	1.47	1.53

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	A6	301	GTG	C5E-C4E-C3E	-10.70	76.70	115.21
55	A6	301	GTG	O5E-C5E-C4E	7.31	133.90	108.99
55	A6	301	GTG	C2E-C3E-C4E	7.30	116.72	102.61
55	A6	301	GTG	PG-O5E-C5E	6.71	159.81	121.35
53	r	1500	GTP	C5-C4-N3	-6.55	117.96	128.39
55	A6	301	GTG	O4E-C4E-C3E	-5.95	93.35	105.15
53	r	1500	GTP	N9-C4-N3	5.75	137.44	125.95
53	r	1500	GTP	C2-N3-C4	5.53	121.82	112.30
55	A6	301	GTG	O2A-PA-O5D	-5.43	82.94	107.57
55	A6	301	GTG	O5E-PG-O1G	-5.07	88.84	108.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	A6	301	GTG	O2B-PB-O3A	-4.89	94.06	107.27
55	A6	301	GTG	O5D-PA-O1A	-4.88	89.59	108.94
55	A6	301	GTG	O3B-PB-O1B	-4.24	97.96	110.70
55	A6	301	GTG	O3B-PG-O1G	-4.10	98.36	110.70
55	A6	301	GTG	O2B-PB-O3B	-4.07	96.27	107.27
55	A6	301	GTG	C7X-N7A-C5A	3.96	131.74	126.80
53	r	1500	GTP	O6-C6-C5	-3.84	116.39	126.53
55	A6	301	GTG	C4E-O4E-C1E	3.50	117.19	109.47
55	A6	301	GTG	C3E-C2E-C1E	3.46	108.02	101.46
55	A6	301	GTG	O2G-PG-O5E	-3.37	92.28	107.57
52	A	3001	IHP	O12-C2-C1	3.26	115.69	108.76
53	r	1500	GTP	C5-C6-N1	3.15	121.28	113.25
55	A6	301	GTG	O5D-C5D-C4D	3.04	119.35	108.99
55	A6	301	GTG	O3A-PA-O1A	3.04	119.85	110.70
53	r	1500	GTP	C2-N1-C6	-3.00	119.68	125.11
55	A6	301	GTG	O4E-C1E-N9B	2.93	115.01	108.36
55	A6	301	GTG	C8A-N7A-C5A	-2.91	104.14	107.78
55	A6	301	GTG	O2A-PA-O3A	2.82	114.89	107.27
55	A6	301	GTG	O2G-PG-O3B	2.77	114.77	107.27
53	r	1500	GTP	C6-C5-N7	2.62	135.06	130.29
55	A6	301	GTG	C2D-C3D-C4D	2.62	107.67	102.61
53	r	1500	GTP	O2G-PG-O3B	2.43	112.79	104.64
52	A	3001	IHP	P3-O13-C3	-2.12	117.77	123.43
53	r	1500	GTP	C8-N9-C4	2.07	109.91	106.03

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
52	A	3001	IHP	C1-C2-O12-P2
53	r	1500	GTP	C5'-O5'-PA-O3A
53	r	1500	GTP	C5'-O5'-PA-O1A
53	r	1500	GTP	C5'-O5'-PA-O2A
53	r	1500	GTP	O4'-C4'-C5'-O5'
55	A6	301	GTG	C5D-O5D-PA-O1A
55	A6	301	GTG	C5D-O5D-PA-O2A
55	A6	301	GTG	C5D-O5D-PA-O3A
55	A6	301	GTG	C5E-O5E-PG-O1G
55	A6	301	GTG	C5E-O5E-PG-O2G
55	A6	301	GTG	C4E-C5E-O5E-PG
53	r	1500	GTP	C3'-C4'-C5'-O5'
55	A6	301	GTG	O4D-C4D-C5D-O5D

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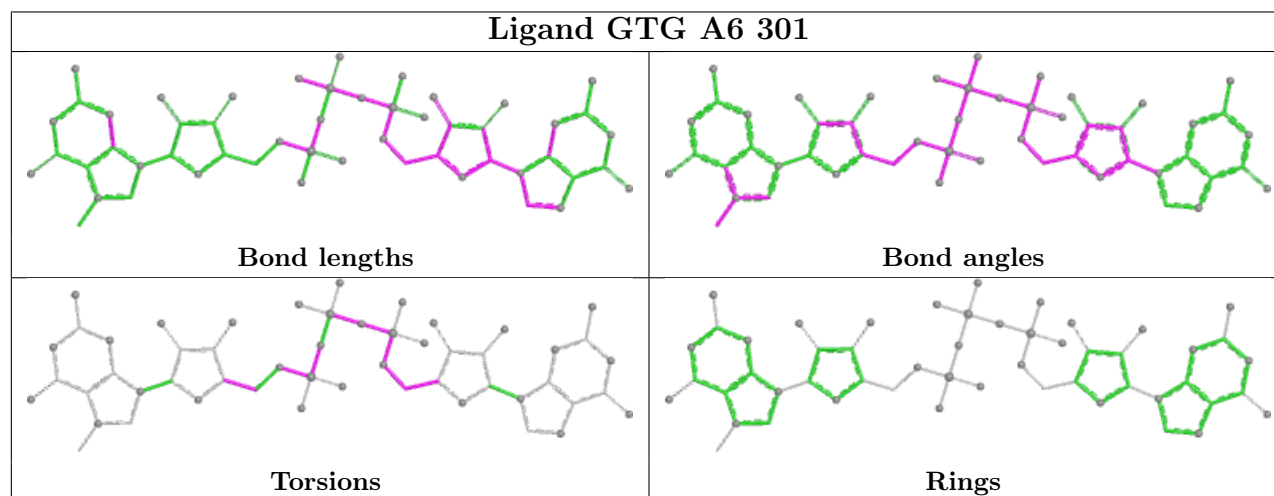
Mol	Chain	Res	Type	Atoms
55	A6	301	GTG	C3D-C4D-C5D-O5D
52	A	3001	IHP	C4-O14-P4-O24
55	A6	301	GTG	PB-O3B-PG-O5E
52	A	3001	IHP	C3-C2-O12-P2
53	r	1500	GTP	PB-O3B-PG-O3G
55	A6	301	GTG	C5E-O5E-PG-O3B
55	A6	301	GTG	C3E-C4E-C5E-O5E
53	r	1500	GTP	PG-O3B-PB-O1B
55	A6	301	GTG	PB-O3A-PA-O2A
55	A6	301	GTG	PG-O3B-PB-O2B

