



Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 08:00 am GMT

PDB ID : 5GAN
EMDB ID : EMD-8012
Title : The overall structure of the yeast spliceosomal U4/U6.U5 tri-snRNP at 3.7 Angstrom
Authors : Nguyen, T.H.D.; Galej, W.P.; Bai, X.C.; Oubridge, C.; Scheres, S.H.W.; Newman, A.J.; Nagai, K.
Deposited on : 2015-12-15
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

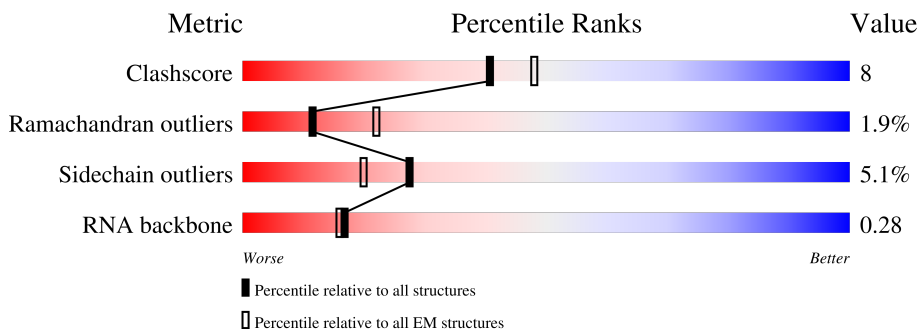
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 3.60 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	V	160	
2	W	112	
3	A	2413	
4	H	465	
5	J	899	
6	D	143	
7	F	494	




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Mol	Chain	Length	Quality of chain
8	G	469	9% 55% 11% 32%
9	B	2163	68% 71% 10% 18%
10	x	100	12% 100%
11	b	196	26% 41% 59%
11	k	196	41% 38% 59%
12	h	146	39% 54% 44%
12	l	146	62% 58% 38%
13	j	110	70% 82% 15%
13	m	110	85% 83% 15%
14	d	101	34% 78% 19%
14	n	101	81% 78% 19%
15	e	94	60% 73% 6% 20%
15	p	94	80% 74% 5% 20%
16	f	86	64% 80% 16%
16	q	86	84% 83% 16%
17	g	77	55% 88% 10%
17	r	77	90% 88% 10%
18	E	328	96% 99%
19	U	214	12% 23% 25% 17% 34%
20	K	126	60% 95% 34%
21	2	95	73% 87% 21% 5%
22	3	89	79% 7% 13%
23	4	187	40% 37% 60%
24	5	93	81% 76% 19%
25	6	86	86% 80% 6% 14%

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Mol	Chain	Length	Quality of chain
26	7	115	
27	8	109	
28	C	1008	

2 Entry composition i

There are 29 unique types of molecules in this entry. The entry contains 77370 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called U4 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	V	124	2635	1179	459	873	124	0	0

- Molecule 2 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	W	80	1697	759	293	565	80	0	0

- Molecule 3 is a protein called Pre-mRNA-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	A	2196	17778	11444	3045	3226	63	0	0

- Molecule 4 is a protein called U4/U6 small nuclear ribonucleoprotein PRP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	H	357	2789	1743	501	532	13	0	0

- Molecule 5 is a protein called Pre-mRNA-splicing factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	J	729	5822	3726	992	1079	25	0	0

- Molecule 6 is a protein called Spliceosomal protein DIB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	D	140	1151	728	200	212	11	0	0

- Molecule 7 is a protein called Pre-mRNA-processing factor 31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	F	415	3218	2052	575	580	11	0	0

- Molecule 8 is a protein called U4/U6 small nuclear ribonucleoprotein PRP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	G	318	2632	1659	469	488	16	0	0

- Molecule 9 is a protein called Pre-mRNA-splicing helicase BRR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	B	1781	14212	9098	2372	2685	57	1	0

- Molecule 10 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	x	100	500	300	100	100	0	0

- Molecule 11 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	k	80	631	403	114	111	3	0	0
11	b	80	631	403	114	111	3	0	0

- Molecule 12 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	l	91	720	455	129	134	2	0	0
12	h	82	644	409	110	123	2	0	0

- Molecule 13 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	94	Total	C	N	O	S	0	0
			737	474	140	119	4		
13	j	94	Total	C	N	O	S	0	0
			741	477	141	119	4		

- Molecule 14 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	82	Total	C	N	O	S	0	0
			625	399	109	115	2		
14	d	82	Total	C	N	O	S	0	0
			625	399	109	115	2		

- Molecule 15 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	p	75	Total	C	N	O	S	0	0
			575	379	92	101	3		
15	e	75	Total	C	N	O	S	0	0
			575	379	92	101	3		

- Molecule 16 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	q	72	Total	C	N	O	S	0	0
			573	368	101	103	1		
16	f	72	Total	C	N	O	S	0	0
			573	368	101	103	1		

- Molecule 17 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	r	69	Total	C	N	O	S	0	0
			526	336	93	95	2		
17	g	69	Total	C	N	O	S	0	0
			529	337	93	97	2		

- Molecule 18 is a protein called Snu66.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	E	328	Total	C	N	O	0	0
			1713	1033	342	338		

- Molecule 19 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
19	U	141	2999	1342	530	986	141	0	0

- Molecule 20 is a protein called 13 kDa ribonucleoprotein-associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	K	124	936	597	161	174	4	0	0

- Molecule 21 is a protein called U6 snRNA-associated Sm-like protein LSm2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	2	90	735	469	124	139	3	0	0

- Molecule 22 is a protein called U6 snRNA-associated Sm-like protein LSm3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	3	77	611	382	105	121	3	0	0

- Molecule 23 is a protein called U6 snRNA-associated Sm-like protein LSm4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	4	74	588	381	96	108	3	0	0

- Molecule 24 is a protein called U6 snRNA-associated Sm-like protein LSm5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	5	75	588	378	98	110	2	0	0

- Molecule 25 is a protein called U6 snRNA-associated Sm-like protein LSm6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	6	74	577	364	95	116	2	0	0

- Molecule 26 is a protein called U6 snRNA-associated Sm-like protein LSm7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	7	66	504	325	85	91	3	0	0

- Molecule 27 is a protein called U6 snRNA-associated Sm-like protein LSm8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	8	64	498	320	86	90	2	0	0

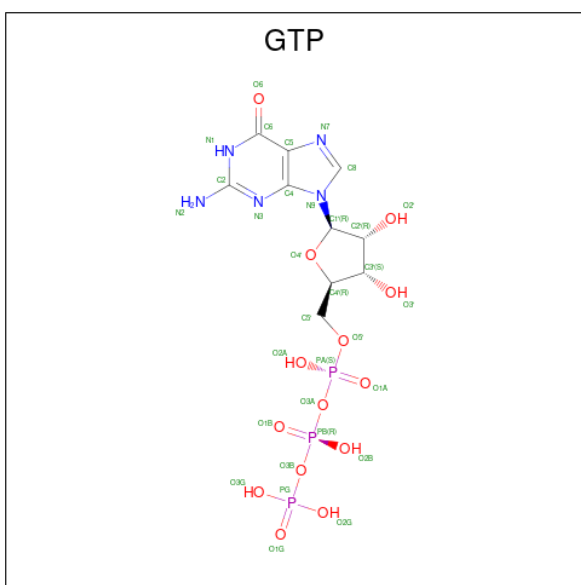
- Molecule 28 is a protein called Pre-mRNA-splicing factor SNU114.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	C	855	6450	4195	1089	1143	23	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	530	SER	GLU	conflict	UNP P36048
C	531	LYS	ASP	conflict	UNP P36048
C	532	THR	ASP	conflict	UNP P36048

- Molecule 29 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

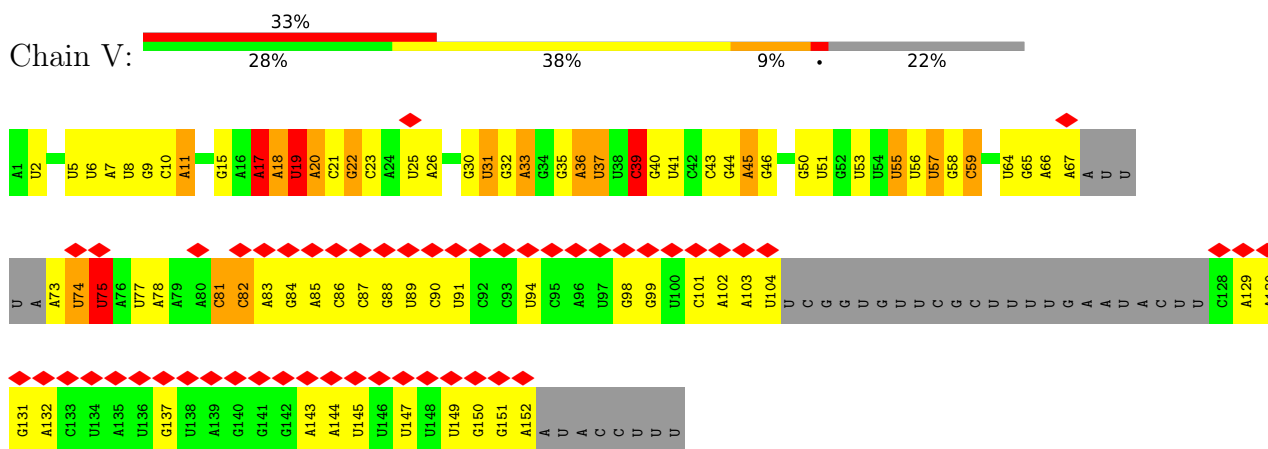


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
29	C	1	32	10	5	14	3	0

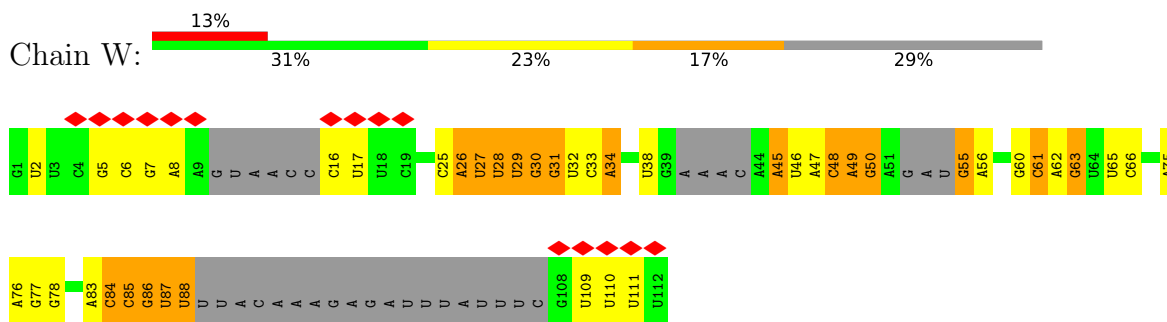
3 Residue-property plots i

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

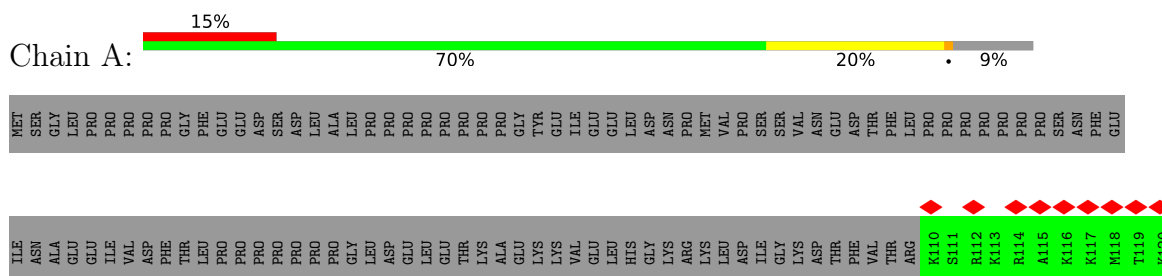
• Molecule 1: U4 snRNA

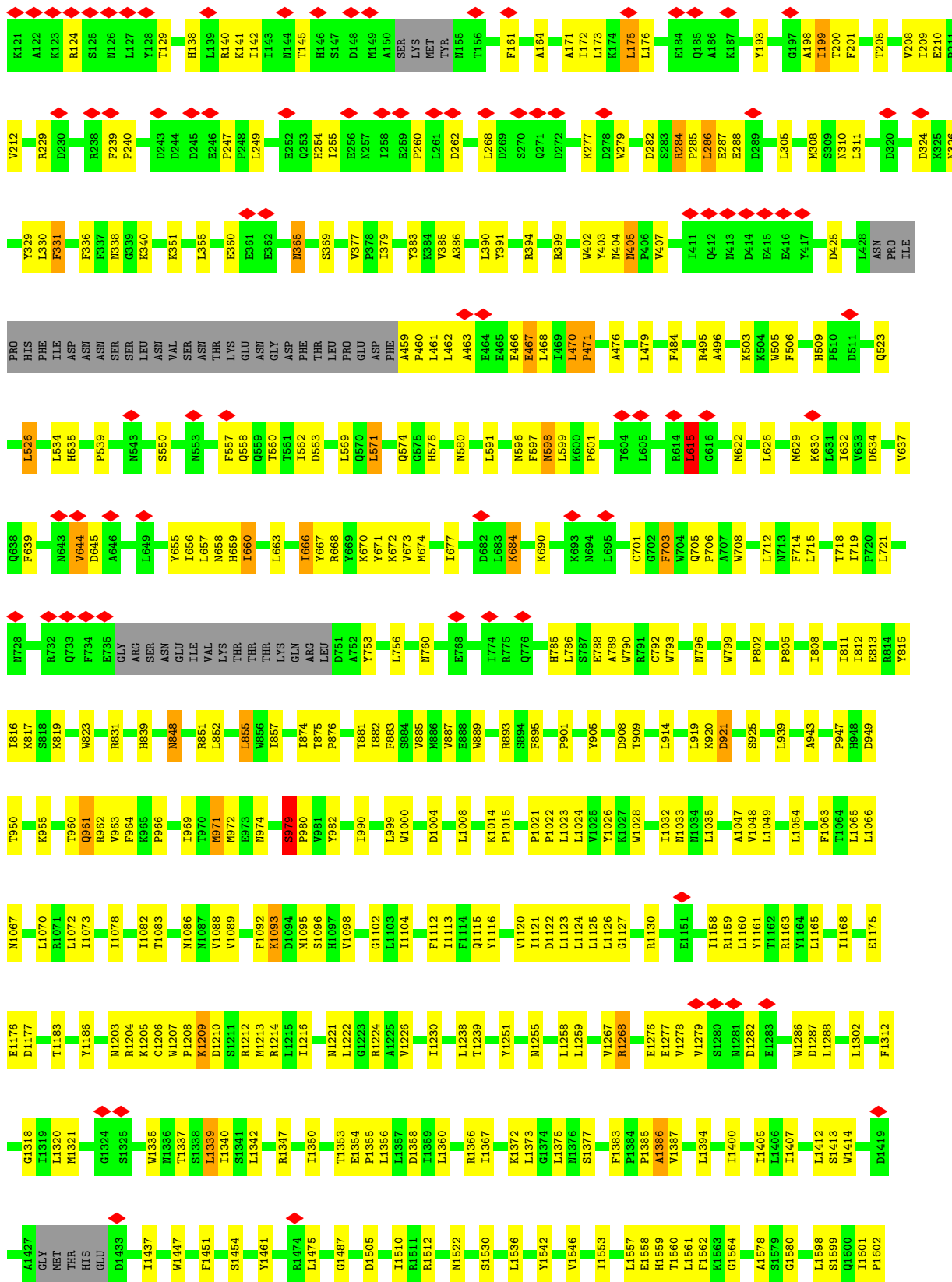


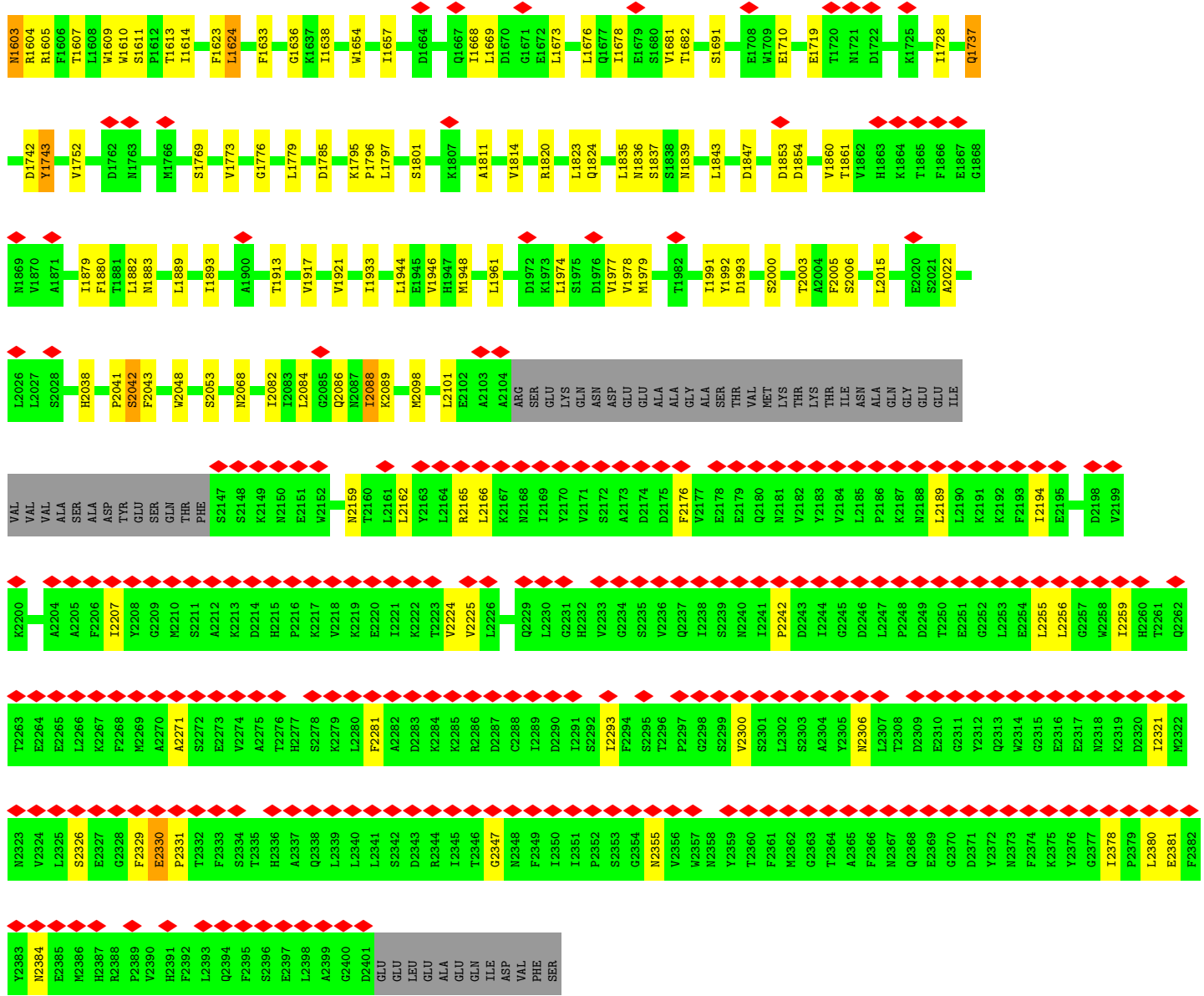
• Molecule 2: U6 snRNA



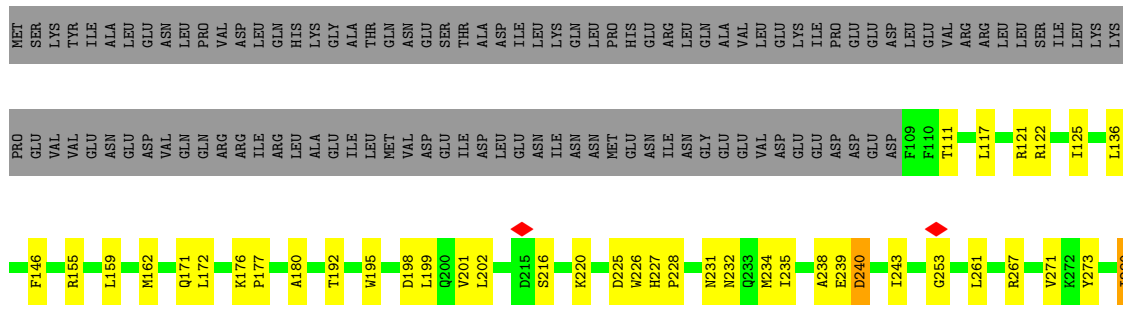
• Molecule 3: Pre-mRNA-splicing factor 8