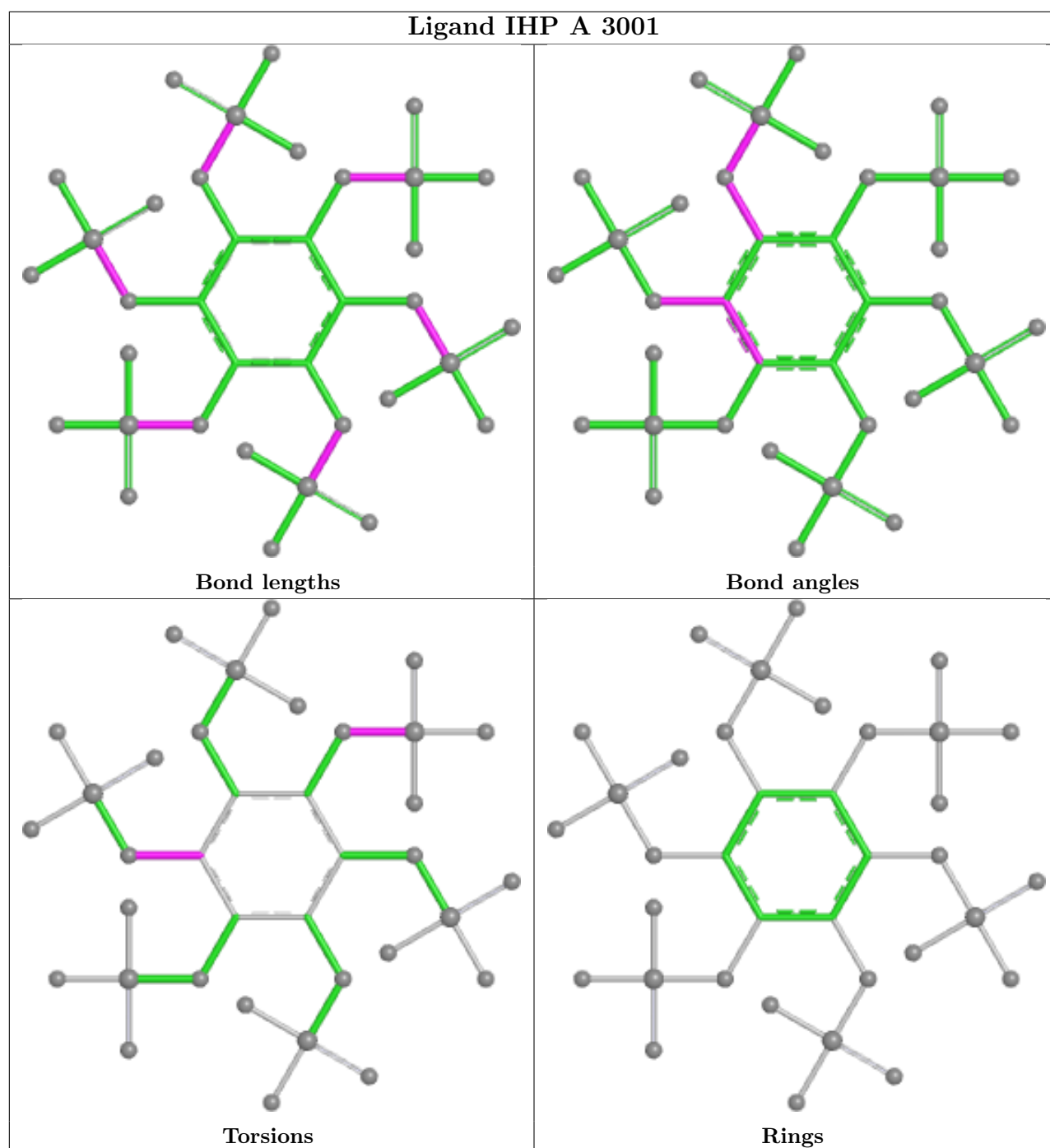
There are no ring outliers.