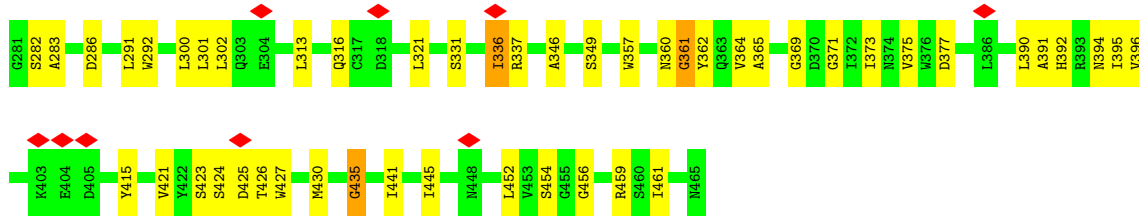




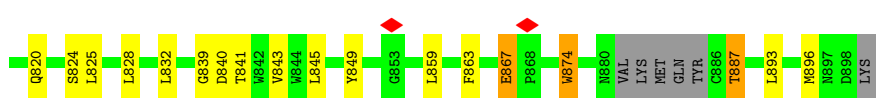
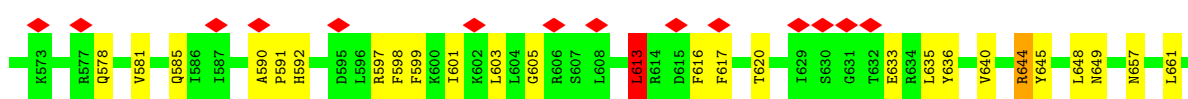
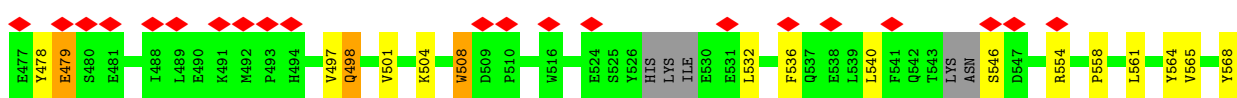
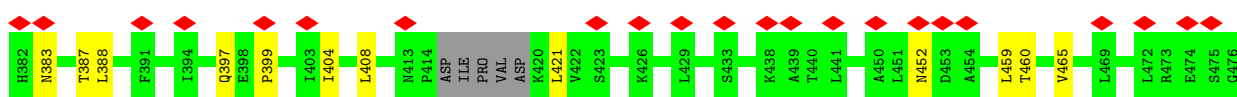
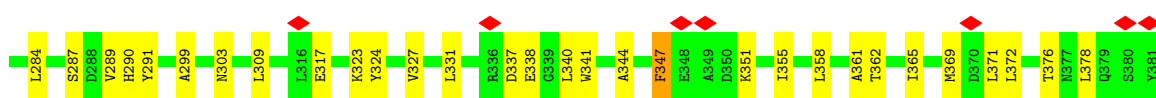
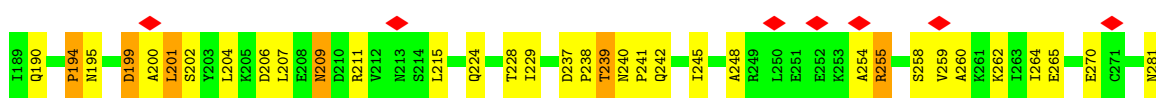
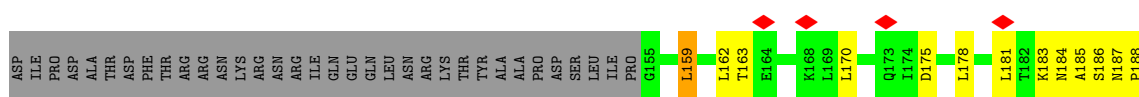


● Molecule 4: U4/U6 small nuclear ribonucleoprotein PRP4



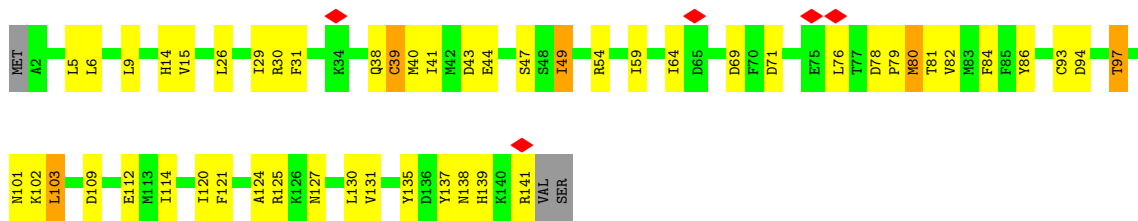


• Molecule 5: Pre-mRNA-splicing factor 6

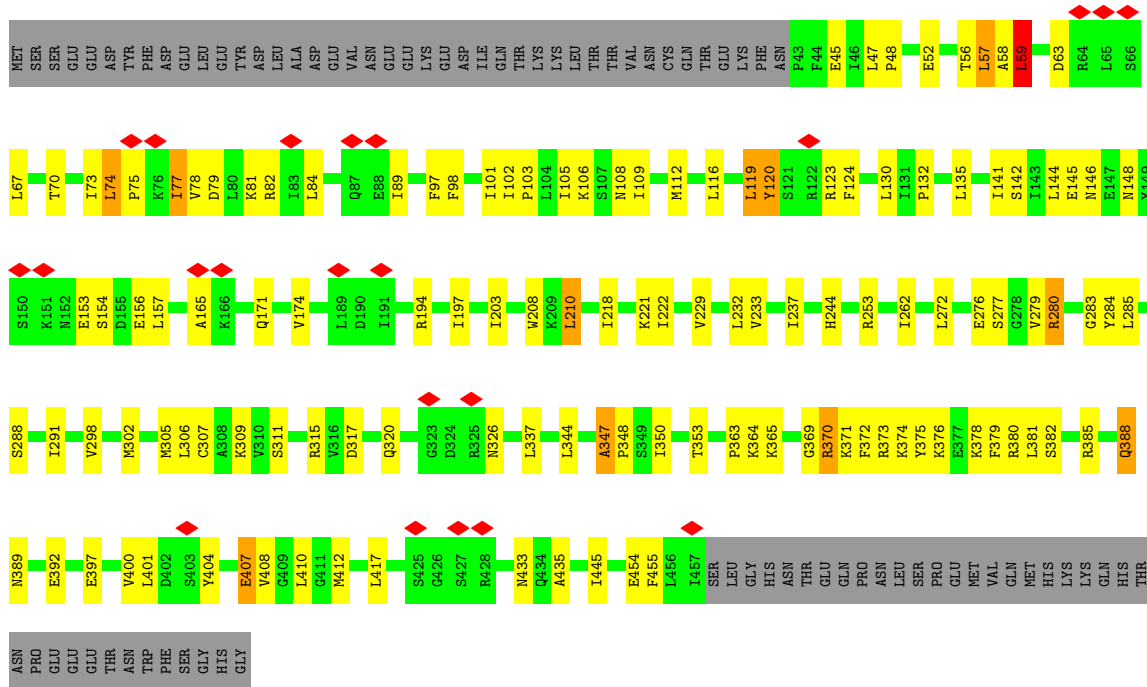


• Molecule 6: Spliceosomal protein DIB1

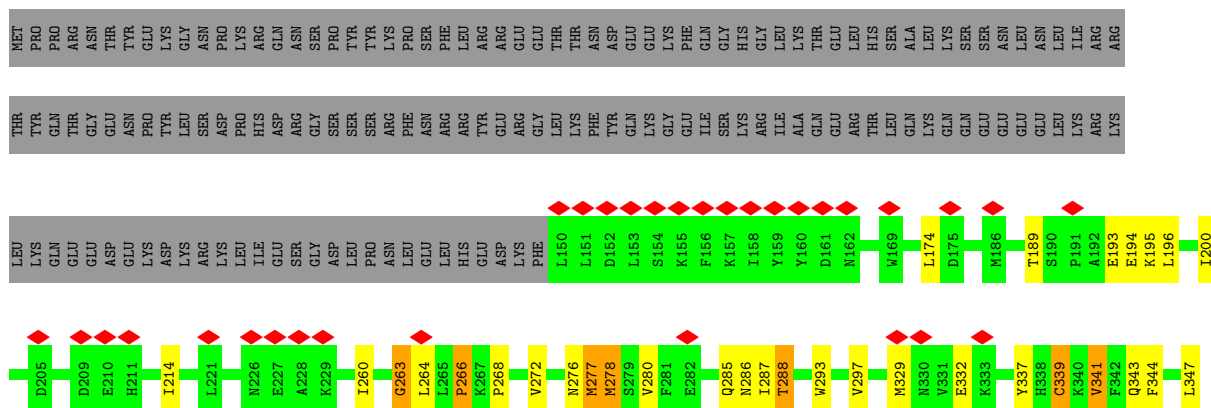


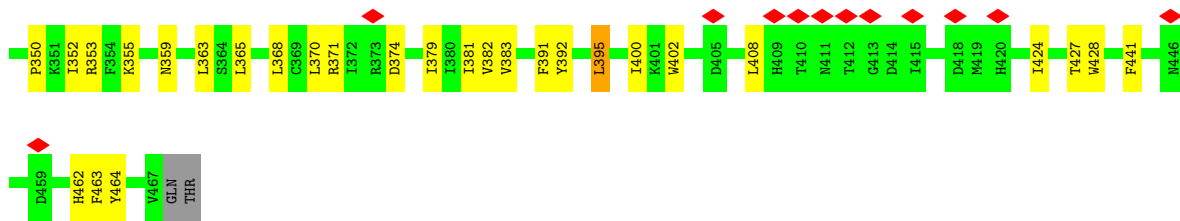


• Molecule 7: Pre-mRNA-processing factor 31

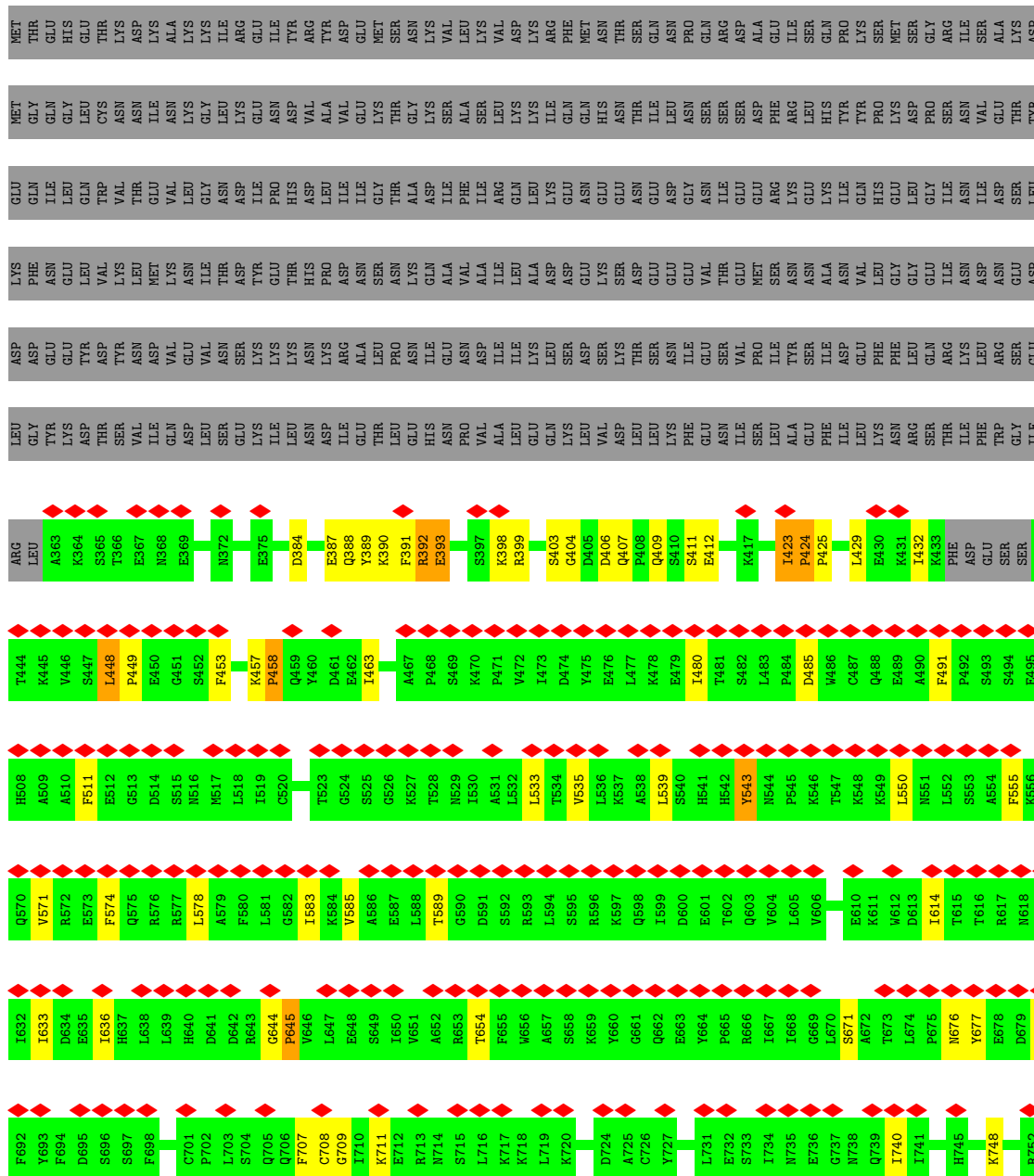


• Molecule 8: U4/U6 small nuclear ribonucleoprotein PRP3





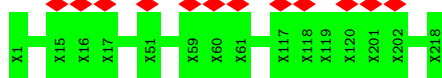
• Molecule 9: Pre-mRNA-splicing helicase BRR2



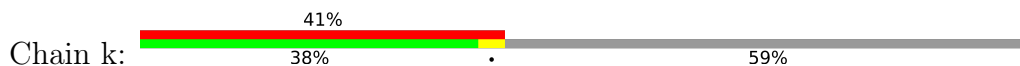
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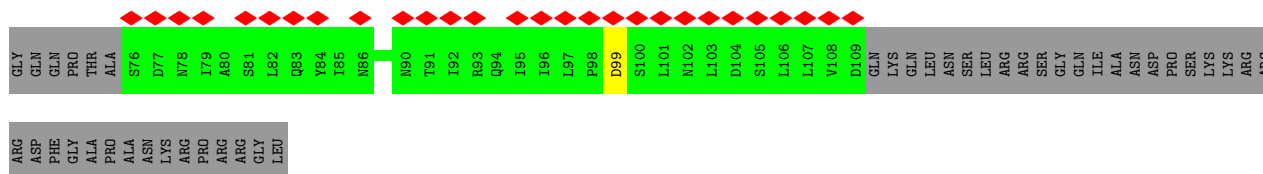
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P1632	AI631	A1691	HI751	LI811	S1871	Q1931	D1991	V2051	L2111	
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Y1656	E1655	SI715	YI775	ASP	R1895	V1955	T2015	L2075	S2135	
E1657	Y1656	M1716	SI776	ASP	K1896	L1956	T2016	G2136	G2137	
VI658	E1657	A1717	YI777	GLU	G1897	V1957	V2017	R2077	T2138	
GI659	VI658	G1718	FI778	GLU	R1898	L1958	D2018	D2078	H2138	
A1660	GI659	K1719	YI779	ALA	R1899	I1959	I2019	V2079	N2139	
V1661	A1660	LI720	RI780	ALA	A1900	V1960	M2020	E2080	L2140	
S1662	V1661	I1721	RI781	TI841	LI901	V1961	A2021	P2081	T2141	
VI663	S1662	I1722	HI782	II843	L1902	V1962	L2022	E2082	I2142	
	VI663	L1723	HI783		V1903	L1963	E2023	N2083	W2143	

● Molecule 10: Unknown protein

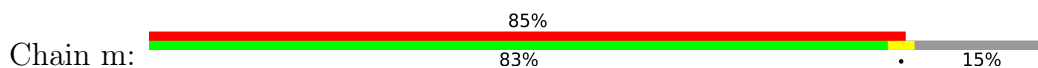


● Molecule 11: Small nuclear ribonucleoprotein-associated protein B

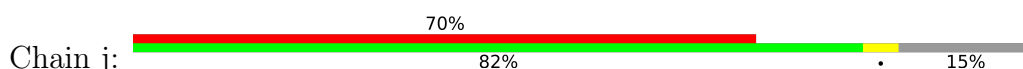




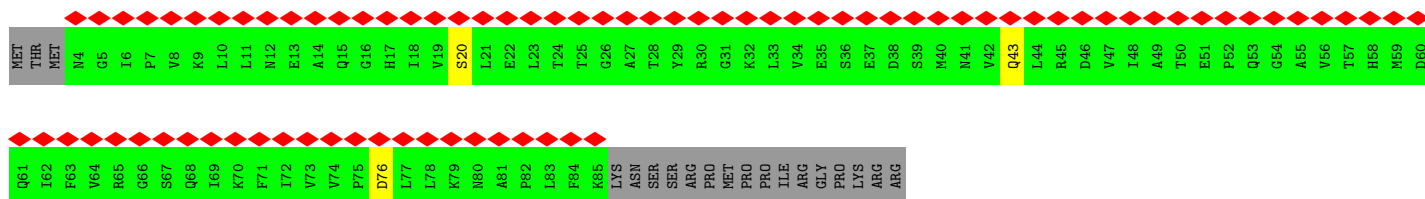
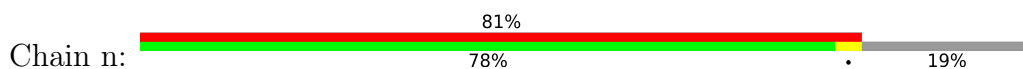
• Molecule 13: Small nuclear ribonucleoprotein Sm D2



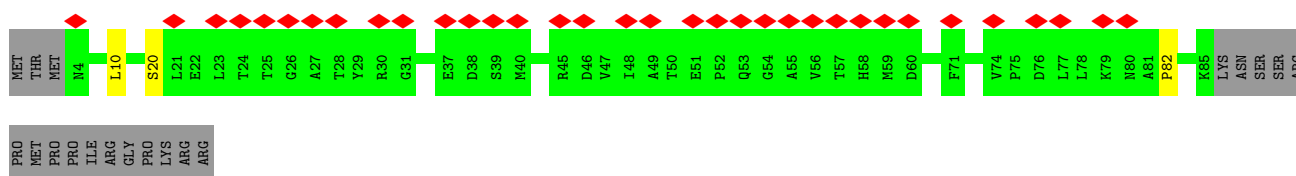
• Molecule 13: Small nuclear ribonucleoprotein Sm D2



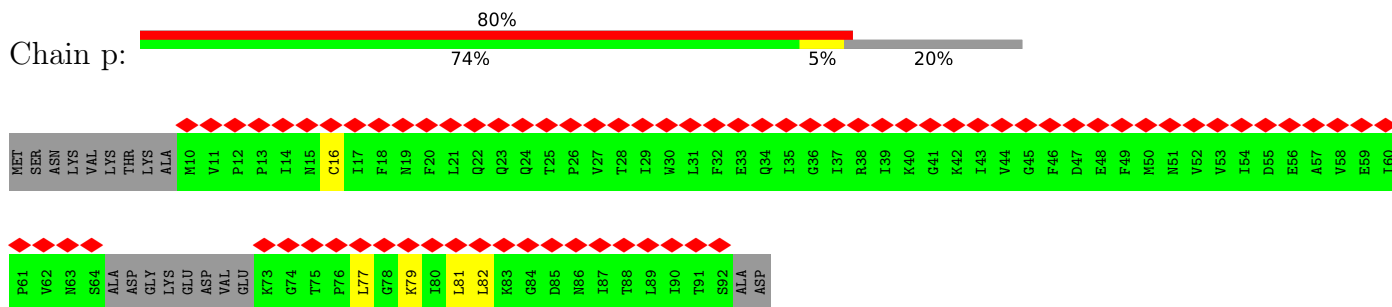
• Molecule 14: Small nuclear ribonucleoprotein Sm D3



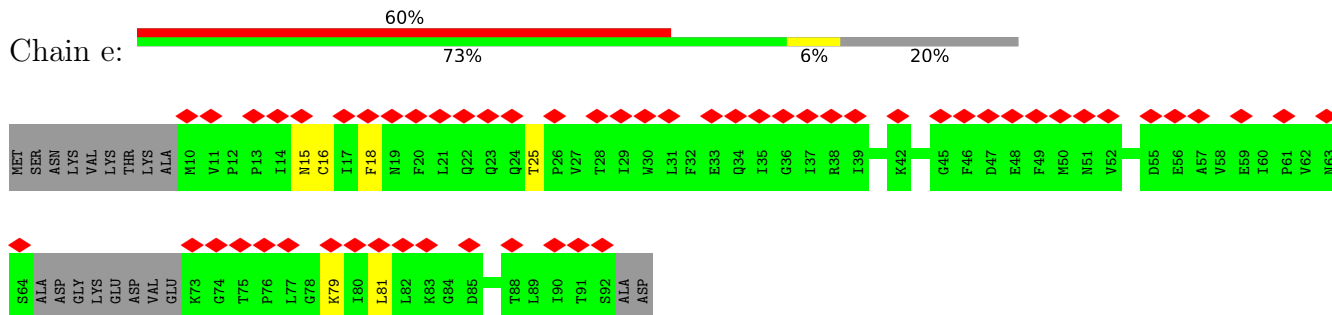
• Molecule 14: Small nuclear ribonucleoprotein Sm D3



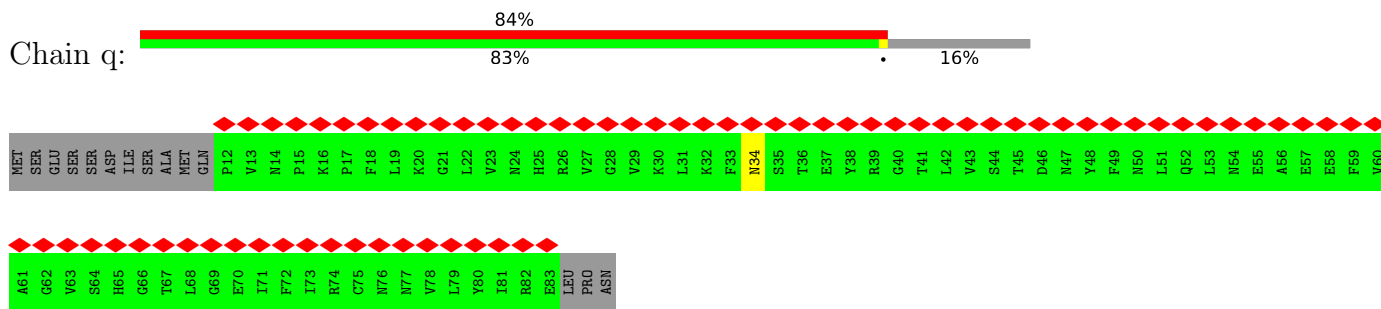
• Molecule 15: Small nuclear ribonucleoprotein E



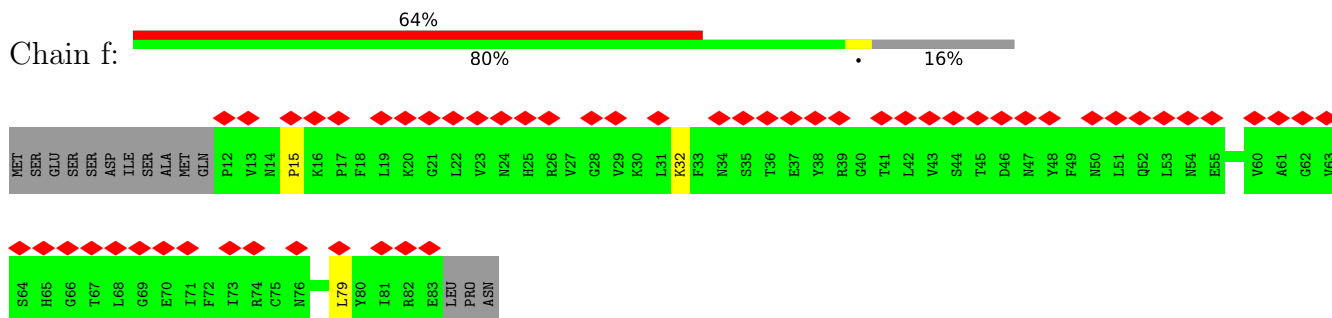
• Molecule 15: Small nuclear ribonucleoprotein E



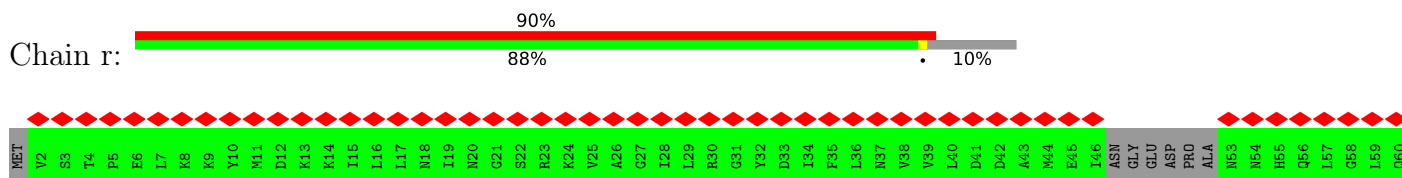
• Molecule 16: Small nuclear ribonucleoprotein F

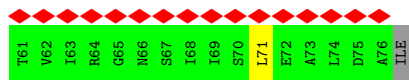


• Molecule 16: Small nuclear ribonucleoprotein F

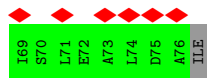
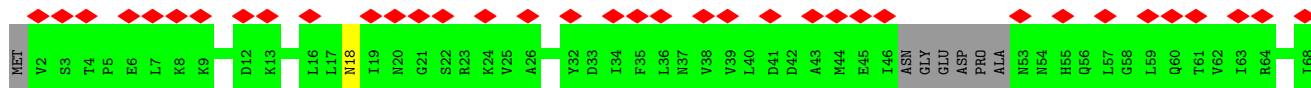
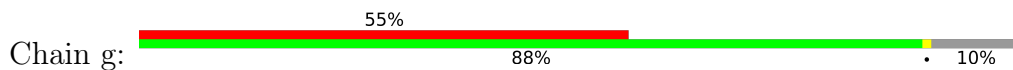


• Molecule 17: Small nuclear ribonucleoprotein G

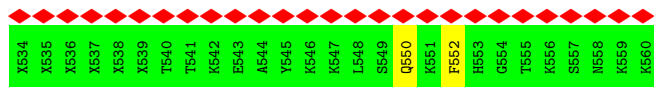
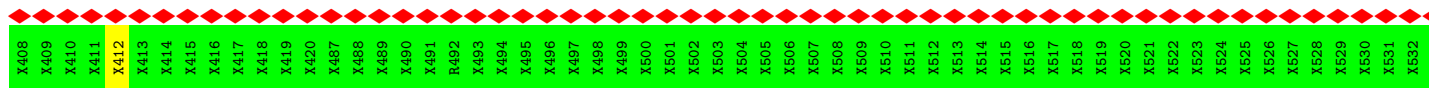
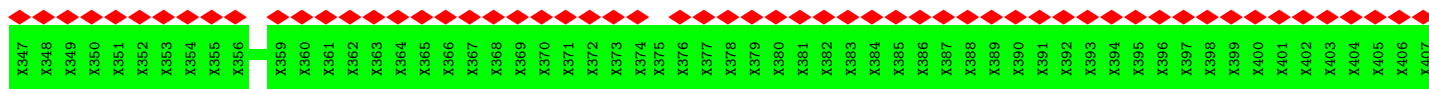
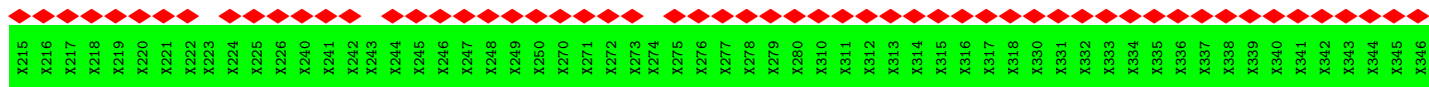
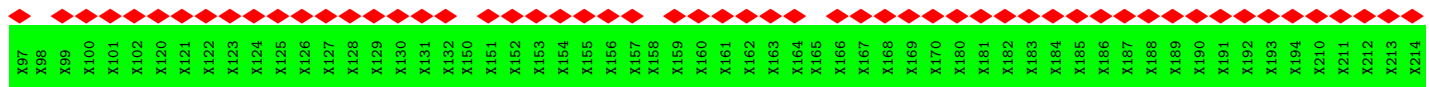
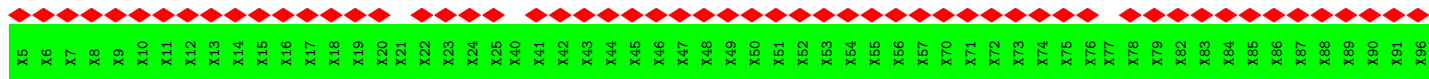




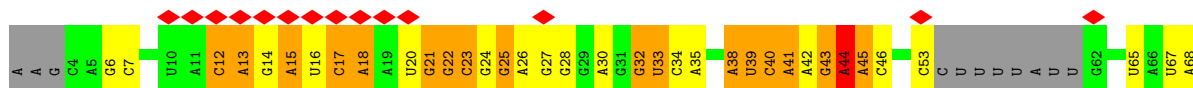
● Molecule 17: Small nuclear ribonucleoprotein G



● Molecule 18: Smu66

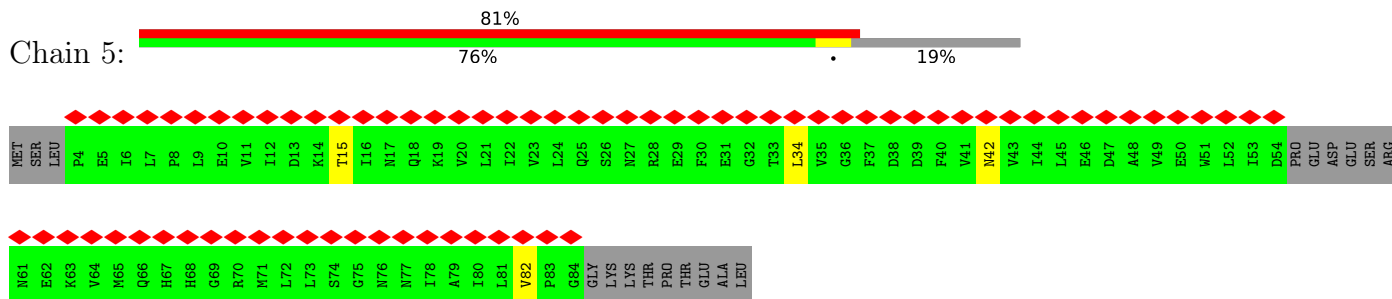


● Molecule 19: U5 snRNA

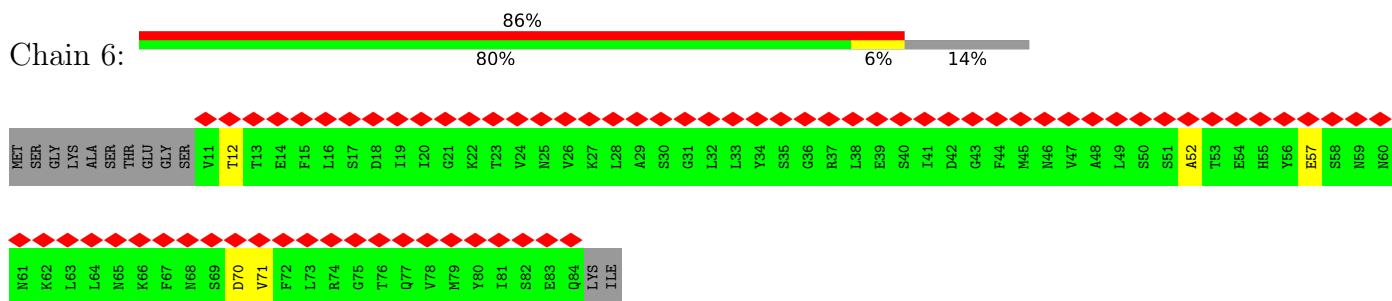


SER
PRO
GLN
LYS
VAL
GLU
PHE

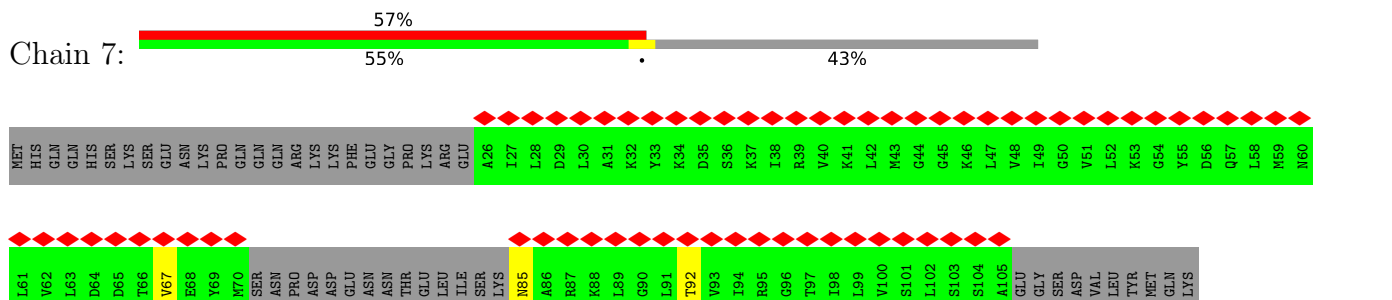
• Molecule 24: U6 snRNA-associated Sm-like protein LSm5



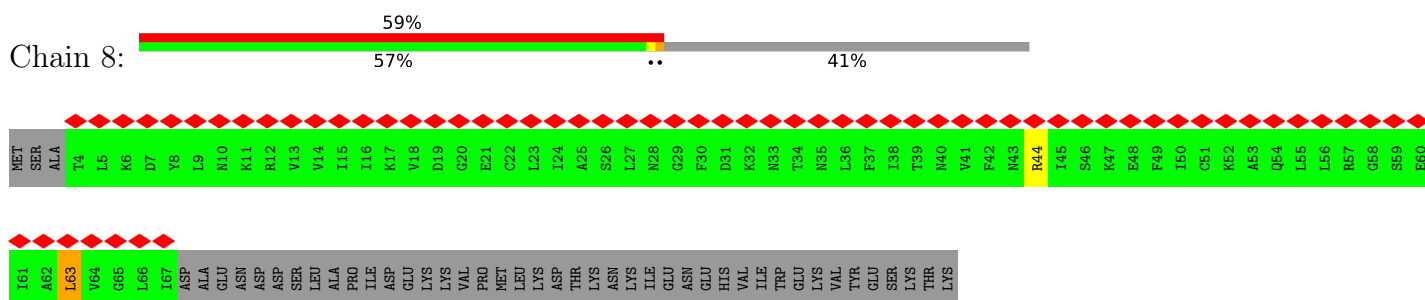
• Molecule 25: U6 snRNA-associated Sm-like protein LSm6



• Molecule 26: U6 snRNA-associated Sm-like protein LSm7



• Molecule 27: U6 snRNA-associated Sm-like protein LSm8



• Molecule 28: Pre-mRNA-splicing factor SNU114



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	140155	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	38	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	35714	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.243	Depositor
Minimum map value	-0.122	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.036	Depositor
Map size (\AA)	543.39996, 543.39996, 543.39996	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.43, 1.43, 1.43	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	V	0.37	0/2943	0.78	4/4577 (0.1%)
2	W	0.33	0/1891	0.82	3/2933 (0.1%)
3	A	0.47	0/18226	0.77	4/24737 (0.0%)
4	H	0.43	0/2845	0.76	0/3843
5	J	0.47	0/5934	0.82	3/8039 (0.0%)
6	D	0.49	0/1172	0.85	1/1578 (0.1%)
7	F	0.48	0/3273	0.85	0/4413
8	G	0.46	0/2687	0.74	0/3611
9	B	0.42	0/14518	0.64	0/19682
11	b	0.37	0/636	0.61	0/856
11	k	0.40	0/636	0.62	0/856
12	h	0.38	0/649	0.56	0/880
12	l	0.43	0/725	0.62	0/980
13	j	0.41	0/753	0.64	0/1013
13	m	0.42	0/749	0.61	0/1009
14	d	0.38	0/634	0.61	0/859
14	n	0.41	0/634	0.55	0/859
15	e	0.42	0/585	0.58	0/795
15	p	0.44	0/585	0.57	0/795
16	f	0.42	0/585	0.60	0/791
16	q	0.44	0/585	0.59	0/791
17	g	0.37	0/532	0.56	0/715
17	r	0.41	0/529	0.54	0/711
18	E	0.44	0/184	0.65	0/238
19	U	0.33	0/3350	0.80	2/5209 (0.0%)
20	K	0.49	0/949	0.84	0/1292
21	2	0.46	0/745	0.72	0/1005
22	3	0.43	0/617	0.64	0/836
23	4	0.42	0/594	0.54	0/802
24	5	0.41	0/595	0.57	0/806
25	6	0.43	0/584	0.53	0/787
26	7	0.39	0/505	0.57	0/675

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
27	8	0.43	0/501	0.53	0/673
28	C	0.45	0/6590	0.78	1/8975 (0.0%)
All	All	0.44	0/77520	0.73	18/106621 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	A	0	9
5	J	0	2
7	F	0	1
9	B	0	2
11	k	0	1
28	C	0	2
All	All	0	17

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	17	A	C2'-C3'-O3'	7.97	127.03	109.50
5	J	613	LEU	CA-CB-CG	7.34	132.18	115.30
2	W	45	A	C2'-C3'-O3'	6.66	124.35	113.70
6	D	103	LEU	CA-CB-CG	6.55	130.37	115.30
19	U	128	A	C2'-C3'-O3'	5.94	123.21	113.70
3	A	979	SER	C-N-CD	-5.93	107.55	120.60
2	W	55	G	C2'-C3'-O3'	5.84	123.05	113.70
3	A	1268	ARG	NE-CZ-NH1	5.58	123.09	120.30
2	W	48	C	C2'-C3'-O3'	5.48	122.47	113.70
3	A	615	LEU	CA-CB-CG	5.42	127.76	115.30
1	V	75	U	N1-C1'-C2'	5.33	120.93	114.00
1	V	19	U	C2'-C3'-O3'	5.24	122.09	113.70
19	U	44	A	C1'-O4'-C4'	-5.20	105.74	109.90
3	A	425	ASP	CB-CG-OD2	5.16	122.94	118.30
5	J	199	ASP	N-CA-C	-5.13	97.16	111.00
28	C	273	LEU	CA-CB-CG	5.11	127.04	115.30
1	V	39	C	C2'-C3'-O3'	5.08	121.83	113.70
5	J	532	LEU	CA-CB-CG	5.07	126.96	115.30