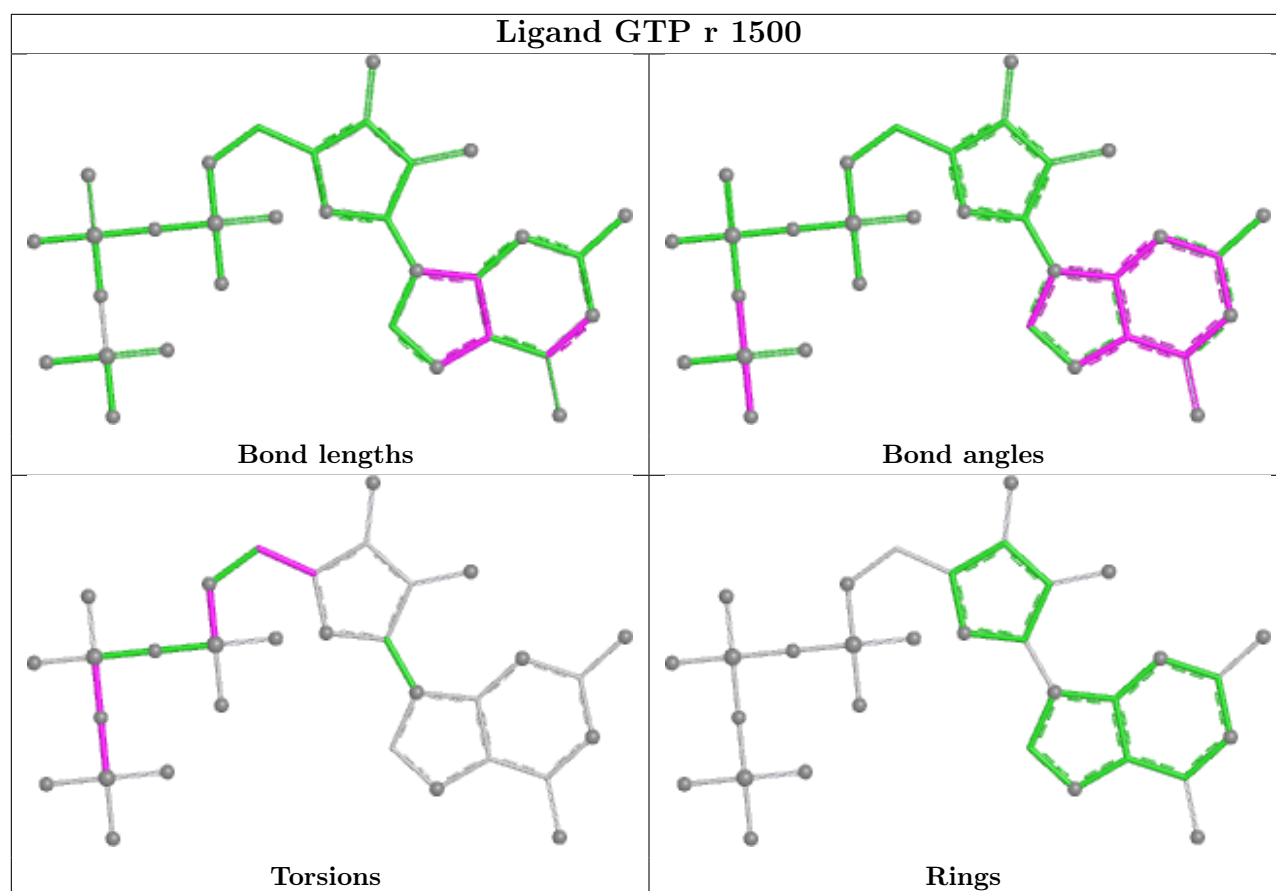
2 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	A6	301	GTG	11	0
53	r	1500	GTP	13	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

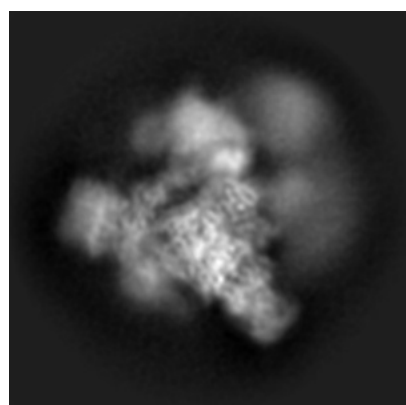
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11695. These allow visual inspection of the internal detail of the map and identification of artifacts.

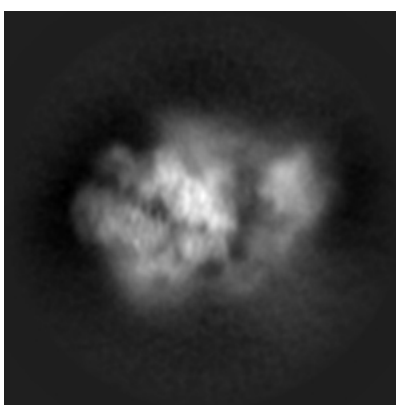
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

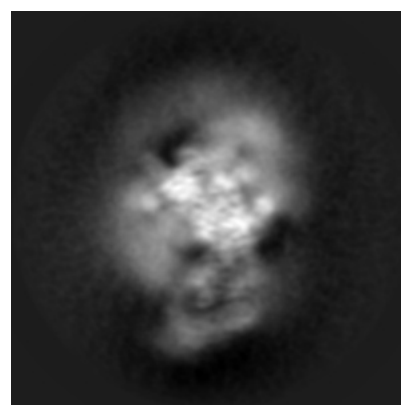
6.1.1 Primary map



X



Y

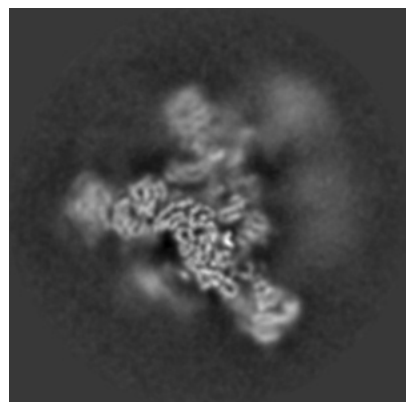


Z

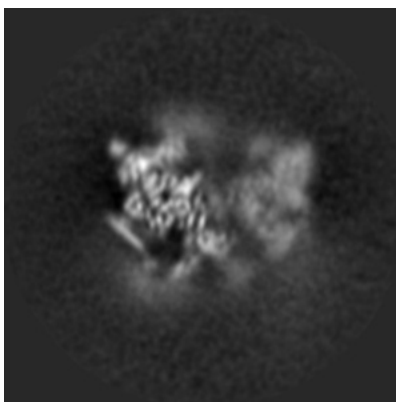
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

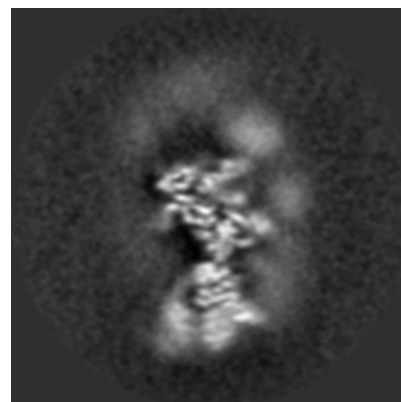
6.2.1 Primary map



X Index: 192



Y Index: 192

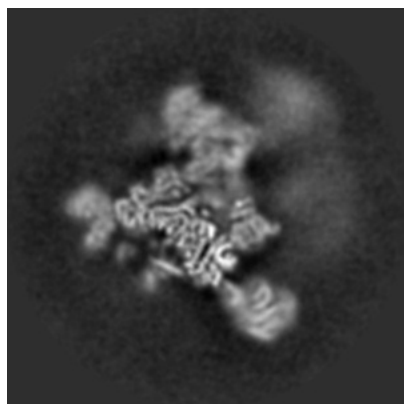


Z Index: 192

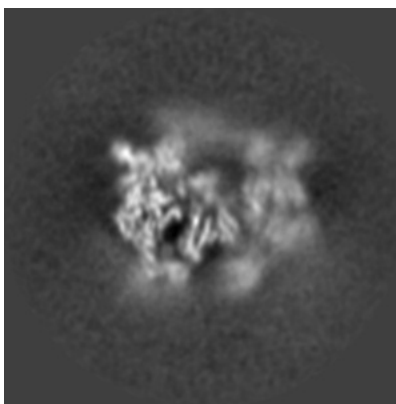
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

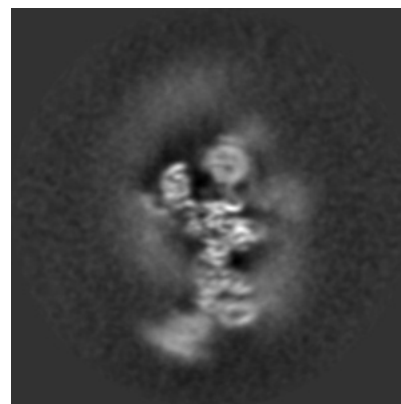
6.3.1 Primary map



X Index: 202



Y Index: 201

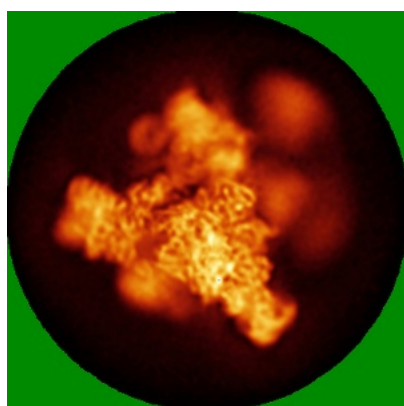


Z Index: 175

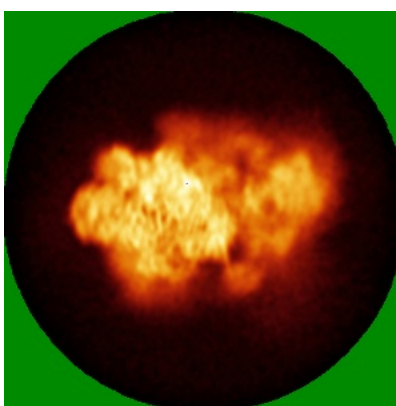
The images above show the largest variance slices of the map in three orthogonal directions.