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	1096	SER	Peptide
3	A	1216	ILE	Peptide
3	A	1279	VAL	Peptide
3	A	1522	ASN	Peptide
3	A	286	LEU	Peptide
3	A	467	GLU	Peptide
3	A	557	PHE	Peptide
3	A	974	ASN	Peptide
3	A	979	SER	Peptide
9	B	423	ILE	Peptide
9	B	458	PRO	Peptide
28	C	607	LEU	Peptide
28	C	958	PRO	Peptide
7	F	154	SER	Peptide
5	J	201	LEU	Peptide
5	J	820	GLN	Peptide
11	k	84	LEU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	V	2635	0	1328	39	0
2	W	1697	0	858	79	0
3	A	17778	0	17575	405	0
4	H	2789	0	2725	58	0
5	J	5822	0	5792	124	0
6	D	1151	0	1138	27	0
7	F	3218	0	3297	72	0
8	G	2632	0	2599	42	0
9	B	14212	0	14210	106	0
10	x	500	0	110	0	0
11	b	631	0	670	0	0
11	k	631	0	670	0	0
12	h	644	0	686	0	0
12	l	720	0	772	0	0
13	j	741	0	778	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	m	737	0	767	0	0
14	d	625	0	647	0	0
14	n	625	0	647	0	0
15	e	575	0	597	0	0
15	p	575	0	597	0	0
16	f	573	0	572	0	0
16	q	573	0	572	0	0
17	g	529	0	557	0	0
17	r	526	0	555	0	0
18	E	1713	0	567	1	0
19	U	2999	0	1516	55	0
20	K	936	0	987	42	0
21	2	735	0	744	11	0
22	3	611	0	620	4	0
23	4	588	0	602	2	0
24	5	588	0	594	3	0
25	6	577	0	572	2	0
26	7	504	0	557	1	0
27	8	498	0	533	1	0
28	C	6450	0	6419	167	0
29	C	32	0	12	0	0
All	All	77370	0	72442	1076	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 (1076) 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)
3:A:462:LEU:CD2	28:C:403:ASN:HD22	1.12	1.53
3:A:459:ALA:C	28:C:376:PHE:HE1	1.22	1.43
2:W:26:A:C5	3:A:671:TYR:CD1	2.10	1.39
3:A:462:LEU:CD2	28:C:403:ASN:ND2	1.77	1.38
3:A:462:LEU:HD21	28:C:403:ASN:ND2	1.35	1.32
3:A:459:ALA:C	28:C:376:PHE:CE1	2.03	1.32
2:W:26:A:C8	3:A:671:TYR:CE1	2.18	1.28
2:W:26:A:N3	3:A:667:TYR:O	1.66	1.27
3:A:459:ALA:O	28:C:376:PHE:HE1	1.13	1.26
2:W:26:A:C2	3:A:667:TYR:O	1.89	1.25
3:A:459:ALA:HB1	3:A:460:PRO:CD	1.67	1.22
3:A:459:ALA:O	28:C:376:PHE:CE1	1.94	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:459:ALA:CB	3:A:460:PRO:HD2	1.74	1.16
2:W:26:A:C4	3:A:671:TYR:CD1	2.34	1.14
3:A:462:LEU:HD22	28:C:403:ASN:ND2	1.63	1.11
2:W:26:A:C6	3:A:671:TYR:HB2	1.88	1.07
3:A:1578:ALA:HB1	3:A:1602:PRO:HB3	1.36	1.07
3:A:459:ALA:HB1	3:A:460:PRO:HD2	1.15	1.07
2:W:26:A:C6	3:A:671:TYR:CG	2.45	1.05
3:A:470:LEU:HB3	3:A:471:PRO:HD2	1.36	1.04
2:W:26:A:C8	3:A:671:TYR:CZ	2.45	1.03
3:A:461:LEU:HD21	28:C:380:PRO:HB3	1.40	1.03
2:W:26:A:C5	3:A:671:TYR:CE1	2.50	0.98
3:A:461:LEU:HD12	3:A:462:LEU:HG	1.47	0.97
2:W:26:A:N7	3:A:671:TYR:CE1	2.32	0.96
2:W:31:G:C5	3:A:1623:PHE:HD2	1.84	0.95
3:A:467:GLU:N	3:A:467:GLU:OE1	2.00	0.95
20:K:16:LEU:HD21	20:K:124:LEU:HD11	1.48	0.95
3:A:470:LEU:HB3	3:A:471:PRO:CD	1.96	0.95
3:A:1599:SER:O	3:A:1602:PRO:HD2	1.67	0.95
8:G:272:VAL:HG12	8:G:280:VAL:HG21	1.49	0.94
9:B:1700:ILE:HD11	9:B:1740:LEU:HD13	1.49	0.94
2:W:26:A:C4	3:A:671:TYR:CE1	2.55	0.94
2:W:26:A:C5	3:A:671:TYR:CG	2.56	0.94
3:A:461:LEU:CD1	3:A:462:LEU:HG	1.98	0.93
2:W:26:A:N9	3:A:671:TYR:CE1	2.36	0.92
2:W:26:A:C6	3:A:671:TYR:CB	2.53	0.92
2:W:26:A:C6	3:A:671:TYR:CD1	2.58	0.90
2:W:31:G:C6	3:A:1623:PHE:CD2	2.61	0.89
2:W:31:G:C6	3:A:1623:PHE:HD2	1.91	0.89
2:W:26:A:N7	3:A:671:TYR:CZ	2.42	0.88
3:A:461:LEU:HD12	3:A:462:LEU:N	1.89	0.87
3:A:2259:ILE:HD11	3:A:2293:ILE:HD11	1.55	0.87
2:W:26:A:N6	3:A:671:TYR:HB2	1.90	0.86
3:A:468:LEU:HD11	28:C:382:TYR:HB3	1.58	0.85
3:A:460:PRO:N	28:C:376:PHE:CE1	2.44	0.84
4:H:441:ILE:HG22	4:H:456:GLY:HA2	1.60	0.83
3:A:462:LEU:HD22	28:C:403:ASN:HD21	1.40	0.83
2:W:26:A:N1	3:A:671:TYR:HB2	1.94	0.83
2:W:29:U:C2	19:U:98:U:C2	2.67	0.82
2:W:26:A:O2'	3:A:667:TYR:CE1	2.32	0.82
2:W:31:G:C5	3:A:1623:PHE:CD2	2.67	0.81
3:A:1350:ILE:HG23	3:A:1356:LEU:HD23	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:164:ALA:HB1	3:A:199:ILE:HG21	1.62	0.80
3:A:673:VAL:HG22	3:A:714:PHE:CZ	2.18	0.79
3:A:468:LEU:O	3:A:468:LEU:HD23	1.82	0.79
28:C:323:THR:HG21	28:C:438:ALA:HB2	1.65	0.79
2:W:29:U:C4	19:U:98:U:C4	2.71	0.78
28:C:710:VAL:HG22	28:C:820:LEU:HD23	1.67	0.77
8:G:368:LEU:HD13	8:G:370:LEU:HD13	1.66	0.77
7:F:388:GLN:HG2	7:F:410:LEU:O	1.83	0.77
2:W:29:U:C4	19:U:98:U:N3	2.53	0.76
3:A:459:ALA:HB1	3:A:460:PRO:HD3	1.67	0.76
2:W:26:A:N6	3:A:671:TYR:CB	2.49	0.76
3:A:461:LEU:HD21	28:C:380:PRO:CB	2.15	0.75
2:W:30:G:H5'	2:W:31:G:H5''	1.68	0.74
1:V:18:A:OP2	7:F:378:LYS:NZ	2.20	0.74
28:C:235:VAL:HG23	28:C:261:VAL:HG11	1.69	0.74
3:A:460:PRO:HA	28:C:376:PHE:CD1	2.22	0.73
3:A:460:PRO:CG	3:A:463:ALA:HB2	2.18	0.73
28:C:836:SER:O	28:C:840:PRO:HD2	1.87	0.73
2:W:88:U:H1'	21:2:80:ASN:HB3	1.71	0.72
5:J:199:ASP:O	5:J:201:LEU:N	2.22	0.72
3:A:715:LEU:O	3:A:719:ILE:HG23	1.89	0.72
3:A:1320:LEU:HD11	3:A:1366:ARG:HB3	1.70	0.72
3:A:470:LEU:CB	3:A:471:PRO:CD	2.68	0.72
5:J:299:ALA:HB1	5:J:309:LEU:HD13	1.71	0.71
3:A:1206:CYS:SG	3:A:1207:TRP:N	2.63	0.71
28:C:345:THR:HA	28:C:348:LEU:HD12	1.71	0.71
5:J:361:ALA:HB1	5:J:371:LEU:HD13	1.73	0.71
3:A:171:ALA:HB1	3:A:201:PHE:HB3	1.72	0.70
2:W:26:A:O2'	3:A:667:TYR:HE1	1.71	0.70
3:A:1047:ALA:HB3	3:A:1251:TYR:HB3	1.72	0.70
3:A:1578:ALA:CB	3:A:1602:PRO:HB3	2.19	0.70
3:A:1335:TRP:CZ2	3:A:1339:LEU:HD13	2.26	0.70
2:W:31:G:N3	3:A:1636:GLY:HA2	1.83	0.69
7:F:233:VAL:HG11	7:F:237:ILE:HG21	1.73	0.69
1:V:50:G:H2'	1:V:51:U:O4'	1.93	0.69
2:W:27:U:C4'	3:A:668:ARG:HG2	2.23	0.68
3:A:330:LEU:HD21	3:A:386:ALA:HB2	1.74	0.68
7:F:347:ALA:HB1	7:F:348:PRO:CD	2.23	0.68
3:A:390:LEU:HD22	3:A:391:TYR:CE1	2.28	0.68
28:C:229:LEU:HD23	28:C:235:VAL:HG21	1.75	0.68
2:W:31:G:O6	3:A:1623:PHE:N	2.22	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:330:LEU:HD22	3:A:385:VAL:HG23	1.73	0.68
4:H:192:THR:HG21	4:H:461:ILE:CD1	2.24	0.68
5:J:597:ARG:HE	5:J:620:THR:HG22	1.59	0.67
28:C:866:ILE:HG22	28:C:868:VAL:HG13	1.76	0.67
3:A:461:LEU:HD12	3:A:461:LEU:C	2.14	0.67
19:U:41:A:H2'	19:U:42:A:C8	2.29	0.67
28:C:615:LEU:N	28:C:616:PRO:HD2	2.10	0.67
3:A:176:LEU:HD23	3:A:715:LEU:HD12	1.77	0.67
3:A:2330:GLU:CB	3:A:2331:PRO:CD	2.73	0.67
3:A:658:ASN:HD22	3:A:684:LYS:HB2	1.60	0.66
2:W:26:A:C4	3:A:671:TYR:HD1	2.09	0.66
3:A:1126:LEU:HD21	3:A:1161:TYR:CD2	2.30	0.66
6:D:86:TYR:CD2	6:D:124:ALA:HB1	2.30	0.66
5:J:264:ILE:HD13	5:J:284:LEU:HD11	1.76	0.66
5:J:327:VAL:HG11	5:J:344:ALA:HB2	1.77	0.66
7:F:253:ARG:HD2	20:K:70:LEU:HD13	1.76	0.66
5:J:598:PHE:HA	5:J:601:ILE:HD12	1.77	0.66
5:J:849:TYR:CD2	5:J:859:LEU:HD11	2.29	0.66
2:W:26:A:H1'	3:A:667:TYR:HD1	1.61	0.66
4:H:227:HIS:CD2	4:H:228:PRO:HD2	2.29	0.66
3:A:468:LEU:HD11	28:C:382:TYR:CB	2.25	0.65
20:K:98:ILE:HD12	20:K:99:ALA:N	2.11	0.65
3:A:1035:LEU:HD11	3:A:1160:LEU:HG	1.78	0.65
9:B:636:ILE:HG22	9:B:671:SER:HB2	1.78	0.65
3:A:462:LEU:HD21	28:C:403:ASN:HD22	0.49	0.65
5:J:215:LEU:CD2	7:F:400:VAL:HG22	2.27	0.64
3:A:460:PRO:HG3	3:A:463:ALA:HB2	1.79	0.64
7:F:74:LEU:HB3	7:F:75:PRO:HD3	1.80	0.64
7:F:119:LEU:HD12	7:F:197:ILE:HG22	1.79	0.64
28:C:493:LEU:HB3	28:C:556:ALA:HB3	1.80	0.64
3:A:459:ALA:HB3	3:A:460:PRO:HD2	1.73	0.64
3:A:960:THR:HG21	7:F:455:PHE:CZ	2.33	0.64
3:A:1175:GLU:O	3:A:1177:ASP:N	2.31	0.63
5:J:843:VAL:HG21	5:J:896:MET:HE2	1.79	0.63
19:U:129:G:H4'	19:U:130:A:H4'	1.80	0.63
2:W:26:A:N6	3:A:671:TYR:CG	2.66	0.63
3:A:461:LEU:HB3	28:C:332:TYR:OH	1.98	0.63
28:C:234:LEU:HD13	28:C:439:ILE:HG23	1.81	0.63
28:C:864:VAL:HG22	28:C:930:LEU:HD22	1.80	0.63
21:2:77:VAL:HG11	22:3:65:MET:HG2	1.79	0.63
3:A:1067:ASN:HB2	3:A:1083:THR:HG21	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1387:VAL:HG12	3:A:1610:TRP:CD2	2.33	0.62
20:K:40:ALA:O	20:K:43:THR:OG1	2.16	0.62
3:A:876:PRO:HB2	7:F:157:LEU:HD13	1.80	0.62
7:F:369:GLY:O	7:F:370:ARG:C	2.37	0.62
3:A:1603:ASN:C	3:A:1605:ARG:H	2.01	0.62
8:G:368:LEU:HD11	8:G:381:ILE:HD12	1.81	0.62
28:C:251:GLN:HG2	28:C:933:TRP:CD2	2.35	0.62
4:H:425:ASP:HB2	8:G:174:LEU:HD23	1.82	0.62
8:G:276:ASN:O	8:G:278:MET:N	2.33	0.62
2:W:49:A:O2'	2:W:50:G:OP2	2.16	0.62
5:J:758:LEU:HD21	20:K:75:ASN:HB2	1.80	0.62
20:K:16:LEU:CD2	20:K:124:LEU:HD11	2.25	0.62
28:C:288:LEU:HD13	28:C:313:PHE:CE2	2.34	0.61
28:C:873:LEU:HD22	28:C:900:LEU:HD13	1.81	0.61
28:C:360:ARG:HA	28:C:361:THR:HG22	1.81	0.61
2:W:31:G:N7	3:A:1623:PHE:CE2	2.68	0.61
5:J:465:VAL:HG11	5:J:501:VAL:HG22	1.82	0.61
5:J:737:VAL:HG22	5:J:767:PHE:CD2	2.35	0.61
9:B:1220:ILE:HD13	9:B:1241:LEU:HD11	1.82	0.61
3:A:813:GLU:O	3:A:816:ILE:HG13	1.99	0.61
3:A:1092:PHE:O	3:A:1093:LYS:C	2.38	0.61
5:J:351:LYS:O	5:J:355:ILE:HG13	2.01	0.61
3:A:175:LEU:HD13	3:A:571:LEU:HD12	1.82	0.61
3:A:939:LEU:HD21	7:F:445:ILE:HD11	1.82	0.61
7:F:347:ALA:HB1	7:F:348:PRO:HD2	1.81	0.61
2:W:26:A:O2'	3:A:667:TYR:CD1	2.50	0.61
2:W:26:A:N7	3:A:671:TYR:CD1	2.60	0.61
9:B:1022:LEU:HD23	9:B:1034:ILE:HD13	1.82	0.61
9:B:1544:LEU:HD21	9:B:1720:VAL:CG2	2.30	0.61
28:C:869:HIS:CD2	28:C:925:LEU:HD22	2.35	0.61
3:A:1835:LEU:HD21	3:A:1843:LEU:HD11	1.82	0.61
7:F:369:GLY:O	7:F:372:PHE:N	2.34	0.61
28:C:193:LEU:HD11	28:C:213:LEU:HB3	1.83	0.61
28:C:659:LEU:CD2	28:C:668:ILE:HD13	2.31	0.60
20:K:23:VAL:HG21	20:K:117:VAL:HG21	1.83	0.60
2:W:27:U:H4'	3:A:668:ARG:HG2	1.83	0.60
3:A:714:PHE:CZ	3:A:718:THR:HG21	2.36	0.60
1:V:35:G:N2	1:V:43:C:C2	2.70	0.60
3:A:960:THR:O	3:A:961:GLN:C	2.40	0.60
28:C:857:LEU:O	28:C:940:VAL:HG22	2.01	0.60
3:A:1603:ASN:O	3:A:1605:ARG:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:271:VAL:HG12	4:H:282:SER:HB3	1.84	0.60
5:J:341:TRP:CD1	5:J:365:ILE:HD11	2.37	0.60
5:J:613:LEU:O	5:J:617:PHE:CD2	2.55	0.60
3:A:1559:HIS:HB3	3:A:1613:THR:HG21	1.84	0.60
3:A:284:ARG:NH2	19:U:33:U:O4	2.35	0.59
3:A:1320:LEU:CD2	3:A:1367:ILE:HD13	2.32	0.59
9:B:1479:ILE:HG22	9:B:1488:TYR:HB3	1.84	0.59
3:A:330:LEU:HD12	28:C:920:LEU:HD21	1.84	0.59
20:K:37:ALA:HB2	20:K:98:ILE:HD11	1.83	0.59
9:B:1585:LEU:HD21	9:B:1683:LEU:HD23	1.84	0.59
3:A:1070:LEU:HD21	3:A:1113:ILE:CD1	2.31	0.59
3:A:1259:LEU:HD23	3:A:1268:ARG:HA	1.85	0.59
21:2:43:ILE:HD11	21:2:60:ILE:HG12	1.84	0.59
28:C:723:LEU:HB3	28:C:773:VAL:HG21	1.84	0.59
3:A:1921:VAL:HG21	3:A:1948:MET:HE1	1.84	0.59
3:A:460:PRO:HG2	3:A:463:ALA:HB2	1.83	0.58
5:J:616:PHE:O	5:J:620:THR:HG23	2.02	0.58
28:C:615:LEU:H	28:C:616:PRO:HD2	1.68	0.58
28:C:712:ALA:HB1	28:C:816:VAL:CG1	2.33	0.58
28:C:868:VAL:HG11	28:C:876:VAL:HG21	1.85	0.58
5:J:190:GLN:O	5:J:194:PRO:HD2	2.03	0.58
3:A:1614:ILE:HG22	3:A:1614:ILE:O	2.03	0.58
9:B:1291:THR:HG23	9:B:1303:GLU:HB3	1.85	0.58
3:A:1668:ILE:HD13	3:A:1801:SER:HB3	1.83	0.58
4:H:121:ARG:O	4:H:125:ILE:HG23	2.03	0.58
5:J:199:ASP:C	5:J:201:LEU:H	2.07	0.58
5:J:204:LEU:HD23	7:F:433:ASN:HD22	1.68	0.58
28:C:712:ALA:HB2	28:C:818:TYR:CD1	2.38	0.58
1:V:58:G:H2'	1:V:59:C:O4'	2.04	0.58
2:W:27:U:H1'	3:A:668:ARG:O	2.03	0.58
3:A:1063:PHE:CZ	3:A:1086:ASN:HB3	2.38	0.58
9:B:948:MET:HB3	9:B:966:LEU:HD11	1.84	0.58
3:A:1598:LEU:HA	3:A:1601:ILE:HD12	1.86	0.58
3:A:1123:LEU:O	3:A:1127:GLY:N	2.37	0.58
3:A:403:TYR:CD2	28:C:189:LEU:HD11	2.38	0.57
3:A:982:TYR:CD2	3:A:1104:ILE:HG23	2.38	0.57
3:A:1082:ILE:HD13	3:A:1113:ILE:HD11	1.86	0.57
8:G:365:LEU:HD22	8:G:382:VAL:HG12	1.85	0.57
4:H:392:HIS:HD2	4:H:396:VAL:HG22	1.68	0.57
22:3:26:LEU:HD13	22:3:68:ILE:HD11	1.85	0.57
3:A:470:LEU:CB	3:A:471:PRO:HD2	2.23	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:29:U:H2'	2:W:30:G:O4'	2.04	0.57
3:A:961:GLN:O	3:A:962:ARG:NH1	2.37	0.57
3:A:1207:TRP:O	3:A:1212:ARG:NH1	2.37	0.57
3:A:1405:ILE:HB	3:A:1437:ILE:HB	1.86	0.57
6:D:31:PHE:HB3	6:D:64:ILE:HD13	1.86	0.57
3:A:788:GLU:HB2	5:J:181:LEU:HD23	1.86	0.57
3:A:1063:PHE:CE1	3:A:1086:ASN:HB3	2.40	0.57
8:G:382:VAL:HG21	8:G:392:TYR:CD2	2.40	0.57
28:C:470:ALA:HB1	28:C:486:VAL:HG12	1.87	0.57
28:C:155:ILE:HA	28:C:161:ILE:HD11	1.85	0.57
3:A:1023:LEU:HD13	3:A:1451:PHE:CD1	2.39	0.57
3:A:1033:ASN:HB2	3:A:1288:LEU:HD23	1.85	0.57
3:A:1447:TRP:HB3	3:A:1451:PHE:CE2	2.40	0.57
5:J:238:PRO:C	5:J:240:ASN:HA	2.26	0.57
5:J:376:THR:HG22	5:J:388:LEU:HD13	1.86	0.57
7:F:106:LYS:O	7:F:109:ILE:HG22	2.05	0.57
2:W:26:A:N9	3:A:671:TYR:HE1	1.96	0.56
28:C:191:ILE:HG12	28:C:221:PHE:CZ	2.40	0.56
3:A:569:LEU:HD11	3:A:637:VAL:CG2	2.35	0.56
3:A:1560:THR:HG21	3:A:1609:TRP:NE1	2.20	0.56
5:J:702:PRO:O	5:J:706:VAL:HG23	2.05	0.56
28:C:602:VAL:HG11	28:C:908:VAL:HG21	1.86	0.56
28:C:862:TYR:CE2	28:C:908:VAL:HG13	2.40	0.56
3:A:670:LYS:O	3:A:673:VAL:HG23	2.06	0.56
5:J:323:LYS:O	5:J:327:VAL:HG23	2.06	0.56
5:J:590:ALA:HB3	5:J:591:PRO:HD3	1.87	0.56
7:F:298:VAL:HG12	7:F:302:MET:HB2	1.87	0.56
9:B:1804:SER:O	9:B:1807:VAL:HG22	2.06	0.56
28:C:200:CYS:HB3	28:C:436:VAL:HG21	1.87	0.56
2:W:84:C:H3'	8:G:350:PRO:HB3	1.88	0.56
5:J:452:ASN:CB	5:J:497:VAL:HG21	2.36	0.56
5:J:824:SER:O	5:J:828:LEU:HG	2.05	0.56
2:W:31:G:O6	3:A:1623:PHE:CD2	2.58	0.56
3:A:811:ILE:HA	5:J:162:LEU:HD23	1.86	0.56
3:A:1335:TRP:CD1	3:A:1367:ILE:HG13	2.41	0.56
19:U:46:C:H4'	28:C:111:LYS:CG	2.36	0.56
3:A:468:LEU:HD23	3:A:468:LEU:C	2.26	0.56
3:A:874:ILE:HD13	3:A:1065:LEU:HD22	1.88	0.56
3:A:2082:ILE:HD12	8:G:288:THR:HA	1.87	0.56
5:J:778:ILE:HG23	5:J:794:PHE:CE1	2.41	0.56
1:V:55:U:OP2	5:J:201:LEU:HD11	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2380:LEU:HB3	3:A:2384:ASN:HD22	1.70	0.56
4:H:261:LEU:HB3	4:H:292:TRP:CZ3	2.41	0.56
5:J:536:PHE:HB3	5:J:564:TYR:CZ	2.41	0.56
9:B:708:CYS:SG	9:B:709:GLY:N	2.78	0.56
28:C:680:SER:O	28:C:856:ILE:N	2.39	0.56
3:A:1210:ASP:CB	3:A:1278:VAL:HG11	2.37	0.55
28:C:472:VAL:HB	28:C:575:ALA:HB3	1.87	0.55
28:C:596:ASP:O	28:C:598:ILE:N	2.39	0.55
3:A:1603:ASN:C	3:A:1605:ARG:N	2.60	0.55
9:B:985:GLU:HG3	9:B:1001:LEU:HD22	1.87	0.55
20:K:64:LEU:O	20:K:66:HIS:N	2.39	0.55
24:5:15:THR:HG23	24:5:34:LEU:HD22	1.87	0.55
6:D:26:LEU:HD21	6:D:120:ILE:HD11	1.88	0.55
3:A:459:ALA:O	28:C:376:PHE:CD1	2.54	0.55
3:A:460:PRO:CA	28:C:376:PHE:CE1	2.88	0.55
3:A:889:TRP:CH2	3:A:893:ARG:HD3	2.42	0.55
8:G:341:VAL:HG11	8:G:463:PHE:CD1	2.42	0.55
9:B:391:PHE:O	9:B:392:ARG:C	2.45	0.55
24:5:82:VAL:HG22	26:7:92:THR:HG22	1.89	0.55
3:A:963:VAL:C	3:A:964:PHE:CD1	2.80	0.55
3:A:1115:GLN:HA	3:A:1115:GLN:OE1	2.06	0.55
3:A:1946:VAL:HG21	5:J:229:ILE:HG21	1.88	0.55
9:B:1950:ILE:O	9:B:1954:VAL:HG13	2.07	0.55
20:K:108:SER:OG	20:K:110:ILE:N	2.39	0.55
28:C:235:VAL:CG2	28:C:261:VAL:HG11	2.37	0.55
28:C:911:SER:OG	28:C:912:ALA:N	2.39	0.55
3:A:639:PHE:HA	3:A:644:VAL:HG11	1.88	0.55
2:W:61:C:H2'	2:W:62:A:C8	2.42	0.55
3:A:673:VAL:HG22	3:A:714:PHE:CE1	2.42	0.55
9:B:1035:PHE:CD2	9:B:1080:LEU:HD22	2.42	0.55
3:A:1414:TRP:HA	3:A:1558:GLU:HG2	1.89	0.55
28:C:712:ALA:HB2	28:C:818:TYR:CE1	2.42	0.55
3:A:503:LYS:HA	3:A:506:PHE:CE2	2.42	0.54
3:A:1375:LEU:O	3:A:1638:ILE:HG23	2.07	0.54
5:J:617:PHE:CD2	5:J:644:ARG:CZ	2.90	0.54
28:C:659:LEU:HD21	28:C:668:ILE:HD13	1.89	0.54
3:A:390:LEU:HD22	3:A:391:TYR:CD1	2.41	0.54
3:A:819:LYS:O	3:A:823:TRP:HB2	2.06	0.54
3:A:1407:ILE:HG21	3:A:1412:LEU:HD21	1.90	0.54
28:C:223:ASP:OD2	28:C:631:GLY:N	2.40	0.54
3:A:1383:PHE:HE1	3:A:1614:ILE:HG23	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1542:TYR:O	3:A:1546:VAL:HG23	2.07	0.54
5:J:248:ALA:HA	5:J:264:ILE:HD11	1.89	0.54
22:3:18:ILE:HD12	22:3:41:LEU:HD11	1.89	0.54
24:5:42:ASN:HB2	25:6:12:THR:HG21	1.90	0.54
28:C:656:LEU:HD22	28:C:670:ILE:HD11	1.90	0.54
3:A:883:PHE:O	3:A:887:VAL:HG23	2.08	0.54
3:A:1578:ALA:HB1	3:A:1602:PRO:CB	2.25	0.54
7:F:98:PHE:HA	7:F:101:ILE:HG22	1.89	0.54
20:K:54:MET:HG2	20:K:64:LEU:HD12	1.89	0.54
4:H:291:LEU:HD22	4:H:336:ILE:HG21	1.89	0.54
5:J:183:LYS:CG	7:F:350:ILE:HG22	2.38	0.54
6:D:80:MET:SD	6:D:80:MET:N	2.81	0.54
6:D:94:ASP:HB2	6:D:130:LEU:HD11	1.90	0.54
19:U:98:U:H2'	19:U:99:U:O4'	2.07	0.54
28:C:856:ILE:HG21	28:C:939:LYS:HG3	1.89	0.54
3:A:1853:ASP:HB3	3:A:1880:PHE:HB3	1.90	0.54
5:J:159:LEU:O	5:J:163:THR:HG23	2.08	0.54
20:K:24:VAL:HG13	20:K:33:LEU:CD1	2.38	0.54
3:A:656:ILE:O	3:A:660:ILE:HD12	2.08	0.53
3:A:1854:ASP:HB3	3:A:1913:THR:HG21	1.90	0.53
19:U:40:C:N3	19:U:115:G:C6	2.77	0.53
28:C:108:GLN:O	28:C:111:LYS:HD3	2.08	0.53
28:C:385:PHE:CE1	28:C:425:LEU:HD11	2.44	0.53
1:V:33:A:C8	1:V:45:A:C6	2.96	0.53
3:A:1222:LEU:O	3:A:1226:VAL:HG23	2.09	0.53
3:A:1286:TRP:CE2	3:A:1302:LEU:HD11	2.43	0.53
3:A:1342:LEU:CD2	3:A:1360:LEU:HD21	2.38	0.53
5:J:239:THR:N	5:J:240:ASN:HA	2.23	0.53
28:C:318:LEU:HB3	28:C:425:LEU:HD12	1.90	0.53
28:C:685:SER:CB	28:C:711:ALA:HB1	2.38	0.53
3:A:1014:LYS:HB3	3:A:1015:PRO:HA	1.90	0.53
5:J:207:LEU:HD12	7:F:382:SER:HB2	1.90	0.53
7:F:218:ILE:O	7:F:222:ILE:HG23	2.08	0.53
9:B:981:LEU:HD23	9:B:986:LEU:HD12	1.91	0.53
9:B:1782:ILE:HD11	9:B:1791:VAL:HG21	1.90	0.53
3:A:1340:ILE:HD11	3:A:1400:ILE:CD1	2.39	0.53
4:H:226:TRP:CE3	4:H:234:MET:HB3	2.43	0.53
4:H:235:ILE:HD11	4:H:243:ILE:HG13	1.91	0.53
5:J:337:ASP:HB3	5:J:340:LEU:HD12	1.89	0.53
9:B:1101:ILE:O	9:B:1105:ALA:N	2.41	0.53
9:B:1402:GLY:HA2	9:B:1405:ILE:HD12	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:U:99:U:C5	19:U:100:A:C4	2.97	0.53
28:C:856:ILE:HD13	28:C:939:LYS:HG3	1.90	0.53
3:A:305:LEU:HD21	3:A:476:ALA:HB2	1.91	0.53
3:A:901:PRO:HD3	3:A:1078:ILE:HD11	1.91	0.53
3:A:1394:LEU:HD11	3:A:1553:ILE:CD1	2.39	0.53
3:A:1669:LEU:HB3	3:A:1681:VAL:HG21	1.91	0.53
5:J:260:ALA:HB1	5:J:264:ILE:HD12	1.90	0.53