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

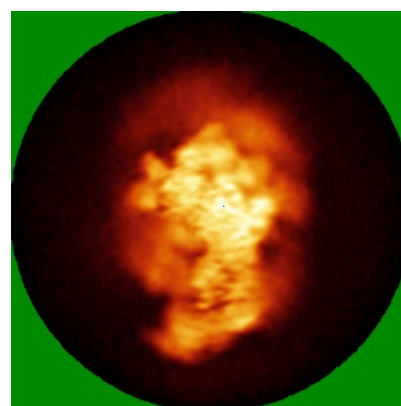
6.4.1 Primary map



X



Y

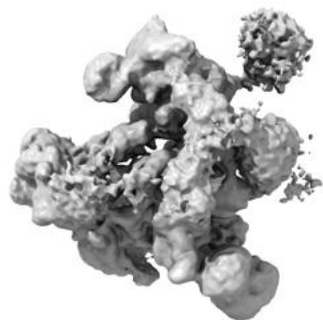


Z

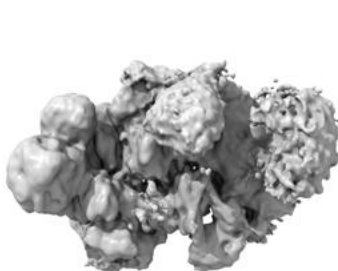
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

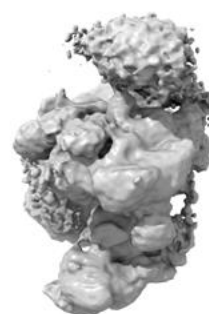
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0095. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

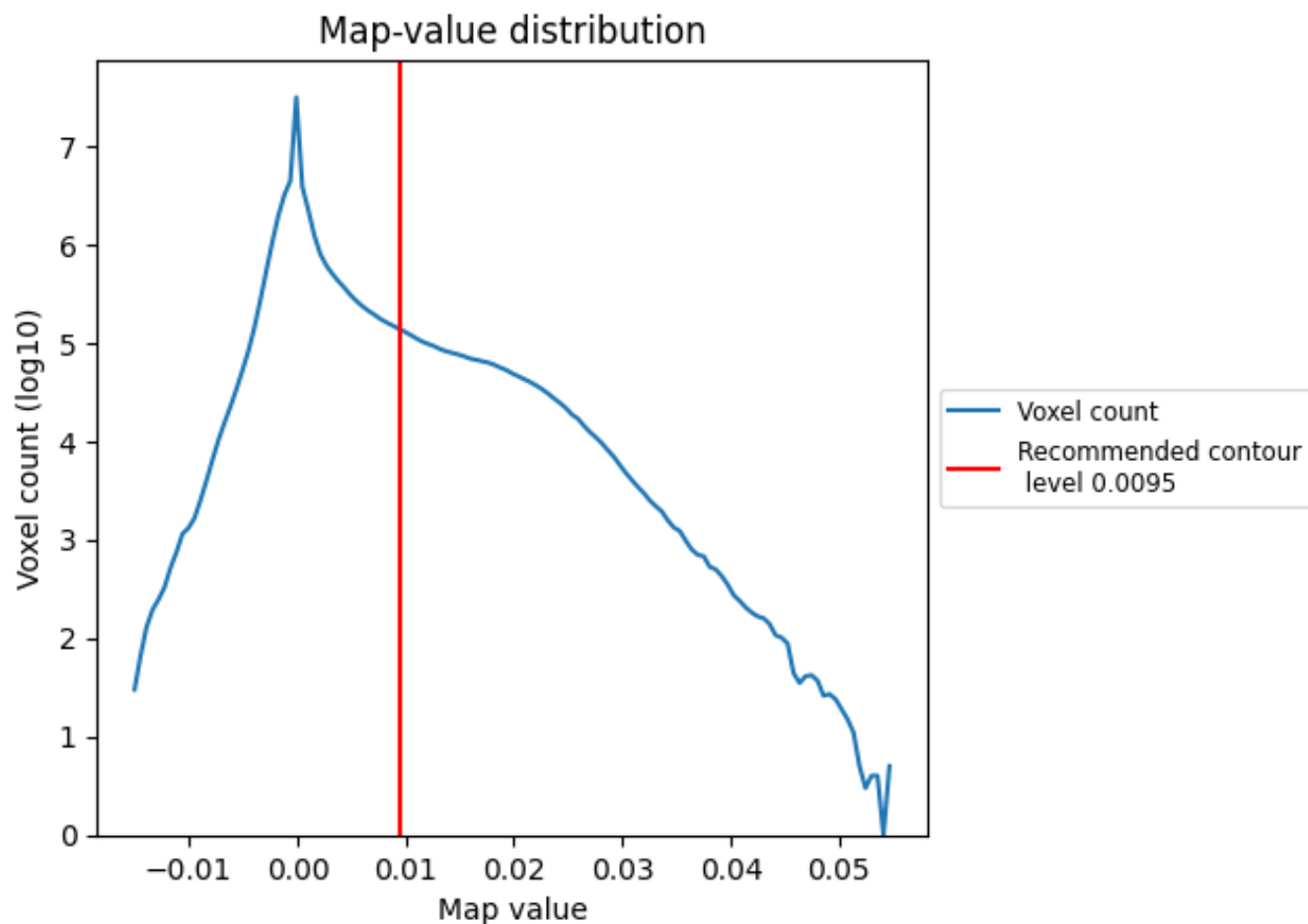
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