9:B:933:ASN:O	9:B:936:VAL:HG22	2.08	0.53
9:B:1456:SER:HA	9:B:1465:ILE:HD13	1.90	0.53
9:B:1930:LEU:HD22	9:B:1983:LEU:HD21	1.89	0.53
20:K:36:GLY:N	20:K:99:ALA:O	2.38	0.53
28:C:774:LEU:HD22	28:C:803:VAL:HB	1.91	0.53
3:A:1354:GLU:N	3:A:1355:PRO:CD	2.72	0.53
3:A:1820:ARG:O	3:A:1824:GLN:N	2.40	0.53
9:B:1398:ILE:HD13	9:B:1491:LEU:HD21	1.91	0.53
28:C:761:ALA:O	28:C:765:VAL:HG13	2.09	0.53
3:A:1879:ILE:HG12	3:A:1913:THR:HG23	1.91	0.53
5:J:204:LEU:CD1	7:F:381:LEU:HD23	2.39	0.53
3:A:461:LEU:HB3	28:C:332:TYR:CZ	2.44	0.52
3:A:461:LEU:O	3:A:462:LEU:HD23	2.09	0.52
3:A:1125:LEU:HD13	3:A:1168:ILE:HD12	1.91	0.52
4:H:125:ILE:HG22	4:H:337:ARG:HB3	1.91	0.52
2:W:29:U:N3	19:U:98:U:C2	2.78	0.52
3:A:284:ARG:N	3:A:285:PRO:HA	2.25	0.52
3:A:1913:THR:O	3:A:1917:VAL:HG23	2.09	0.52
5:J:498:GLN:HE21	5:J:498:GLN:N	2.07	0.52
9:B:1399:ASN:O	9:B:1405:ILE:HD11	2.09	0.52
19:U:15:A:H4'	19:U:15:A:OP1	2.08	0.52
3:A:459:ALA:CB	3:A:460:PRO:CD	2.37	0.52
28:C:219:VAL:HG11	28:C:931:TYR:HB3	1.91	0.52
1:V:99:G:H5''	9:B:1177:ALA:HB2	1.92	0.52
2:W:30:G:H5'	2:W:31:G:C5'	2.38	0.52
4:H:459:ARG:NH2	20:K:72:GLU:O	2.43	0.52
6:D:86:TYR:CG	6:D:124:ALA:HB1	2.43	0.52
7:F:57:LEU:HD21	7:F:108:ASN:HA	1.91	0.52
21:2:6:PHE:CZ	21:2:10:LEU:HD11	2.45	0.52
1:V:20:A:H2'	1:V:21:C:O4'	2.09	0.52
7:F:123:ARG:NH1	7:F:145:GLU:OE2	2.42	0.52
9:B:1095:ASN:O	9:B:1098:ILE:HG22	2.10	0.52
3:A:2189:LEU:HD13	3:A:2224:VAL:HG23	1.91	0.52
7:F:102:ILE:N	7:F:103:PRO:CD	2.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:574:PHE:CB	9:B:585:VAL:HG11	2.40	0.52
21:2:25:ILE:HD12	27:8:63:LEU:HD11	1.91	0.52
3:A:790:TRP:CZ3	3:A:793:TRP:CE3	2.98	0.52
6:D:121:PHE:CE2	6:D:125:ARG:HD2	2.45	0.52
9:B:404:GLY:O	9:B:407:GLN:HB2	2.10	0.52
2:W:31:G:N7	3:A:1623:PHE:CD2	2.78	0.51
3:A:1893:ILE:HD12	3:A:1978:VAL:HG22	1.91	0.51
5:J:849:TYR:CE2	5:J:859:LEU:HD11	2.45	0.51
2:W:30:G:C2	19:U:97:U:C2	2.99	0.51
3:A:379:ILE:HG23	3:A:379:ILE:O	2.11	0.51
3:A:467:GLU:H	3:A:467:GLU:CD	2.12	0.51
3:A:562:ILE:HG22	3:A:563:ASP:O	2.10	0.51
3:A:1026:TYR:HA	3:A:1286:TRP:CZ3	2.45	0.51
3:A:2330:GLU:CB	3:A:2331:PRO:HD3	2.40	0.51
19:U:40:C:C2	19:U:115:G:N1	2.78	0.51
20:K:39:GLU:O	20:K:43:THR:HG23	2.10	0.51
28:C:723:LEU:HD12	28:C:773:VAL:HG11	1.92	0.51
2:W:31:G:N7	3:A:1623:PHE:HE2	2.09	0.51
3:A:460:PRO:HA	28:C:376:PHE:CE1	2.46	0.51
3:A:1318:GLY:O	3:A:1321:MET:O	2.27	0.51
3:A:1992:TYR:OH	3:A:2005:PHE:HA	2.10	0.51
8:G:392:TYR:HA	8:G:395:LEU:HD23	1.93	0.51
2:W:29:U:O4	19:U:98:U:C4	2.63	0.51
4:H:371:GLY:HA2	4:H:396:VAL:HG23	1.92	0.51
9:B:1032:PHE:CD2	9:B:1080:LEU:HD23	2.45	0.51
3:A:1183:THR:HG23	3:A:1221:ASN:HB3	1.92	0.51
3:A:1654:TRP:HA	3:A:1657:ILE:HD12	1.92	0.51
3:A:1657:ILE:HA	3:A:1811:ALA:CB	2.40	0.51
4:H:192:THR:HG21	4:H:461:ILE:HD13	1.92	0.51
9:B:423:ILE:HG23	9:B:424:PRO:HD3	1.93	0.51
3:A:1676:LEU:HD12	3:A:1678:ILE:HD11	1.92	0.51
3:A:2084:LEU:HB3	3:A:2086:GLN:HB3	1.92	0.51
7:F:381:LEU:HD22	7:F:385:ARG:HB3	1.92	0.51
28:C:470:ALA:HB3	28:C:577:LEU:CD1	2.40	0.51
2:W:26:A:H1'	3:A:667:TYR:CD1	2.43	0.51
3:A:632:ILE:HG23	3:A:656:ILE:HG21	1.92	0.51
3:A:919:LEU:CD1	3:A:990:ILE:HD13	2.41	0.51
4:H:243:ILE:HG13	4:H:261:LEU:HD13	1.92	0.51
5:J:372:LEU:O	5:J:376:THR:HG23	2.11	0.51
5:J:601:ILE:HG12	5:J:617:PHE:CE1	2.46	0.51
6:D:120:ILE:HG22	6:D:131:VAL:HG11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:U:12:C:H2'	19:U:13:A:C8	2.45	0.51
3:A:1387:VAL:HG12	3:A:1610:TRP:CE3	2.45	0.51
28:C:864:VAL:HG22	28:C:930:LEU:CD2	2.41	0.51
5:J:687:SER:O	5:J:690:THR:OG1	2.23	0.51
3:A:461:LEU:HD12	3:A:462:LEU:CG	2.29	0.50
8:G:379:ILE:HD12	8:G:464:TYR:HA	1.93	0.50
28:C:879:LEU:HD11	28:C:921:SER:OG	2.11	0.50
3:A:919:LEU:HD13	3:A:990:ILE:HD13	1.92	0.50
5:J:863:PHE:CE1	5:J:893:LEU:HD11	2.47	0.50
9:B:535:VAL:HG13	9:B:557:ILE:HD13	1.93	0.50
4:H:171:GLN:NE2	4:H:172:LEU:O	2.44	0.50
5:J:465:VAL:CG1	5:J:501:VAL:HG22	2.42	0.50
8:G:195:LYS:HB2	8:G:196:LEU:HD12	1.92	0.50
28:C:360:ARG:HA	28:C:361:THR:CB	2.41	0.50
3:A:971:MET:SD	3:A:979:SER:OG	2.58	0.50
3:A:1454:SER:HA	3:A:1487:GLY:HA2	1.92	0.50
5:J:540:LEU:O	5:J:546:SER:N	2.45	0.50
7:F:135:LEU:HD22	7:F:208:TRP:CD1	2.46	0.50
19:U:23:C:H2'	19:U:24:G:O4'	2.11	0.50
28:C:360:ARG:HA	28:C:361:THR:CG2	2.41	0.50
1:V:22:G:C2	1:V:23:C:C2	2.99	0.50
2:W:26:A:N7	3:A:671:TYR:CE2	2.79	0.50
1:V:7:A:H2'	1:V:8:U:O4'	2.10	0.50
3:A:390:LEU:HD21	28:C:605:ILE:HD11	1.94	0.50
3:A:756:LEU:HD13	6:D:44:GLU:HG3	1.92	0.50
3:A:1413:SER:N	3:A:1743:TYR:OH	2.44	0.50
4:H:243:ILE:HG12	4:H:261:LEU:HB2	1.92	0.50
19:U:98:U:C4	19:U:99:U:C5	3.00	0.50
8:G:352:ILE:HD12	8:G:400:ILE:HG23	1.94	0.50
9:B:1982:MET:O	9:B:1986:GLY:N	2.45	0.50
19:U:38:A:H2'	19:U:39:U:C6	2.47	0.50
1:V:19:U:O2	1:V:19:U:O5'	2.30	0.50
20:K:35:LYS:HG2	20:K:91:CYS:HB3	1.94	0.50
1:V:30:G:C8	20:K:35:LYS:HD2	2.47	0.49
2:W:86:G:C6	2:W:87:U:C5	3.00	0.49
3:A:630:LYS:O	3:A:634:ASP:N	2.39	0.49
3:A:708:TRP:CZ2	3:A:712:LEU:HD11	2.47	0.49
6:D:81:THR:HG21	6:D:102:LYS:HD2	1.94	0.49
9:B:1001:LEU:HD23	9:B:1015:MET:HE2	1.94	0.49
28:C:872:LEU:HD13	28:C:922:THR:HG22	1.93	0.49
2:W:34:A:C6	2:W:50:G:C6	3.01	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:403:TYR:CE2	28:C:650:LEU:HD13	2.47	0.49
4:H:390:LEU:HB3	8:G:428:TRP:CE3	2.47	0.49
28:C:966:PHE:O	28:C:970:THR:HG23	2.11	0.49
1:V:58:G:C6	1:V:59:C:C4	3.01	0.49
3:A:786:LEU:HG	3:A:815:TYR:CE2	2.47	0.49
3:A:1811:ALA:HA	3:A:2101:LEU:HD13	1.95	0.49
6:D:5:LEU:HD13	6:D:47:SER:HB2	1.93	0.49
19:U:74:U:H2'	19:U:75:A:H4'	1.95	0.49
3:A:1098:VAL:HG21	7:F:276:GLU:N	2.27	0.49
7:F:194:ARG:O	7:F:197:ILE:HG13	2.12	0.49
28:C:193:LEU:HD21	28:C:213:LEU:HD13	1.95	0.49
5:J:686:MET:O	5:J:690:THR:HG23	2.13	0.49
28:C:621:ALA:CB	28:C:664:ALA:HB2	2.43	0.49
3:A:1394:LEU:HD11	3:A:1553:ILE:HD13	1.95	0.49
7:F:298:VAL:HG13	7:F:344:LEU:HD13	1.93	0.49
8:G:293:TRP:O	8:G:297:VAL:HG13	2.13	0.49
9:B:574:PHE:HB3	9:B:585:VAL:HG11	1.94	0.49
9:B:1001:LEU:HD23	9:B:1015:MET:CE	2.43	0.49
9:B:1544:LEU:HD21	9:B:1720:VAL:HG23	1.94	0.49
19:U:46:C:H4'	28:C:111:LYS:HG3	1.95	0.49
2:W:30:G:C2	19:U:97:U:O2	2.66	0.49
3:A:1836:ASN:N	3:A:1839:ASN:OD1	2.46	0.49
3:A:2207:ILE:HD12	3:A:2256:LEU:HB2	1.95	0.49
4:H:180:ALA:O	4:H:192:THR:HA	2.13	0.49
5:J:781:PHE:CE2	5:J:793:ILE:HG13	2.48	0.49
20:K:21:LEU:HD13	20:K:90:ALA:HB2	1.95	0.49
28:C:154:VAL:HG11	28:C:177:TYR:CD2	2.47	0.49
28:C:236:LEU:HD23	28:C:264:CYS:HB3	1.95	0.49
1:V:58:G:N1	1:V:59:C:C2	2.81	0.49
3:A:209:ILE:HB	3:A:212:VAL:HB	1.93	0.49
3:A:1580:GLY:HA3	7:F:389:ASN:CG	2.33	0.49
5:J:170:LEU:HD13	5:J:175:ASP:OD2	2.13	0.49
5:J:183:LYS:HG2	7:F:350:ILE:HG22	1.95	0.49
28:C:320:PHE:CE1	28:C:425:LEU:HD13	2.48	0.49
6:D:9:LEU:HD13	6:D:15:VAL:HA	1.95	0.49
20:K:67:LEU:N	20:K:68:PRO:CD	2.75	0.49
28:C:471:HIS:HB2	28:C:592:PHE:CZ	2.48	0.49
1:V:35:G:C2	1:V:43:C:C2	3.01	0.48
3:A:172:ILE:HA	3:A:571:LEU:HD11	1.95	0.48
3:A:1372:LYS:HG2	3:A:1383:PHE:CE2	2.48	0.48
5:J:763:ALA:HB1	5:J:773:LEU:CD1	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:1273:THR:HG21	9:B:1731:TYR:CD1	2.48	0.48
3:A:331:PHE:CD2	3:A:336:PHE:HZ	2.31	0.48
3:A:816:ILE:HD12	3:A:817:LYS:N	2.28	0.48
4:H:125:ILE:HG22	4:H:337:ARG:CB	2.43	0.48
5:J:260:ALA:HB1	5:J:264:ILE:CD1	2.43	0.48
5:J:331:LEU:HD13	5:J:341:TRP:CH2	2.47	0.48
7:F:105:ILE:HD13	7:F:210:LEU:HD21	1.95	0.48
9:B:499:LEU:HD23	9:B:503:GLN:HB3	1.95	0.48
28:C:621:ALA:HB2	28:C:664:ALA:HB2	1.95	0.48
3:A:831:ARG:HD2	3:A:831:ARG:HA	1.70	0.48
3:A:1073:ILE:HD13	3:A:1116:TYR:CE1	2.48	0.48
28:C:270:LEU:HD11	28:C:313:PHE:HB3	1.95	0.48
4:H:195:TRP:CG	4:H:220:LYS:HG3	2.49	0.48
4:H:390:LEU:HD13	8:G:428:TRP:HB2	1.95	0.48
9:B:567:VAL:O	9:B:571:VAL:HG23	2.12	0.48
9:B:1367:PHE:HB3	9:B:1532:ILE:HA	1.95	0.48
9:B:1707:VAL:N	9:B:1708:GLY:HA3	2.28	0.48
3:A:2189:LEU:HD11	3:A:2347:GLY:HA3	1.95	0.48
19:U:125:C:H2'	19:U:126:A:O4'	2.14	0.48
2:W:61:C:H2'	2:W:62:A:O4'	2.14	0.48
3:A:1312:PHE:CE2	3:A:1360:LEU:HD23	2.49	0.48
28:C:227:VAL:HG11	28:C:474:LYS:HD3	1.95	0.48
3:A:172:ILE:HD11	3:A:626:LEU:CD2	2.43	0.48
3:A:1088:VAL:HG22	3:A:1104:ILE:HD11	1.95	0.48
7:F:277:SER:HB2	7:F:279:VAL:HG12	1.94	0.48
9:B:1291:THR:HG22	9:B:1293:ILE:HD11	1.96	0.48
9:B:2113:ALA:HB2	9:B:2130:PHE:HB3	1.95	0.48
28:C:234:LEU:HD21	28:C:264:CYS:HB2	1.96	0.48
28:C:567:ILE:HG22	28:C:571:TYR:CE1	2.49	0.48
3:A:405:ASN:C	3:A:405:ASN:HD22	2.16	0.48
3:A:789:ALA:HB2	3:A:799:TRP:CE2	2.49	0.48
21:2:8:LYS:O	21:2:11:VAL:HG23	2.13	0.48
3:A:268:LEU:HD13	3:A:277:LYS:HB3	1.96	0.48
3:A:1598:LEU:O	3:A:1602:PRO:HD3	2.12	0.48
5:J:561:LEU:O	5:J:565:VAL:HG23	2.14	0.48
4:H:369:GLY:O	4:H:395:ILE:HG22	2.13	0.48
9:B:836:TRP:HA	9:B:836:TRP:CE3	2.49	0.48
19:U:87:G:H2'	19:U:88:U:C6	2.49	0.48
19:U:93:G:C6	19:U:94:C:N4	2.82	0.48
23:4:17:ILE:HD13	23:4:79:ILE:HG23	1.96	0.48
2:W:29:U:C5	19:U:98:U:N3	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:631:LEU:HD22	9:B:654:THR:HG21	1.96	0.47
20:K:121:ILE:HA	20:K:124:LEU:HD12	1.96	0.47
28:C:869:HIS:HB2	28:C:872:LEU:HD12	1.96	0.47
1:V:50:G:OP1	5:J:188:PRO:HG2	2.14	0.47
3:A:173:LEU:HD13	3:A:715:LEU:HB3	1.95	0.47
3:A:383:TYR:O	3:A:386:ALA:N	2.47	0.47
3:A:925:SER:HA	7:F:408:VAL:HG21	1.97	0.47
3:A:1795:LYS:N	3:A:1796:PRO:CD	2.77	0.47
4:H:176:LYS:HB3	4:H:177:PRO:HD2	1.96	0.47
5:J:674:LEU:CD2	5:J:690:THR:HG21	2.44	0.47
20:K:64:LEU:HD21	20:K:98:ILE:HB	1.96	0.47
3:A:569:LEU:HD11	3:A:637:VAL:HG22	1.96	0.47
3:A:1230:ILE:HD13	3:A:1230:ILE:HA	1.80	0.47
3:A:1946:VAL:HG21	5:J:229:ILE:CG2	2.44	0.47
6:D:79:PRO:O	6:D:81:THR:HG23	2.15	0.47
28:C:219:VAL:HG13	28:C:933:TRP:CH2	2.49	0.47
28:C:864:VAL:HG21	28:C:906:VAL:CG2	2.44	0.47
28:C:154:VAL:O	28:C:157:SER:OG	2.32	0.47
2:W:65:U:H2'	2:W:66:C:C6	2.49	0.47
3:A:1383:PHE:CE1	3:A:1614:ILE:HG23	2.48	0.47
4:H:271:VAL:HG12	4:H:282:SER:CB	2.43	0.47
5:J:691:TYR:CE2	5:J:711:ILE:HD11	2.50	0.47
9:B:543:TYR:HB2	9:B:550:LEU:HD12	1.96	0.47
9:B:558:VAL:HB	9:B:631:LEU:HD12	1.96	0.47
1:V:18:A:C5'	1:V:19:U:OP1	2.63	0.47
3:A:466:GLU:HG2	3:A:467:GLU:N	2.28	0.47
3:A:657:LEU:HD13	3:A:708:TRP:HA	1.97	0.47
3:A:1654:TRP:CZ3	3:A:1779:LEU:HD12	2.49	0.47
3:A:1961:LEU:HG	3:A:2084:LEU:HG	1.95	0.47
7:F:57:LEU:O	7:F:59:LEU:HD23	2.15	0.47
23:4:29:LEU:HD21	23:4:32:VAL:CG2	2.45	0.47
1:V:5:U:H2'	1:V:6:U:C6	2.50	0.47
3:A:792:CYS:SG	5:J:184:ASN:HB2	2.55	0.47
3:A:1795:LYS:HB3	3:A:1796:PRO:HD3	1.97	0.47
4:H:155:ARG:HD3	8:G:174:LEU:HD22	1.97	0.47
6:D:39:CYS:SG	6:D:40:MET:N	2.87	0.47
7:F:244:HIS:CD2	7:F:262:ILE:HG23	2.50	0.47
3:A:943:ALA:O	3:A:947:PRO:HA	2.15	0.47
6:D:97:THR:O	6:D:141:ARG:NH2	2.46	0.47
7:F:102:ILE:HG22	7:F:103:PRO:HD3	1.96	0.47
9:B:384:ASP:O	9:B:387:GLU:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:161:PHE:CE2	3:A:198:ALA:HB2	2.50	0.47
3:A:966:PRO:HB3	3:A:1089:VAL:HB	1.95	0.47
3:A:1605:ARG:HG2	3:A:1823:LEU:HA	1.97	0.47
5:J:209:ASN:CG	5:J:209:ASN:O	2.54	0.47
5:J:617:PHE:CE2	5:J:644:ARG:NH1	2.83	0.47
5:J:645:TYR:O	5:J:649:ASN:N	2.47	0.47
5:J:843:VAL:HG21	5:J:896:MET:CE	2.45	0.47
6:D:6:LEU:HD22	6:D:59:ILE:CG2	2.44	0.47
9:B:1482:GLY:O	9:B:1483:VAL:HG13	2.15	0.47
19:U:79:C:C2	19:U:114:G:N2	2.82	0.47
28:C:274:ILE:HG21	28:C:385:PHE:CD2	2.50	0.47
1:V:8:U:H2'	1:V:9:G:C8	2.50	0.47
5:J:229:ILE:HD12	7:F:417:LEU:HD21	1.97	0.47
19:U:132:A:O2'	19:U:133:C:OP1	2.28	0.47
25:6:52:ALA:HB3	25:6:71:VAL:HG21	1.97	0.47
28:C:133:ILE:HG23	28:C:209:MET:SD	2.55	0.47
28:C:320:PHE:CD1	28:C:425:LEU:HD13	2.50	0.47
28:C:539:VAL:HG13	28:C:564:ILE:CG2	2.45	0.47
3:A:823:TRP:NE1	3:A:851:ARG:HD3	2.30	0.46
3:A:882:ILE:CD1	3:A:1238:LEU:HD21	2.46	0.46
3:A:1974:LEU:O	3:A:1977:VAL:HG22	2.15	0.46
3:A:2041:PRO:O	3:A:2042:SER:C	2.54	0.46
4:H:424:SER:HA	4:H:427:TRP:CZ3	2.51	0.46
28:C:374:VAL:HG12	28:C:379:ILE:HG12	1.97	0.46
1:V:58:G:C2	1:V:59:C:C2	3.04	0.46
2:W:26:A:H2	3:A:667:TYR:O	1.78	0.46
3:A:1353:THR:HG23	3:A:1356:LEU:HB3	1.97	0.46
4:H:201:VAL:C	4:H:202:LEU:HD12	2.36	0.46
7:F:373:ARG:O	7:F:374:LYS:C	2.53	0.46
9:B:820:PHE:CD1	9:B:840:LEU:HD21	2.50	0.46
28:C:628:TYR:O	28:C:630:PRO:HD3	2.16	0.46
1:V:77:U:H3'	9:B:833:THR:HG22	1.96	0.46
2:W:31:G:OP1	3:A:1377:SER:OG	2.24	0.46
3:A:176:LEU:HD13	3:A:632:ILE:CD1	2.46	0.46
5:J:195:ASN:O	5:J:199:ASP:N	2.48	0.46
6:D:121:PHE:CZ	6:D:125:ARG:HD2	2.50	0.46
28:C:473:LEU:HB2	28:C:485:LEU:HD23	1.98	0.46
28:C:873:LEU:N	28:C:874:PRO:CD	2.79	0.46
3:A:140:ARG:NE	3:A:255:ILE:HD11	2.31	0.46
3:A:1607:THR:O	3:A:1611:SER:N	2.48	0.46
3:A:2015:LEU:HD23	3:A:2022:ALA:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:239:GLU:HA	4:H:267:ARG:CB	2.45	0.46
9:B:1409:LEU:HD22	9:B:1427:LYS:HB2	1.97	0.46
19:U:40:C:O2	19:U:115:G:C2	2.69	0.46
2:W:88:U:C1'	21:2:80:ASN:HB3	2.44	0.46
4:H:159:LEU:HD13	4:H:430:MET:CE	2.46	0.46
9:B:1226:TRP:CH2	9:B:1259:ILE:HG21	2.51	0.46
28:C:231:ALA:O	28:C:487:ARG:NH1	2.49	0.46
3:A:208:VAL:CG1	3:A:496:ALA:HB2	2.46	0.46
4:H:395:ILE:HD11	4:H:415:TYR:CD1	2.51	0.46
5:J:358:LEU:O	5:J:362:THR:HG23	2.15	0.46
1:V:35:G:C2	1:V:36:A:C8	3.04	0.46
3:A:193:TYR:CE1	3:A:560:THR:HG23	2.51	0.46
3:A:819:LYS:O	3:A:823:TRP:N	2.47	0.46
3:A:1676:LEU:HD11	3:A:1797:LEU:HD22	1.97	0.46
4:H:357:TRP:CZ3	4:H:364:VAL:HG22	2.51	0.46
5:J:601:ILE:HD13	5:J:640:VAL:HG11	1.96	0.46
8:G:193:GLU:O	8:G:196:LEU:N	2.49	0.46
3:A:138:HIS:NE2	3:A:142:ILE:HD11	2.30	0.46
3:A:550:SER:OG	3:A:558:GLN:NE2	2.49	0.46
3:A:672:LYS:N	19:U:101:C:OP1	2.43	0.46
3:A:1214:ARG:N	3:A:1255:ASN:OD1	2.47	0.46
19:U:129:G:H4'	19:U:130:A:C4'	2.46	0.46
2:W:27:U:H2'	2:W:28:U:C6	2.51	0.46
3:A:329:TYR:CD1	3:A:330:LEU:HG	2.51	0.46
3:A:1070:LEU:HD11	3:A:1113:ILE:HD12	1.97	0.46
5:J:792:THR:OG1	20:K:46:ARG:NE	2.49	0.46
8:G:264:LEU:HD12	9:B:458:PRO:HA	1.97	0.46
9:B:845:VAL:HG21	9:B:874:ARG:O	2.16	0.46
9:B:1656:TYR:CZ	9:B:1677:THR:HG22	2.50	0.46
28:C:615:LEU:N	28:C:616:PRO:CD	2.77	0.46
28:C:762:SER:O	28:C:765:VAL:HG22	2.15	0.46
1:V:57:U:O2'	1:V:58:G:H5'	2.16	0.45
3:A:355:LEU:HD13	3:A:355:LEU:O	2.16	0.45
9:B:480:ILE:HD12	9:B:491:PHE:CD1	2.52	0.45
28:C:862:TYR:N	28:C:906:VAL:O	2.46	0.45
28:C:866:ILE:HB	28:C:902:VAL:HG13	1.98	0.45
3:A:268:LEU:HD13	3:A:277:LYS:CB	2.46	0.45
5:J:254:ALA:N	5:J:255:ARG:HA	2.31	0.45
9:B:932:ARG:O	9:B:936:VAL:HG13	2.17	0.45
28:C:389:LEU:HD21	28:C:421:LEU:HD12	1.99	0.45
3:A:666:ILE:CG2	3:A:673:VAL:HG21	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:788:GLU:CB	5:J:181:LEU:HD23	2.46	0.45
3:A:819:LYS:O	3:A:823:TRP:CB	2.64	0.45
5:J:404:ILE:O	5:J:408:LEU:HG	2.16	0.45
5:J:561:LEU:HD23	5:J:585:GLN:HE21	1.82	0.45
5:J:601:ILE:HG12	5:J:617:PHE:HE1	1.81	0.45
8:G:402:TRP:CD1	8:G:424:ILE:HG21	2.51	0.45
9:B:793:LEU:HD12	9:B:803:THR:HG23	1.98	0.45
20:K:64:LEU:HD21	20:K:98:ILE:HD13	1.98	0.45
2:W:26:A:HO2'	3:A:667:TYR:HD1	1.50	0.45
3:A:1032:ILE:HG21	3:A:1258:LEU:CD2	2.46	0.45
3:A:1066:LEU:HD11	3:A:1113:ILE:HG23	1.99	0.45
3:A:1933:ILE:HG21	3:A:1944:LEU:HD21	1.98	0.45
3:A:2271:ALA:HB2	3:A:2326:SER:OG	2.16	0.45
4:H:283:ALA:HB2	4:H:313:LEU:HG	1.97	0.45
5:J:187:ASN:N	5:J:188:PRO:CD	2.79	0.45
9:B:539:LEU:HD11	9:B:555:PHE:CE1	2.51	0.45
9:B:633:ILE:HG21	9:B:636:ILE:HD13	1.99	0.45
3:A:305:LEU:HD22	28:C:390:SER:HA	1.99	0.45
5:J:211:ARG:CB	7:F:400:VAL:HG21	2.47	0.45
5:J:242:GLN:HA	5:J:245:ILE:HD12	1.99	0.45
5:J:536:PHE:HB3	5:J:564:TYR:CE2	2.51	0.45
6:D:82:VAL:CG2	6:D:103:LEU:HG	2.46	0.45
7:F:309:LYS:HG3	7:F:337:LEU:HD21	1.97	0.45
28:C:360:ARG:HA	28:C:361:THR:HB	1.99	0.45
28:C:685:SER:HB2	28:C:711:ALA:HB1	1.98	0.45
3:A:208:VAL:HG13	3:A:496:ALA:HB2	1.98	0.45
4:H:243:ILE:HD11	4:H:261:LEU:HD22	1.99	0.45
7:F:400:VAL:HG23	7:F:410:LEU:HG	1.99	0.45
19:U:115:G:H2'	19:U:116:U:C6	2.52	0.45
21:2:83:GLN:HG2	22:3:12:LEU:HD22	1.98	0.45
28:C:844:LYS:O	28:C:848:VAL:HG23	2.17	0.45
2:W:5:G:C6	2:W:6:C:N4	2.85	0.45
3:A:656:ILE:HA	3:A:663:LEU:HD12	1.98	0.45
3:A:963:VAL:C	3:A:964:PHE:CG	2.90	0.45
3:A:1320:LEU:HD21	3:A:1367:ILE:HD13	1.99	0.45
3:A:1752:VAL:HG11	3:A:1785:ASP:O	2.17	0.45
5:J:224:GLN:O	5:J:228:THR:HG23	2.17	0.45
5:J:605:GLY:HA3	5:J:887:THR:HG21	1.99	0.45
8:G:355:LYS:O	8:G:359:ASN:ND2	2.50	0.45
28:C:241:VAL:HG11	28:C:273:LEU:HD23	1.99	0.45
3:A:212:VAL:HA	3:A:311:LEU:HD22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:526:LEU:HD23	3:A:526:LEU:HA	1.90	0.45
3:A:885:VAL:HG21	3:A:1124:LEU:CD2	2.47	0.45
5:J:204:LEU:HD11	7:F:381:LEU:HD23	1.98	0.45
20:K:64:LEU:CD2	20:K:98:ILE:HD13	2.46	0.45
3:A:1599:SER:O	3:A:1602:PRO:CD	2.53	0.45
4:H:198:ASP:OD1	4:H:198:ASP:N	2.50	0.45
7:F:253:ARG:CD	20:K:70:LEU:HD13	2.46	0.45
28:C:161:ILE:HD12	28:C:164:MET:SD	2.57	0.45
28:C:861:ILE:HD12	28:C:936:ILE:CG2	2.47	0.45
1:V:10:C:H2'	1:V:11:A:O4'	2.16	0.45
3:A:805:PRO:HD3	5:J:178:LEU:CD2	2.47	0.45
3:A:1461:TYR:CE1	3:A:1475:LEU:HD23	2.52	0.45
28:C:210:ILE:HD11	28:C:436:VAL:HG13	1.98	0.45
28:C:634:ILE:HG13	28:C:644:ILE:HG23	1.99	0.45
5:J:259:VAL:HA	5:J:262:LYS:HD2	1.99	0.44
5:J:674:LEU:HD22	5:J:690:THR:HG21	1.99	0.44
8:G:264:LEU:HD13	9:B:711:LYS:HD3	1.98	0.44
9:B:1084:PHE:CE2	9:B:1131:LEU:HD13	2.52	0.44
4:H:316:GLN:HE21	4:H:361:GLY:HA3	1.82	0.44
6:D:49:ILE:HG23	6:D:114:ILE:HG12	1.99	0.44