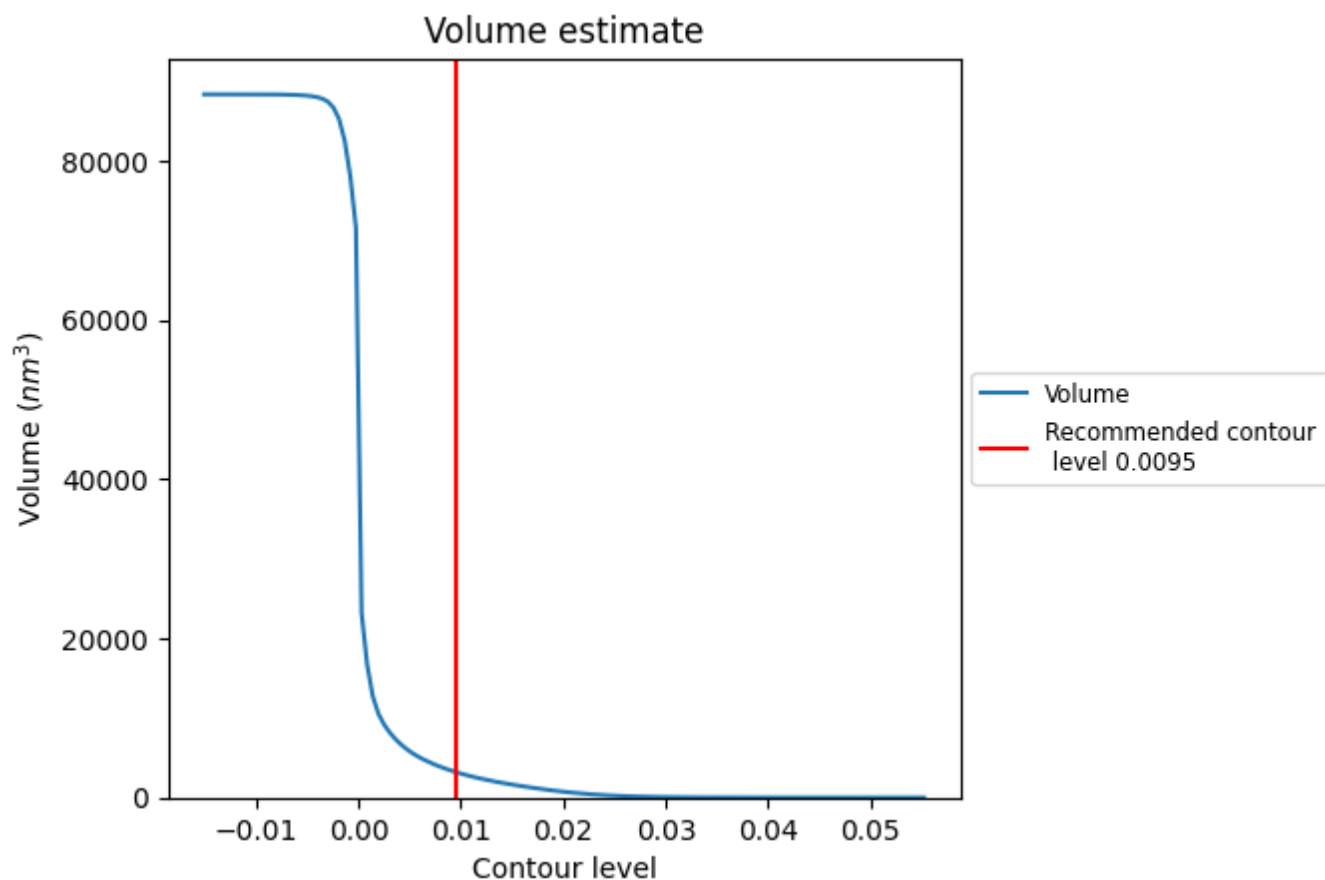
This section contains the results of statistical analysis of the map.

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.