8:G:347:LEU:HD11	8:G:371:ARG:CD	2.47	0.44
3:A:173:LEU:HA	3:A:715:LEU:HD13	1.98	0.44
3:A:1063:PHE:HD2	7:F:272:LEU:HD11	1.82	0.44
3:A:1536:LEU:HD23	3:A:1536:LEU:HA	1.84	0.44
8:G:363:LEU:HD11	8:G:391:PHE:CD2	2.52	0.44
19:U:73:U:H2'	19:U:74:U:N1	2.32	0.44
20:K:53:ILE:HD11	20:K:102:ILE:HG12	1.99	0.44
2:W:77:G:H2'	2:W:78:G:O4'	2.17	0.44
3:A:468:LEU:C	3:A:468:LEU:CD2	2.86	0.44
5:J:215:LEU:HD22	7:F:400:VAL:HG22	1.99	0.44
8:G:347:LEU:HD11	8:G:371:ARG:HD3	2.00	0.44
19:U:6:G:C6	19:U:7:C:N4	2.86	0.44
28:C:774:LEU:HD13	28:C:803:VAL:HG23	2.00	0.44
2:W:85:C:OP2	8:G:353:ARG:CZ	2.65	0.44
3:A:1557:LEU:O	3:A:1560:THR:N	2.49	0.44
5:J:201:LEU:HD23	7:F:379:PHE:CZ	2.52	0.44
5:J:378:LEU:C	5:J:378:LEU:HD13	2.38	0.44
1:V:75:U:O2	1:V:75:U:C2'	2.65	0.44
2:W:84:C:C2	2:W:85:C:C5	3.05	0.44
3:A:405:ASN:C	3:A:405:ASN:ND2	2.71	0.44
3:A:674:MET:HA	3:A:677:ILE:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1350:ILE:HG23	3:A:1356:LEU:CD2	2.38	0.44
5:J:568:TYR:CZ	5:J:581:VAL:HG21	2.53	0.44
9:B:708:CYS:SG	9:B:889:ILE:HA	2.58	0.44
9:B:1703:LEU:O	9:B:1707:VAL:HG22	2.18	0.44
19:U:32:G:O6	19:U:120:G:O6	2.35	0.44
28:C:341:ILE:O	28:C:345:THR:HG23	2.17	0.44
1:V:59:C:H5''	1:V:59:C:H6	1.83	0.44
3:A:326:ASN:ND2	3:A:404:ASN:OD1	2.49	0.44
3:A:591:LEU:HD22	3:A:599:LEU:HD21	1.99	0.44
3:A:1335:TRP:CH2	3:A:1339:LEU:HD13	2.52	0.44
5:J:204:LEU:HD22	7:F:380:ARG:O	2.18	0.44
28:C:322:PHE:CE2	28:C:381:LEU:HD11	2.52	0.44
28:C:656:LEU:HD13	28:C:670:ILE:HD13	2.00	0.44
3:A:703:PHE:CE2	3:A:706:PRO:HD3	2.53	0.44
3:A:1320:LEU:HD23	3:A:1367:ILE:HD13	1.98	0.44
3:A:1603:ASN:OD1	3:A:1603:ASN:N	2.51	0.44
5:J:698:VAL:HG23	5:J:698:VAL:O	2.18	0.44
7:F:77:ILE:HG22	7:F:78:VAL:HG23	2.00	0.44
9:B:740:ILE:HD11	9:B:846:ILE:HD12	1.99	0.44
20:K:98:ILE:HD12	20:K:99:ALA:CB	2.48	0.44
3:A:459:ALA:CA	28:C:376:PHE:CE1	2.97	0.44
5:J:780:LEU:O	5:J:783:HIS:HB2	2.18	0.44
6:D:93:CYS:SG	6:D:120:ILE:HG21	2.58	0.44
6:D:109:ASP:HB2	6:D:112:GLU:CB	2.48	0.44
7:F:47:LEU:HD13	7:F:97:PHE:HB3	1.99	0.44
28:C:872:LEU:HB3	28:C:922:THR:HG23	2.00	0.44
3:A:308:MET:CG	3:A:479:LEU:HD21	2.48	0.43
3:A:534:LEU:HD23	3:A:535:HIS:CE1	2.53	0.43
19:U:74:U:C2	19:U:75:A:H4'	2.53	0.43
20:K:117:VAL:O	20:K:121:ILE:HG13	2.18	0.43
1:V:75:U:O2	1:V:75:U:H2'	2.17	0.43
3:A:1860:VAL:HA	3:A:1861:THR:HA	2.00	0.43
4:H:357:TRP:CH2	4:H:364:VAL:HG22	2.52	0.43
6:D:112:GLU:CD	6:D:137:TYR:OH	2.57	0.43
8:G:339:CYS:HB2	8:G:383:VAL:HG22	2.00	0.43
9:B:1183:ILE:HD11	9:B:1192:VAL:HG11	1.98	0.43
19:U:132:A:C2'	19:U:133:C:OP1	2.66	0.43
28:C:227:VAL:HG22	28:C:595:LEU:HD12	2.00	0.43
28:C:492:LEU:HD12	28:C:492:LEU:O	2.18	0.43
28:C:774:LEU:HD21	28:C:813:ILE:HG21	2.01	0.43
2:W:50:G:N3	2:W:50:G:C2'	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:162:MET:HB3	4:H:421:VAL:HG21	2.00	0.43
5:J:289:VAL:HG23	5:J:290:HIS:N	2.33	0.43
5:J:324:TYR:CD1	5:J:347:PHE:CE2	3.07	0.43
9:B:589:THR:HG23	9:B:589:THR:O	2.18	0.43
19:U:22:G:N1	19:U:131:A:C2	2.86	0.43
21:2:25:ILE:HD11	21:2:52:PRO:HG3	1.99	0.43
3:A:808:ILE:HA	3:A:811:ILE:HG22	2.00	0.43
3:A:1737:GLN:HE21	3:A:1737:GLN:HA	1.83	0.43
28:C:314:ALA:CB	28:C:321:THR:HG22	2.48	0.43
2:W:5:G:C2	2:W:6:C:C2	3.05	0.43
3:A:338:ASN:OD1	3:A:399:ARG:N	2.51	0.43
3:A:2003:THR:O	3:A:2006:SER:OG	2.31	0.43
4:H:172:LEU:HD22	5:J:755:GLN:HG3	2.01	0.43
4:H:243:ILE:CG1	4:H:261:LEU:HD13	2.49	0.43
4:H:445:ILE:HA	4:H:452:LEU:HD23	2.00	0.43
5:J:764:LEU:HD13	5:J:774:TRP:CZ2	2.53	0.43
8:G:287:ILE:HD12	8:G:287:ILE:N	2.32	0.43
19:U:41:A:C2	19:U:42:A:N1	2.86	0.43
1:V:30:G:O2'	20:K:97:VAL:HG22	2.18	0.43
3:A:200:THR:N	3:A:574:GLN:OE1	2.46	0.43
3:A:883:PHE:CZ	3:A:1072:LEU:HD11	2.54	0.43
3:A:920:LYS:O	3:A:921:ASP:C	2.57	0.43
3:A:1054:LEU:HD13	3:A:1121:ILE:HG21	2.00	0.43
3:A:1204:ARG:O	3:A:1206:CYS:N	2.51	0.43
7:F:52:GLU:O	7:F:56:THR:HG23	2.19	0.43
9:B:1109:LEU:HD22	9:B:1131:LEU:HD12	2.00	0.43
20:K:71:CYS:O	20:K:75:ASN:N	2.52	0.43
28:C:197:THR:O	28:C:198:LEU:HD23	2.19	0.43
1:V:31:U:O4'	20:K:63:ILE:HD12	2.19	0.43
2:W:29:U:N3	19:U:98:U:N3	2.67	0.43
3:A:141:LYS:O	3:A:145:THR:HG23	2.19	0.43
3:A:172:ILE:HD11	3:A:626:LEU:HD21	2.01	0.43
3:A:239:PHE:HA	3:A:240:PRO:C	2.38	0.43
3:A:708:TRP:CE2	3:A:712:LEU:HD11	2.54	0.43
3:A:1203:ASN:ND2	3:A:1213:MET:O	2.50	0.43
3:A:1598:LEU:O	3:A:1601:ILE:HB	2.18	0.43
3:A:1676:LEU:HD11	3:A:1797:LEU:CD2	2.49	0.43
7:F:374:LYS:O	7:F:375:TYR:C	2.57	0.43
19:U:43:G:C2'	19:U:44:A:H5'	2.49	0.43
1:V:74:U:O2	1:V:74:U:C2'	2.66	0.43
3:A:831:ARG:HH11	3:A:848:ASN:HD21	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:889:TRP:CZ2	3:A:893:ARG:HD3	2.54	0.43
7:F:120:TYR:CE1	7:F:141:ILE:HG23	2.53	0.43
8:G:276:ASN:O	8:G:277:MET:C	2.57	0.43
19:U:20:U:H2'	19:U:21:G:C1'	2.48	0.43
20:K:20:ILE:HD13	20:K:79:VAL:HG21	2.01	0.43
28:C:234:LEU:HD23	28:C:235:VAL:N	2.34	0.43
3:A:1158:ILE:HG22	3:A:1158:ILE:O	2.19	0.43
3:A:1561:LEU:O	3:A:1564:GLY:N	2.47	0.43
5:J:504:LYS:HG3	5:J:508:TRP:CZ3	2.54	0.43
7:F:229:VAL:HG23	7:F:317:ASP:OD2	2.18	0.43
9:B:644:GLY:N	9:B:645:PRO:HD2	2.33	0.43
9:B:707:PHE:CZ	9:B:902:LEU:HD12	2.54	0.43
19:U:133:C:H2'	19:U:133:C:O2	2.19	0.43
20:K:54:MET:CG	20:K:64:LEU:HD12	2.48	0.43
28:C:472:VAL:HA	28:C:486:VAL:HG22	2.01	0.43
3:A:172:ILE:HG23	3:A:629:MET:HG3	2.00	0.43
3:A:461:LEU:N	28:C:332:TYR:OH	2.52	0.43
3:A:905:TYR:HB3	3:A:908:ASP:HB2	2.01	0.43
3:A:1354:GLU:N	3:A:1355:PRO:HD2	2.34	0.43
5:J:702:PRO:HA	5:J:739:PHE:CZ	2.54	0.43
5:J:839:GLY:O	5:J:841:THR:N	2.52	0.43
9:B:677:TYR:HB2	9:B:691:LEU:HD11	2.01	0.43
9:B:1774:THR:HG21	18:E:412:UNK:HA	2.01	0.43
9:B:1803:LEU:O	9:B:1807:VAL:HG13	2.19	0.43
3:A:365:ASN:OD1	3:A:365:ASN:N	2.52	0.42
4:H:390:LEU:HD13	8:G:428:TRP:CG	2.54	0.42
4:H:435:GLY:N	5:J:731:LEU:HD13	2.34	0.42
5:J:341:TRP:CE3	5:J:361:ALA:HB2	2.54	0.42
5:J:737:VAL:HG13	5:J:773:LEU:HD11	1.99	0.42
7:F:233:VAL:CG1	7:F:237:ILE:HG21	2.46	0.42
9:B:1157:ILE:HD12	9:B:1158:LYS:N	2.34	0.42
9:B:1273:THR:HG21	9:B:1731:TYR:CE1	2.54	0.42
19:U:20:U:H2'	19:U:21:G:O4'	2.19	0.42
19:U:46:C:C5'	28:C:111:LYS:HG2	2.50	0.42
3:A:857:ILE:CD1	3:A:969:ILE:HD11	2.49	0.42
3:A:2165:ARG:HB3	3:A:2300:VAL:HG13	2.00	0.42
5:J:327:VAL:O	5:J:331:LEU:HG	2.19	0.42
5:J:369:MET:HG3	5:J:404:ILE:HD11	2.00	0.42
8:G:200:ILE:HG23	8:G:200:ILE:O	2.19	0.42
9:B:448:LEU:N	9:B:449:PRO:HA	2.34	0.42
3:A:1063:PHE:CD2	7:F:272:LEU:HD11	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1120:VAL:O	3:A:1124:LEU:HG	2.20	0.42
4:H:365:ALA:HB2	4:H:375:VAL:HG13	2.01	0.42
4:H:445:ILE:HG23	4:H:452:LEU:CD2	2.50	0.42
5:J:737:VAL:HG22	5:J:767:PHE:CG	2.54	0.42
7:F:233:VAL:HG11	7:F:237:ILE:CG2	2.44	0.42
28:C:483:TRP:CH2	28:C:550:VAL:HG11	2.54	0.42
4:H:426:THR:OG1	4:H:427:TRP:N	2.52	0.42
6:D:112:GLU:HG2	6:D:135:TYR:CE1	2.54	0.42
9:B:578:LEU:HB3	9:B:583:ILE:HD12	2.01	0.42
1:V:33:A:H1'	1:V:45:A:C2	2.55	0.42
3:A:1946:VAL:CG2	5:J:229:ILE:HG21	2.48	0.42
4:H:117:LEU:HD13	4:H:301:LEU:HD12	2.01	0.42
5:J:561:LEU:O	5:J:564:TYR:HB2	2.19	0.42
7:F:311:SER:O	7:F:315:ARG:HG2	2.19	0.42
7:F:347:ALA:CB	7:F:348:PRO:CD	2.96	0.42
8:G:286:ASN:OD1	8:G:293:TRP:NE1	2.52	0.42
9:B:429:LEU:HA	9:B:432:ILE:HD12	2.02	0.42
9:B:1224:ALA:HB1	9:B:1226:TRP:CZ3	2.53	0.42
3:A:1032:ILE:HG21	3:A:1258:LEU:HD23	2.01	0.42
3:A:1752:VAL:CG1	3:A:1776:GLY:HA3	2.49	0.42
3:A:1835:LEU:CD2	3:A:1843:LEU:HD11	2.49	0.42
7:F:283:GLY:O	7:F:284:TYR:C	2.58	0.42
9:B:1978:ASP:O	9:B:1982:MET:HG3	2.20	0.42
20:K:23:VAL:HG21	20:K:117:VAL:CG2	2.48	0.42
28:C:271:ASP:CB	28:C:318:LEU:HD12	2.50	0.42
28:C:288:LEU:HD13	28:C:313:PHE:HE2	1.83	0.42
28:C:774:LEU:HD21	28:C:813:ILE:CG2	2.50	0.42
2:W:87:U:C5	8:G:441:PHE:CD1	3.08	0.42
3:A:198:ALA:HA	3:A:574:GLN:HG2	2.02	0.42
3:A:330:LEU:HD21	3:A:386:ALA:CB	2.47	0.42
3:A:885:VAL:HG21	3:A:1124:LEU:HD23	2.02	0.42
3:A:1993:ASP:HB2	3:A:2038:HIS:CG	2.54	0.42
3:A:2084:LEU:HD22	3:A:2086:GLN:CD	2.40	0.42
4:H:373:ILE:HG13	4:H:391:ALA:HB2	2.00	0.42
9:B:391:PHE:O	9:B:393:GLU:N	2.53	0.42
9:B:836:TRP:HA	9:B:836:TRP:HE3	1.83	0.42
19:U:70:A:H3'	19:U:71:A:H5''	2.02	0.42
20:K:24:VAL:HG22	20:K:53:ILE:HD13	2.02	0.42
28:C:241:VAL:CG1	28:C:273:LEU:HD23	2.49	0.42
1:V:31:U:OP1	20:K:98:ILE:HG13	2.20	0.42
3:A:591:LEU:HA	3:A:601:PRO:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1028:TRP:NE1	3:A:1032:ILE:HD11	2.34	0.42
3:A:1186:TYR:CE2	3:A:1224:ARG:HB3	2.55	0.42
4:H:195:TRP:O	4:H:220:LYS:HA	2.20	0.42
4:H:238:ALA:HB3	4:H:240:ASP:HB3	2.01	0.42
6:D:29:ILE:HG21	6:D:31:PHE:CE1	2.55	0.42
7:F:70:THR:HA	7:F:73:ILE:HD12	2.01	0.42
7:F:171:GLN:O	7:F:174:VAL:HG22	2.19	0.42
28:C:634:ILE:O	28:C:634:ILE:HG22	2.19	0.42
3:A:2041:PRO:O	3:A:2043:PHE:N	2.53	0.42
5:J:265:GLU:HG2	5:J:281:ASN:HD21	1.84	0.42
9:B:398:LYS:O	9:B:399:ARG:CB	2.68	0.42
19:U:93:G:C2	19:U:94:C:N3	2.87	0.42
28:C:127:ALA:O	28:C:133:ILE:HD11	2.20	0.42
3:A:171:ALA:CB	3:A:201:PHE:HB3	2.44	0.42
3:A:459:ALA:C	28:C:376:PHE:CZ	2.83	0.42
3:A:1092:PHE:O	3:A:1095:MET:N	2.52	0.42
3:A:1126:LEU:O	3:A:1130:ARG:HB3	2.19	0.42
3:A:2225:VAL:HG11	3:A:2242:PRO:HG3	2.02	0.42
4:H:122:ARG:O	4:H:125:ILE:HG12	2.20	0.42
9:B:978:LEU:HD23	9:B:981:LEU:HD12	2.02	0.42
9:B:1812:ASN:HA	9:B:1815:VAL:HG22	2.02	0.42
3:A:377:VAL:HG21	28:C:912:ALA:HB3	2.01	0.41
3:A:999:LEU:HD13	3:A:1112:PHE:CE1	2.55	0.41
5:J:578:GLN:HE21	5:J:603:LEU:CD2	2.33	0.41
9:B:633:ILE:HD12	9:B:633:ILE:N	2.35	0.41
28:C:617:LYS:CB	28:C:666:ILE:HD11	2.49	0.41
28:C:768:PHE:HB3	28:C:775:ILE:HA	2.02	0.41
2:W:29:U:C2	19:U:98:U:O2	2.70	0.41
3:A:596:ASN:O	3:A:598:ASN:N	2.46	0.41
3:A:785:HIS:CD2	5:J:181:LEU:HD22	2.55	0.41
3:A:2255:LEU:HD21	3:A:2281:PHE:CE1	2.54	0.41
5:J:383:ASN:O	5:J:387:THR:HG23	2.20	0.41
6:D:137:TYR:O	6:D:138:ASN:CB	2.68	0.41
8:G:344:PHE:HB3	8:G:424:ILE:HD13	2.03	0.41
9:B:406:ASP:O	9:B:409:GLN:N	2.53	0.41
9:B:491:PHE:HZ	9:B:533:LEU:HD21	1.86	0.41
20:K:79:VAL:HG13	20:K:121:ILE:HG23	2.01	0.41
28:C:108:GLN:O	28:C:111:LYS:CD	2.68	0.41
28:C:255:GLN:HG3	28:C:598:ILE:HD13	2.02	0.41
3:A:644:VAL:HG22	3:A:645:ASP:H	1.85	0.41
3:A:895:PHE:CZ	3:A:1008:LEU:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1206:CYS:SG	3:A:1207:TRP:CD1	3.13	0.41
3:A:1814:VAL:HG23	3:A:2098:MET:HG2	2.01	0.41
5:J:185:ALA:O	5:J:187:ASN:N	2.53	0.41
5:J:733:ASN:OD1	5:J:739:PHE:CE1	2.74	0.41
6:D:84:PHE:HB3	6:D:120:ILE:HD12	2.03	0.41
7:F:320:GLN:HE22	7:F:326:ASN:HB3	1.86	0.41
8:G:214:ILE:O	8:G:214:ILE:HG22	2.19	0.41
9:B:676:ASN:O	9:B:680:VAL:HG23	2.20	0.41
9:B:809:THR:HA	9:B:1092:PHE:CG	2.55	0.41
19:U:41:A:C2	19:U:42:A:C6	3.08	0.41
28:C:418:GLN:HB3	28:C:419:PRO:HD3	2.01	0.41
28:C:470:ALA:HB3	28:C:577:LEU:HD11	2.02	0.41
1:V:36:A:C2	1:V:37:U:C6	3.08	0.41
2:W:62:A:C4	2:W:63:G:C8	3.09	0.41
3:A:1673:LEU:HA	3:A:1678:ILE:HD12	2.01	0.41
5:J:867:GLU:HB2	5:J:874:TRP:CZ3	2.55	0.41
9:B:1095:ASN:O	9:B:1099:VAL:HG23	2.19	0.41
3:A:279:TRP:HB2	3:A:286:LEU:HB3	2.02	0.41
3:A:875:THR:HB	3:A:876:PRO:HD2	2.01	0.41
3:A:2159:ASN:HA	3:A:2162:LEU:HD13	2.03	0.41
3:A:2378:ILE:N	3:A:2378:ILE:HD12	2.35	0.41
5:J:781:PHE:CZ	5:J:793:ILE:HG13	2.56	0.41
7:F:45:GLU:O	7:F:48:PRO:HD2	2.21	0.41
8:G:260:ILE:HD12	8:G:266:PRO:HG2	2.02	0.41
9:B:779:GLN:O	9:B:783:THR:HG23	2.21	0.41
9:B:936:VAL:HG11	9:B:971:GLU:CD	2.40	0.41
1:V:22:G:N2	1:V:23:C:C2	2.89	0.41
3:A:914:LEU:HD22	3:A:1505:ASP:HB2	2.03	0.41
3:A:1000:TRP:NE1	3:A:1112:PHE:HB2	2.36	0.41
4:H:227:HIS:HA	4:H:273:TYR:CD2	2.55	0.41
5:J:190:GLN:O	5:J:194:PRO:CD	2.66	0.41
7:F:315:ARG:HD2	20:K:66:HIS:CE1	2.56	0.41
9:B:491:PHE:CZ	9:B:533:LEU:HD21	2.56	0.41
28:C:120:ARG:HD3	28:C:551:TYR:CE1	2.55	0.41
28:C:251:GLN:HG2	28:C:933:TRP:CG	2.55	0.41
28:C:324:ILE:HG23	28:C:377:ILE:HD11	2.01	0.41
28:C:328:VAL:HG21	28:C:345:THR:HG22	2.03	0.41
1:V:57:U:C4	2:W:63:G:C2	3.09	0.41
3:A:1405:ILE:HG21	3:A:1437:ILE:HG13	2.02	0.41
5:J:565:VAL:HG11	5:J:599:PHE:CB	2.50	0.41
5:J:845:LEU:O	5:J:849:TYR:HD2	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:291:ILE:CD1	7:F:306:LEU:HD22	2.51	0.41
8:G:263:GLY:N	9:B:458:PRO:HG2	2.35	0.41
9:B:1770:VAL:O	9:B:1774:THR:HG23	2.21	0.41
19:U:128:A:N3	19:U:128:A:H2'	2.35	0.41
28:C:469:TRP:CZ3	28:C:590:LYS:HG2	2.56	0.41
28:C:599:THR:HA	28:C:933:TRP:HA	2.02	0.41
1:V:6:U:H2'	1:V:7:A:C8	2.55	0.41
1:V:37:U:H2'	1:V:39:C:C5	2.56	0.41
3:A:404:ASN:CG	3:A:405:ASN:N	2.73	0.41
3:A:1375:LEU:CD2	3:A:1607:THR:HG23	2.51	0.41
3:A:1882:LEU:HD12	3:A:1883:ASN:N	2.35	0.41
9:B:809:THR:HA	9:B:1092:PHE:CD1	2.56	0.41
9:B:1873:THR:HG22	9:B:2109:LYS:HD2	2.03	0.41
21:2:19:LEU:HD12	21:2:23:ILE:CG2	2.50	0.41
28:C:242:VAL:HG22	28:C:277:LEU:HD11	2.02	0.41
1:V:17:A:C2	1:V:18:A:C4	3.09	0.41
2:W:60:G:H2'	2:W:61:C:O4'	2.21	0.41
3:A:963:VAL:HG21	7:F:280:ARG:NH2	2.35	0.41
3:A:1609:TRP:CZ3	3:A:1823:LEU:HD13	2.56	0.41
5:J:763:ALA:HB1	5:J:773:LEU:HD13	2.02	0.41
6:D:79:PRO:HA	6:D:80:MET:CE	2.51	0.41
7:F:285:LEU:HD13	7:F:306:LEU:HD23	2.02	0.41
19:U:45:A:H2'	19:U:45:A:N3	2.35	0.41
20:K:81:VAL:HB	20:K:82:PRO:HD2	2.03	0.41
28:C:139:ILE:O	28:C:237:ILE:HA	2.21	0.41
28:C:227:VAL:HG22	28:C:595:LEU:CD1	2.51	0.41
28:C:856:ILE:HG22	28:C:857:LEU:O	2.20	0.41
3:A:1021:PRO:N	3:A:1022:PRO:CD	2.84	0.41
4:H:172:LEU:HD13	5:J:755:GLN:HG3	2.03	0.41
4:H:395:ILE:CD1	20:K:126:ILE:CD1	2.99	0.41
7:F:135:LEU:HD22	7:F:208:TRP:NE1	2.35	0.41
7:F:369:GLY:O	7:F:371:LYS:N	2.54	0.41
9:B:412:GLU:N	9:B:412:GLU:OE1	2.54	0.41
9:B:924:VAL:HG12	9:B:998:ALA:HB2	2.02	0.41
9:B:1746:LEU:O	9:B:1750:ILE:HG23	2.20	0.41
9:B:2113:ALA:HB2	9:B:2130:PHE:CB	2.51	0.41
19:U:24:G:H2'	19:U:25:G:O5'	2.21	0.41
28:C:142:LEU:HD22	28:C:143:HIS:N	2.36	0.41
3:A:394:ARG:HD3	28:C:610:LEU:HD13	2.04	0.40
3:A:576:HIS:CD2	3:A:580:ASN:HD21	2.40	0.40
3:A:1710:GLU:HG2	3:A:1728:ILE:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:155:ARG:NE	8:G:174:LEU:HD22	2.35	0.40
5:J:299:ALA:O	5:J:303:ASN:N	2.46	0.40
5:J:478:TYR:O	5:J:479:GLU:CB	2.69	0.40
7:F:112:MET:CE	7:F:203:ILE:HD12	2.51	0.40
9:B:940:ALA:HB2	9:B:970:ARG:NH1	2.36	0.40
19:U:17:C:H2'	19:U:18:A:C8	2.56	0.40
21:2:10:LEU:HD22	21:2:13:GLN:HE21	1.85	0.40
28:C:220:ASN:HB3	28:C:651:TYR:HB2	2.03	0.40
28:C:446:PHE:HA	28:C:449:PHE:HB3	2.03	0.40
1:V:81:C:C4	1:V:82:C:C4	3.09	0.40
3:A:330:LEU:CD2	3:A:385:VAL:HG23	2.48	0.40
3:A:461:LEU:HD11	3:A:462:LEU:HG	1.94	0.40
3:A:1122:ASP:CG	3:A:1163:ARG:HE	2.23	0.40
4:H:321:LEU:HD22	8:G:195:LYS:CD	2.51	0.40
19:U:96:U:C4	19:U:97:U:C5	3.09	0.40
28:C:219:VAL:O	28:C:221:PHE:N	2.54	0.40
2:W:27:U:H1'	3:A:668:ARG:HA	2.02	0.40
3:A:1385:PRO:O	3:A:1386:ALA:C	2.58	0.40
3:A:1889:LEU:HD22	3:A:1991:ILE:HD12	2.04	0.40
3:A:2166:LEU:HD11	3:A:2194:ILE:HG21	2.03	0.40
8:G:365:LEU:HD22	8:G:382:VAL:CG1	2.51	0.40
8:G:428:TRP:CE3	8:G:428:TRP:HA	2.57	0.40
9:B:1428:LEU:HB2	9:B:1447:ALA:HB2	2.02	0.40
20:K:20:ILE:O	20:K:24:VAL:HG23	2.21	0.40
20:K:95:ARG:HG3	20:K:96:PRO:HD2	2.03	0.40
3:A:484:PHE:CD1	3:A:484:PHE:C	2.94	0.40
3:A:881:THR:O	3:A:885:VAL:HG23	2.21	0.40
3:A:1837:SER:N	3:A:2084:LEU:HD21	2.37	0.40
4:H:273:TYR:CD1	4:H:280:ILE:HG23	2.56	0.40
9:B:1773:PHE:CD2	9:B:1803:LEU:HD21	2.56	0.40
19:U:93:G:N2	19:U:94:C:C2	2.90	0.40
28:C:941:PRO:O	28:C:963:SER:HB3	2.22	0.40
3:A:324:ASP:HB3	3:A:407:VAL:HG21	2.04	0.40
3:A:461:LEU:CD1	3:A:461:LEU:C	2.85	0.40
3:A:632:ILE:CG2	3:A:656:ILE:HG21	2.51	0.40
3:A:852:LEU:O	3:A:855:LEU:HG	2.21	0.40
3:A:1048:VAL:HG11	3:A:1226:VAL:HG11	2.03	0.40
3:A:1208:PRO:O	3:A:1209:LYS:C	2.58	0.40
3:A:1624:LEU:HD23	3:A:1633:PHE:CG	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	2182/2413 (90%)	1924 (88%)	217 (10%)	41 (2%)	8	42
4	H	355/465 (76%)	301 (85%)	43 (12%)	11 (3%)	4	32
5	J	719/899 (80%)	643 (89%)	59 (8%)	17 (2%)	6	37
6	D	138/143 (96%)	124 (90%)	9 (6%)	5 (4%)	3	29
7	F	413/494 (84%)	361 (87%)	35 (8%)	17 (4%)	3	26
8	G	316/469 (67%)	274 (87%)	34 (11%)	8 (2%)	5	36
9	B	1776/2163 (82%)	1623 (91%)	132 (7%)	21 (1%)	13	51
11	b	76/196 (39%)	67 (88%)	9 (12%)	0	100	100
11	k	76/196 (39%)	70 (92%)	5 (7%)	1 (1%)	12	50
12	h	78/146 (53%)	73 (94%)	4 (5%)	1 (1%)	12	50
12	l	87/146 (60%)	76 (87%)	9 (10%)	2 (2%)	6	38
13	j	92/110 (84%)	87 (95%)	5 (5%)	0	100	100
13	m	92/110 (84%)	87 (95%)	5 (5%)	0	100	100
14	d	80/101 (79%)	72 (90%)	7 (9%)	1 (1%)	12	50
14	n	80/101 (79%)	73 (91%)	7 (9%)	0	100	100
15	e	71/94 (76%)	65 (92%)	6 (8%)	0	100	100
15	p	71/94 (76%)	64 (90%)	7 (10%)	0	100	100
16	f	70/86 (81%)	64 (91%)	4 (6%)	2 (3%)	4	33
16	q	70/86 (81%)	63 (90%)	7 (10%)	0	100	100
17	g	65/77 (84%)	63 (97%)	2 (3%)	0	100	100
17	r	65/77 (84%)	58 (89%)	7 (11%)	0	100	100
18	E	21/328 (6%)	20 (95%)	1 (5%)	0	100	100
20	K	122/126 (97%)	113 (93%)	7 (6%)	2 (2%)	9	46
21	2	88/95 (93%)	76 (86%)	11 (12%)	1 (1%)	14	53
22	3	75/89 (84%)	71 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	4	70/187 (37%)	65 (93%)	5 (7%)	0	100	100
24	5	71/93 (76%)	66 (93%)	5 (7%)	0	100	100
25	6	72/86 (84%)	67 (93%)	4 (6%)	1 (1%)	11	48
26	7	62/115 (54%)	57 (92%)	5 (8%)	0	100	100
27	8	62/109 (57%)	59 (95%)	3 (5%)	0	100	100
28	C	847/1008 (84%)	734 (87%)	82 (10%)	31 (4%)	3	28
All	All	8462/10902 (78%)	7560 (89%)	740 (9%)	162 (2%)	11	42