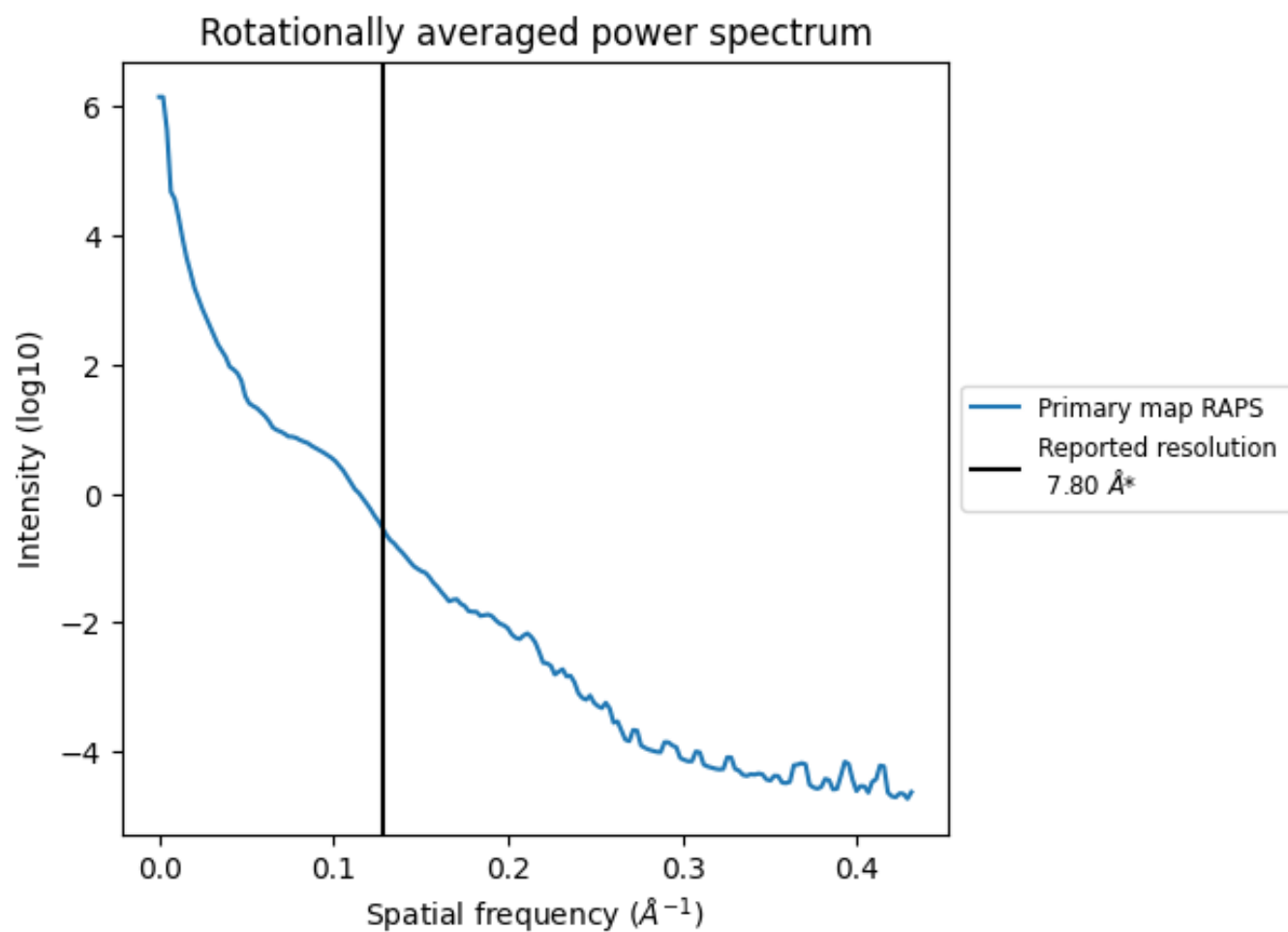
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3218 nm³; this corresponds to an approximate mass of 2907 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.128 Å⁻¹

8 Fourier-Shell correlation

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

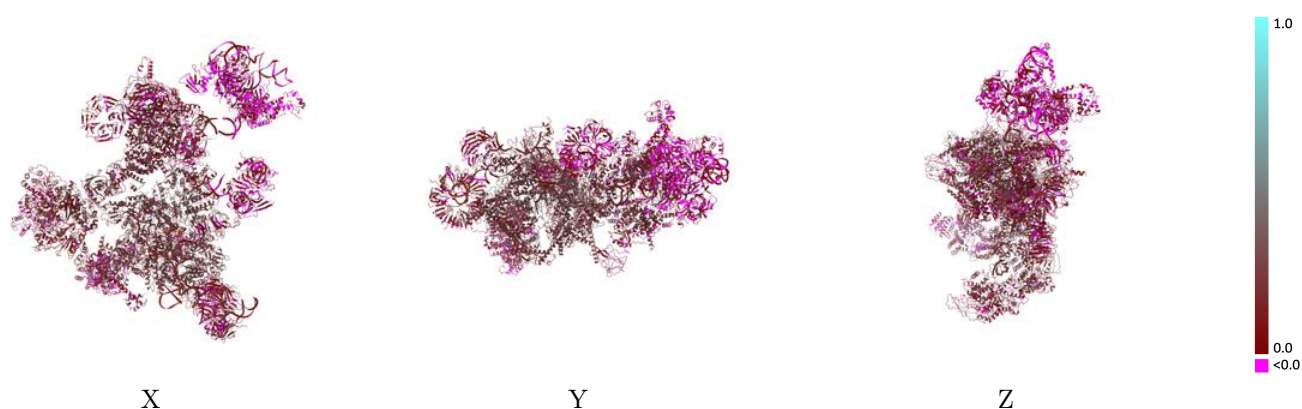
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-11695 and PDB model 7ABG. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)

This section was not generated.