All (162) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	247	PRO
3	A	470	LEU
3	A	471	PRO
3	A	597	PHE
3	A	796	ASN
3	A	980	PRO
3	A	1093	LYS
3	A	1176	GLU
3	A	1209	LYS
3	A	1562	PHE
3	A	2042	SER
3	A	2088	ILE
3	A	2330	GLU
4	H	360	ASN
4	H	361	GLY
4	H	362	TYR
5	J	186	SER
5	J	592	HIS
6	D	54	ARG
7	F	59	LEU
7	F	148	ASN
7	F	407	GLU
8	G	194	GLU
8	G	277	MET
9	B	388	GLN
9	B	392	ARG
9	B	393	GLU
9	B	424	PRO
9	B	448	LEU

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Mol	Chain	Res	Type
9	B	843	HIS
9	B	1264	VAL
9	B	1483	VAL
20	K	65	LEU
28	C	164	MET
28	C	367	VAL
28	C	598	ILE
3	A	495	ARG
3	A	921	ASP
3	A	961	GLN
3	A	1102	GLY
3	A	1159	ARG
3	A	1604	ARG
3	A	2068	ASN
4	H	216	SER
4	H	240	ASP
5	J	200	ALA
5	J	479	GLU
5	J	683	ASN
6	D	127	ASN
7	F	58	ALA
7	F	79	ASP
7	F	146	ASN
7	F	353	THR
7	F	363	PRO
7	F	370	ARG
7	F	435	ALA
8	G	462	HIS
11	k	81	VAL
12	l	78	ASN
16	f	32	LYS
21	2	55	GLY
28	C	175	LEU
28	C	269	LYS
28	C	361	THR
28	C	568	SER
28	C	830	ASN
28	C	963	SER
3	A	360	GLU
3	A	598	ASN
3	A	802	PRO
3	A	839	HIS