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

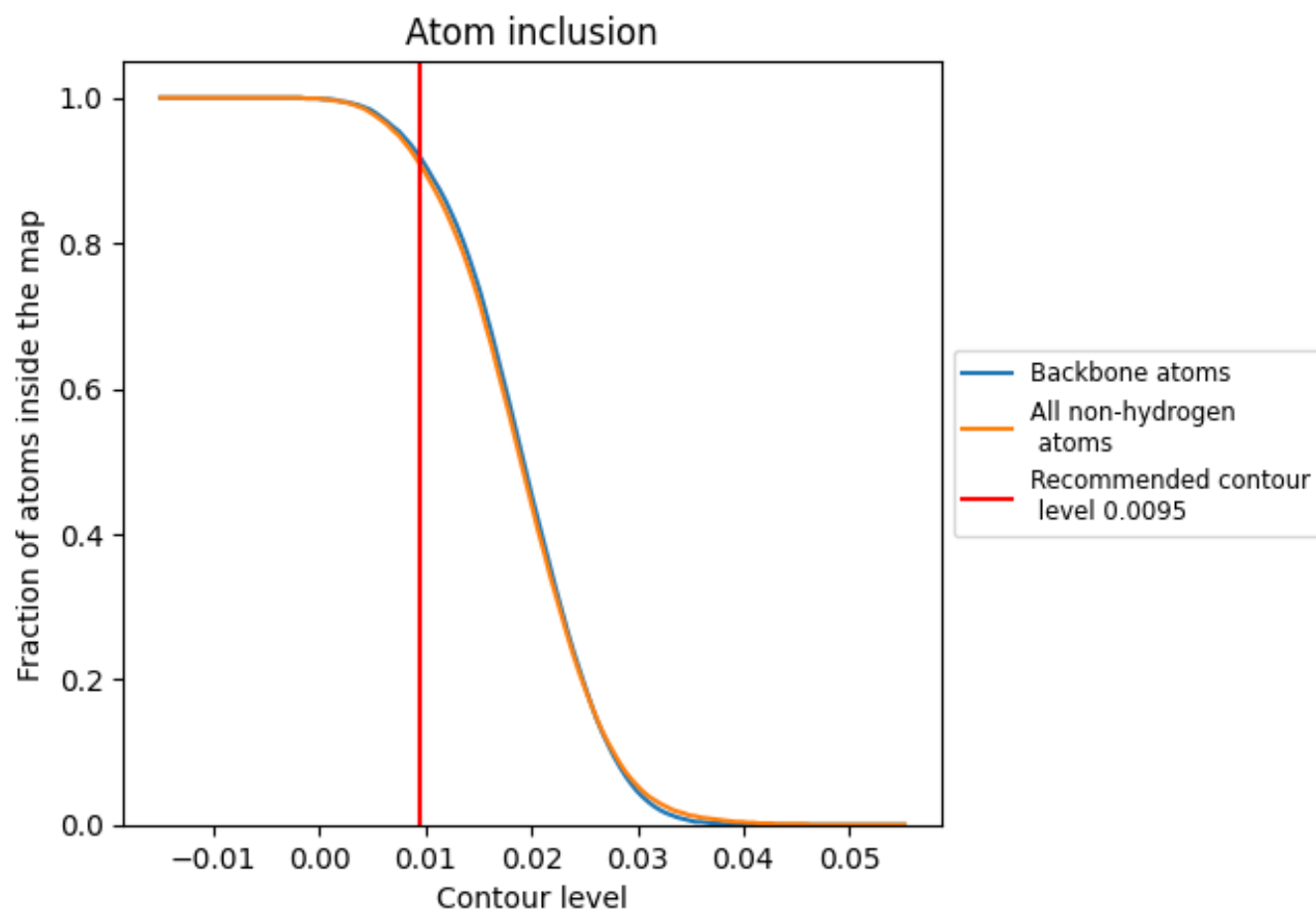


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion ⓘ



At the recommended contour level, 92% of all backbone atoms, 91% 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 (0.0095) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9080	 0.1470
0	 0.9720	 0.0750
2	 0.5410	 0.0490
4	 0.4400	 0.0250
5	 0.9880	 0.1780
6	 0.9690	 0.1550
9	 0.9050	 0.0210
A	 0.9870	 0.2520
A1	 0.9970	 0.0610
A2	 0.9620	 0.0650
A3	 1.0000	 0.0740
A4	 0.9420	 0.1610
A5	 0.9620	 0.0740
A6	 1.0000	 0.0640
B	 0.0010	 -0.0040
C	 0.9880	 0.0570
D	 0.9960	 0.0960
E	 0.9520	 0.1080
F	 0.8800	 0.0670
G	 0.9980	 0.1600
H	 0.8580	 0.0370
I	 0.9970	 0.2580
J	 0.9880	 0.0780
K	 0.9940	 0.2720
L	 0.9480	 0.1760
N	 1.0000	 0.2480
P	 0.9960	 0.1760
Q	 0.9990	 0.2290
R	 0.9560	 0.2570
T	 0.9930	 0.1120
V	 0.9450	 0.0510
W	 0.4860	 0.0180
X	 1.0000	 0.2510
Y	 0.9330	 0.1320
Z	 1.0000	 0.1940



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Chain	Atom inclusion	Q-score
a	 0.9900	 0.1530
b	 0.9560	 0.1180
c	 0.9510	 0.1160
d	 0.9940	 0.1820
e	 0.9970	 0.1990
f	 1.0000	 0.1560
g	 0.9700	 0.1360
h	 0.8750	 -0.0140
i	 0.7600	 0.0090
j	 0.2360	 0.0320
k	 0.1320	 0.0160
l	 0.2020	 0.0100
m	 0.7360	 0.0420
n	 0.9730	 0.0000
p	 0.0200	 0.0700
q	 1.0000	 0.2990
r	 0.9980	 0.2390
s	 0.9870	 0.1560
u	 0.9850	 0.1630
v	 0.9350	 0.2120
w	 0.9850	 0.0730
x	 1.0000	 0.1200
y	 0.9940	 0.1280
z	 0.9040	 0.1010