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Mol	Chain	Res	Type
3	A	1386	ALA
3	A	1530	SER
3	A	1743	TYR
3	A	2321	ILE
5	J	237	ASP
5	J	633	GLU
5	J	867	GLU
7	F	365	LYS
9	B	875	ALA
9	B	1301	GLU
28	C	220	ASN
28	C	432	GLN
28	C	446	PHE
28	C	535	PRO
28	C	600	GLU
28	C	884	ARG
3	A	262	ASP
3	A	539	PRO
3	A	615	LEU
3	A	703	PHE
3	A	1205	LYS
4	H	346	ALA
4	H	377	ASP
4	H	394	ASN
5	J	206	ASP
5	J	287	SER
5	J	840	ASP
6	D	97	THR
6	D	101	ASN
7	F	74	LEU
7	F	165	ALA
8	G	266	PRO
8	G	288	THR
9	B	411	SER
9	B	1422	GLY
9	B	1586	PRO
9	B	1637	VAL
12	h	10	LEU
25	6	57	GLU
28	C	162	PRO
28	C	180	ASN
28	C	371	PRO

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Mol	Chain	Res	Type
28	C	464	PRO
28	C	573	LYS
28	C	597	TYR
28	C	923	ASN
3	A	199	ILE
3	A	260	PRO
3	A	644	VAL
3	A	1165	LEU
3	A	1347	ARG
3	A	2089	LYS
4	H	231	ASN
5	J	202	SER
5	J	241	PRO
5	J	258	SER
6	D	78	ASP
9	B	389	TYR
9	B	791	PRO
9	B	958	PRO
20	K	82	PRO
28	C	369	LYS
28	C	428	ILE
28	C	770	ASN
28	C	886	SER
28	C	949	ALA
5	J	887	THR
7	F	392	GLU
8	G	374	ASP
9	B	1482	GLY
28	C	807	PRO
28	C	951	ILE
3	A	979	SER
4	H	435	GLY
8	G	263	GLY
8	G	268	PRO
9	B	1327	ILE
5	J	558	PRO
7	F	132	PRO
7	F	347	ALA
14	d	82	PRO
5	J	399	PRO
16	f	15	PRO
28	C	547	GLY

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Mol	Chain	Res	Type
28	C	829	VAL
4	H	253	GLY
7	F	89	ILE
9	B	425	PRO
9	B	1062	PRO
3	A	509	HIS
12	l	98	PRO

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	
3	A	1918/2182 (88%)	1836 (96%)	82 (4%)	29	63
4	H	305/410 (74%)	290 (95%)	15 (5%)	25	59
5	J	627/813 (77%)	595 (95%)	32 (5%)	24	58
6	D	129/132 (98%)	117 (91%)	12 (9%)	9	38
7	F	346/445 (78%)	313 (90%)	33 (10%)	8	37
8	G	289/436 (66%)	277 (96%)	12 (4%)	30	63
9	B	1592/1955 (81%)	1522 (96%)	70 (4%)	28	63
11	b	70/176 (40%)	70 (100%)	0	100	100
11	k	70/176 (40%)	67 (96%)	3 (4%)	29	63
12	h	77/129 (60%)	75 (97%)	2 (3%)	46	74
12	l	85/129 (66%)	81 (95%)	4 (5%)	26	61
13	j	79/103 (77%)	75 (95%)	4 (5%)	24	58
13	m	78/103 (76%)	75 (96%)	3 (4%)	33	66
14	d	69/89 (78%)	67 (97%)	2 (3%)	42	72
14	n	69/89 (78%)	66 (96%)	3 (4%)	29	63
15	e	65/83 (78%)	59 (91%)	6 (9%)	9	39
15	p	65/83 (78%)	60 (92%)	5 (8%)	13	45
16	f	63/77 (82%)	62 (98%)	1 (2%)	62	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	q	63/77 (82%)	62 (98%)	1 (2%)	62	83
17	g	58/66 (88%)	57 (98%)	1 (2%)	60	82
17	r	57/66 (86%)	56 (98%)	1 (2%)	59	81
18	E	20/20 (100%)	18 (90%)	2 (10%)	7	35
20	K	102/104 (98%)	92 (90%)	10 (10%)	8	36
21	2	85/91 (93%)	78 (92%)	7 (8%)	11	42
22	3	71/81 (88%)	69 (97%)	2 (3%)	43	72
23	4	64/172 (37%)	63 (98%)	1 (2%)	62	83
24	5	66/84 (79%)	66 (100%)	0	100	100
25	6	66/75 (88%)	65 (98%)	1 (2%)	65	84
26	7	56/103 (54%)	54 (96%)	2 (4%)	35	67
27	8	56/99 (57%)	54 (96%)	2 (4%)	35	67
28	C	673/910 (74%)	616 (92%)	57 (8%)	10	41
All	All	7433/9558 (78%)	7057 (95%)	376 (5%)	27	58

All (376) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	124	ARG
3	A	129	THR
3	A	175	LEU
3	A	205	THR
3	A	210	GLU
3	A	229	ARG
3	A	249	LEU
3	A	254	HIS
3	A	282	ASP
3	A	284	ARG
3	A	287	GLU
3	A	288	GLU
3	A	310	ASN
3	A	331	PHE
3	A	340	LYS
3	A	351	LYS
3	A	365	ASN
3	A	369	SER
3	A	402	TRP

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Mol	Chain	Res	Type
3	A	405	ASN
3	A	505	TRP
3	A	523	GLN
3	A	526	LEU
3	A	571	LEU
3	A	615	LEU
3	A	622	MET
3	A	655	TYR
3	A	659	HIS
3	A	660	ILE
3	A	666	ILE
3	A	684	LYS
3	A	690	LYS
3	A	701	CYS
3	A	705	GLN
3	A	721	LEU
3	A	753	TYR
3	A	760	ASN
3	A	812	ILE
3	A	848	ASN
3	A	855	LEU
3	A	909	THR
3	A	949	ASP
3	A	950	THR
3	A	955	LYS
3	A	971	MET
3	A	972	MET
3	A	979	SER
3	A	1004	ASP
3	A	1024	LEU
3	A	1049	LEU
3	A	1239	THR
3	A	1267	VAL
3	A	1276	GLU
3	A	1277	GLU
3	A	1282	ASP
3	A	1287	ASP
3	A	1337	THR
3	A	1339	LEU
3	A	1358	ASP
3	A	1373	LEU
3	A	1510	ILE

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Mol	Chain	Res	Type
3	A	1512	ARG
3	A	1603	ASN
3	A	1624	LEU
3	A	1682	THR
3	A	1691	SER
3	A	1719	GLU
3	A	1737	GLN
3	A	1742	ASP
3	A	1769	SER
3	A	1773	VAL
3	A	1847	ASP
3	A	1979	MET
3	A	2000	SER
3	A	2048	TRP
3	A	2053	SER
3	A	2088	ILE
3	A	2176	PHE
3	A	2306	ASN
3	A	2329	PHE
3	A	2355	ASN
3	A	2381	GLU
4	H	111	THR
4	H	136	LEU
4	H	146	PHE
4	H	199	LEU
4	H	225	ASP
4	H	232	ASN
4	H	280	ILE
4	H	286	ASP
4	H	300	LEU
4	H	302	LEU
4	H	331	SER
4	H	336	ILE
4	H	349	SER
4	H	423	SER
4	H	454	SER
5	J	159	LEU
5	J	194	PRO
5	J	209	ASN
5	J	239	THR
5	J	255	ARG
5	J	270	GLU

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Mol	Chain	Res	Type
5	J	291	TYR
5	J	317	GLU
5	J	338	GLU
5	J	347	PHE
5	J	397	GLN
5	J	421	LEU
5	J	459	LEU
5	J	460	THR
5	J	498	GLN
5	J	508	TRP
5	J	554	ARG
5	J	613	LEU
5	J	635	LEU
5	J	636	TYR
5	J	644	ARG
5	J	648	LEU
5	J	657	ASN
5	J	661	LEU
5	J	708	LEU
5	J	715	ASP
5	J	767	PHE
5	J	788	SER
5	J	809	LEU
5	J	825	LEU
5	J	832	LEU
5	J	874	TRP
6	D	14	HIS
6	D	30	ARG
6	D	38	GLN
6	D	39	CYS
6	D	41	ILE
6	D	43	ASP
6	D	49	ILE
6	D	69	ASP
6	D	71	ASP
6	D	76	LEU
6	D	80	MET
6	D	139	HIS
7	F	57	LEU
7	F	59	LEU
7	F	63	ASP
7	F	67	LEU

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Mol	Chain	Res	Type
7	F	77	ILE
7	F	81	LYS
7	F	82	ARG
7	F	84	LEU
7	F	116	LEU
7	F	119	LEU
7	F	120	TYR
7	F	124	PHE
7	F	130	LEU
7	F	142	SER
7	F	144	LEU
7	F	153	GLU
7	F	156	GLU
7	F	210	LEU
7	F	221	LYS
7	F	232	LEU
7	F	280	ARG
7	F	288	SER
7	F	305	MET
7	F	307	CYS
7	F	364	LYS
7	F	376	LYS
7	F	388	GLN
7	F	397	GLU
7	F	401	LEU
7	F	404	TYR
7	F	407	GLU
7	F	412	MET
7	F	454	GLU
8	G	189	THR
8	G	278	MET
8	G	285	GLN
8	G	329	MET
8	G	332	GLU
8	G	337	TYR
8	G	339	CYS
8	G	341	VAL
8	G	343	GLN
8	G	395	LEU
8	G	408	LEU
8	G	427	THR
9	B	390	LYS

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Mol	Chain	Res	Type
9	B	403	SER
9	B	440	LEU
9	B	453	PHE
9	B	457	LYS
9	B	463	ILE
9	B	485	ASP
9	B	505	LYS
9	B	511	PHE
9	B	543	TYR
9	B	566	LEU
9	B	614	ILE
9	B	645	PRO
9	B	748	LYS
9	B	778	LYS
9	B	782	LYS
9	B	793	LEU
9	B	836	TRP
9	B	870	GLN
9	B	901	VAL
9	B	902	LEU
9	B	928	ASN
9	B	942	THR
9	B	944	LEU
9	B	956	LYS
9	B	963	ASP
9	B	1015	MET
9	B	1016	ASP
9	B	1039	GLU
9	B	1054	LEU
9	B	1077	ASN
9	B	1086	GLN
9	B	1088	LYS
9	B	1131	LEU
9	B	1137	THR
9	B	1139	MET
9	B	1160	LEU
9	B	1198	ARG
9	B	1240	LEU
9	B	1242	MET
9	B	1280	ASN
9	B	1284	LEU
9	B	1344	GLU

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Mol	Chain	Res	Type
9	B	1408	LEU
9	B	1453	GLU
9	B	1483	VAL
9	B	1488	TYR
9	B	1491	LEU
9	B	1515	LEU
9	B	1519	ARG
9	B	1524	TRP
9	B	1556	HIS
9	B	1561	PHE
9	B	1578	ARG
9	B	1590	ASP
9	B	1610	LEU
9	B	1669	ASP
9	B	1687	LEU
9	B	1689	ASP
9	B	1694	LYS
9	B	1696	MET
9	B	1724	THR
9	B	1743	GLU
9	B	1771	ASP
9	B	1849	ASN
9	B	1917	THR
9	B	1959	ASN
9	B	1975	THR
9	B	2000	PHE
9	B	2131	ASP
11	k	48	CYS
11	k	78	GLU
11	k	82	LEU
12	l	96	ILE
12	l	97	LEU
12	l	104	ASP
12	l	110	GLN
13	m	41	ARG
13	m	52	HIS
13	m	94	LEU
14	n	20	SER
14	n	43	GLN
14	n	76	ASP
15	p	16	CYS
15	p	77	LEU

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Mol	Chain	Res	Type
15	p	79	LYS
15	p	81	LEU
15	p	82	LEU
16	q	34	ASN
17	r	71	LEU
18	E	550	GLN
18	E	552	PHE
15	e	15	ASN
15	e	16	CYS
15	e	18	PHE
15	e	25	THR
15	e	79	LYS
15	e	81	LEU
16	f	79	LEU
17	g	18	ASN
14	d	10	LEU
14	d	20	SER
12	h	30	GLN
12	h	99	ASP
13	j	24	PHE
13	j	49	ARG
13	j	77	THR
13	j	100	SER
20	K	11	LEU
20	K	21	LEU
20	K	22	ASP
20	K	30	LEU
20	K	33	LEU
20	K	35	LYS
20	K	46	ARG
20	K	73	ASP
20	K	93	VAL
20	K	125	LEU
21	2	12	ASP
21	2	13	GLN
21	2	45	CYS
21	2	63	ARG
21	2	66	THR
21	2	68	ARG
21	2	72	LEU
22	3	26	LEU
22	3	34	ASP

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Mol	Chain	Res	Type
23	4	83	ASP
25	6	70	ASP
26	7	67	VAL
26	7	85	ASN
27	8	44	ARG
27	8	63	LEU
28	C	111	LYS
28	C	112	ASN
28	C	113	ILE
28	C	146	LYS
28	C	160	ARG
28	C	173	LYS
28	C	176	ARG
28	C	179	ASP
28	C	181	LEU
28	C	183	GLN
28	C	202	ASP
28	C	233	ASP
28	C	255	GLN
28	C	260	ASN
28	C	264	CYS
28	C	272	ARG
28	C	283	ASP
28	C	315	SER
28	C	327	PHE
28	C	342	ASP
28	C	347	ARG
28	C	361	THR
28	C	406	VAL
28	C	407	ASN
28	C	421	LEU
28	C	431	GLN
28	C	458	ILE
28	C	469	TRP
28	C	475	THR
28	C	478	TYR
28	C	534	THR
28	C	537	CYS
28	C	576	THR
28	C	577	LEU
28	C	590	LYS
28	C	605	ILE

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Mol	Chain	Res	Type
28	C	619	LEU
28	C	634	ILE
28	C	658	ASP
28	C	674	LEU
28	C	681	CYS
28	C	707	SER
28	C	723	LEU
28	C	767	SER
28	C	770	ASN
28	C	772	ASN
28	C	784	SER
28	C	791	TYR
28	C	808	LEU
28	C	851	LEU
28	C	862	TYR
28	C	883	ARG
28	C	909	ILE
28	C	928	CYS
28	C	933	TRP
28	C	971	ARG
28	C	988	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	216	GLN
3	A	326	ASN
3	A	344	ASN
3	A	404	ASN
3	A	405	ASN
3	A	472	ASN
3	A	528	ASN
3	A	558	GLN
3	A	576	HIS
3	A	654	HIS
3	A	705	GLN
3	A	848	ASN
3	A	907	ASN
3	A	1005	GLN
3	A	1190	ASN
3	A	1273	GLN
3	A	1368	GLN

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Mol	Chain	Res	Type
3	A	1677	GLN
3	A	1695	ASN
3	A	1737	GLN
3	A	2168	ASN
4	H	203	ASN
4	H	306	HIS
4	H	374	ASN
4	H	392	HIS
5	J	190	GLN
5	J	209	ASN
5	J	281	ASN
5	J	397	GLN
5	J	498	GLN
5	J	537	GLN
5	J	578	GLN
5	J	585	GLN
5	J	646	GLN
5	J	673	GLN
5	J	733	ASN
7	F	244	HIS
7	F	270	HIS
7	F	320	GLN
7	F	331	HIS
7	F	433	ASN
8	G	276	ASN
8	G	286	ASN
9	B	372	ASN
9	B	570	GLN
9	B	804	HIS
9	B	862	GLN
9	B	921	ASN
9	B	1003	ASN
9	B	1280	ASN
9	B	1349	ASN
9	B	1579	ASN
9	B	1727	ASN
9	B	1959	ASN
9	B	2058	ASN
9	B	2069	GLN
15	e	15	ASN
15	e	34	GLN
17	g	18	ASN

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Mol	Chain	Res	Type
17	g	66	ASN
12	h	86	ASN
20	K	45	ASN
20	K	113	GLN
21	2	13	GLN
23	4	9	ASN
24	5	61	ASN
25	6	59	ASN
28	C	112	ASN
28	C	180	ASN
28	C	194	ASN
28	C	289	ASN
28	C	290	HIS
28	C	403	ASN
28	C	432	GLN
28	C	776	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	V	122/160 (76%)	60 (49%)	13 (10%)
19	U	137/214 (64%)	75 (54%)	21 (15%)
2	W	77/112 (68%)	35 (45%)	12 (15%)
All	All	336/486 (69%)	170 (50%)	46 (13%)

All (170) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	V	2	U
1	V	11	A
1	V	15	G
1	V	18	A
1	V	19	U
1	V	20	A
1	V	22	G
1	V	25	U
1	V	26	A
1	V	31	U
1	V	32	G
1	V	33	A
1	V	36	A

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Mol	Chain	Res	Type
1	V	37	U
1	V	39	C
1	V	40	G
1	V	41	U
1	V	45	A
1	V	46	G
1	V	53	U
1	V	55	U
1	V	56	U
1	V	57	U
1	V	59	C
1	V	64	U
1	V	65	G
1	V	66	A
1	V	67	A
1	V	74	U
1	V	75	U
1	V	78	A
1	V	81	C
1	V	82	C
1	V	83	A
1	V	84	G
1	V	85	A
1	V	86	C
1	V	87	C
1	V	88	G
1	V	89	U
1	V	90	C
1	V	91	U
1	V	94	U
1	V	98	G
1	V	101	C
1	V	102	A
1	V	103	A
1	V	104	U
1	V	129	A
1	V	130	A
1	V	131	G
1	V	132	A
1	V	137	G
1	V	143	A
1	V	144	A

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Mol	Chain	Res	Type
1	V	145	U
1	V	147	U
1	V	149	U
1	V	151	G
1	V	152	A
2	W	2	U
2	W	7	G
2	W	8	A
2	W	17	U
2	W	25	C
2	W	26	A
2	W	27	U
2	W	28	U
2	W	29	U
2	W	30	G
2	W	31	G
2	W	32	U
2	W	33	C
2	W	34	A
2	W	38	U
2	W	45	A
2	W	46	U
2	W	47	A
2	W	48	C
2	W	49	A
2	W	50	G
2	W	56	A
2	W	61	C
2	W	63	G
2	W	75	A
2	W	76	A
2	W	83	A
2	W	84	C
2	W	85	C
2	W	86	G
2	W	87	U
2	W	88	U
2	W	109	U
2	W	110	U
2	W	111	U
19	U	12	C
19	U	13	A

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Mol	Chain	Res	Type
19	U	14	G
19	U	15	A
19	U	16	U
19	U	17	C
19	U	18	A
19	U	21	G
19	U	22	G
19	U	23	C
19	U	25	G
19	U	26	A
19	U	27	G
19	U	28	G
19	U	30	A
19	U	32	G
19	U	33	U
19	U	34	C
19	U	35	A
19	U	38	A
19	U	39	U
19	U	40	C
19	U	41	A
19	U	43	G
19	U	44	A
19	U	45	A
19	U	53	C
19	U	65	U
19	U	67	U
19	U	68	A
19	U	69	G
19	U	70	A
19	U	71	A
19	U	72	C
19	U	73	U
19	U	74	U
19	U	75	A
19	U	76	U
19	U	77	A
19	U	78	A
19	U	79	C
19	U	80	G
19	U	81	A
19	U	82	A

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Mol	Chain	Res	Type
19	U	83	C
19	U	84	A
19	U	87	G
19	U	94	C
19	U	95	C
19	U	96	U
19	U	97	U
19	U	101	C
19	U	104	G
19	U	108	C
19	U	112	C
19	U	115	G
19	U	119	U
19	U	120	G
19	U	121	U
19	U	122	C
19	U	123	U
19	U	125	C
19	U	126	A
19	U	128	A
19	U	129	G
19	U	130	A
19	U	133	C
19	U	134	A
19	U	135	G
19	U	142	C
19	U	143	U
19	U	170	U
19	U	171	U
19	U	172	U
19	U	173	U

All (46) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	V	17	A
1	V	19	U
1	V	31	U
1	V	39	C
1	V	44	G
1	V	73	A
1	V	74	U

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Mol	Chain	Res	Type
1	V	83	A
1	V	88	G
1	V	129	A
1	V	143	A
1	V	145	U
1	V	150	G
2	W	16	C
2	W	25	C
2	W	26	A
2	W	27	U
2	W	31	G
2	W	32	U
2	W	45	A
2	W	48	C
2	W	49	A
2	W	55	G
2	W	83	A
2	W	84	C
19	U	25	G
19	U	26	A
19	U	27	G
19	U	32	G
19	U	40	C
19	U	44	A
19	U	68	A
19	U	75	A
19	U	78	A
19	U	80	G
19	U	82	A
19	U	83	C
19	U	95	C
19	U	103	A
19	U	114	G
19	U	124	C
19	U	128	A
19	U	129	G
19	U	132	A
19	U	133	C
19	U	172	U

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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
29	GTP	C	1101	-	26,34,34	0.82	1 (3%)	32,54,54	1.67	5 (15%)

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
29	GTP	C	1101	-	-	4/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	C	1101	GTP	C6-N1	-2.12	1.34	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	C	1101	GTP	PB-O3B-PG	-4.87	116.11	132.83
29	C	1101	GTP	PA-O3A-PB	-4.14	118.61	132.83
29	C	1101	GTP	C5-C6-N1	2.61	118.55	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	C	1101	GTP	O6-C6-C5	-2.46	119.57	124.37
29	C	1101	GTP	C8-N7-C5	2.27	107.32	102.99

There are no chirality outliers.

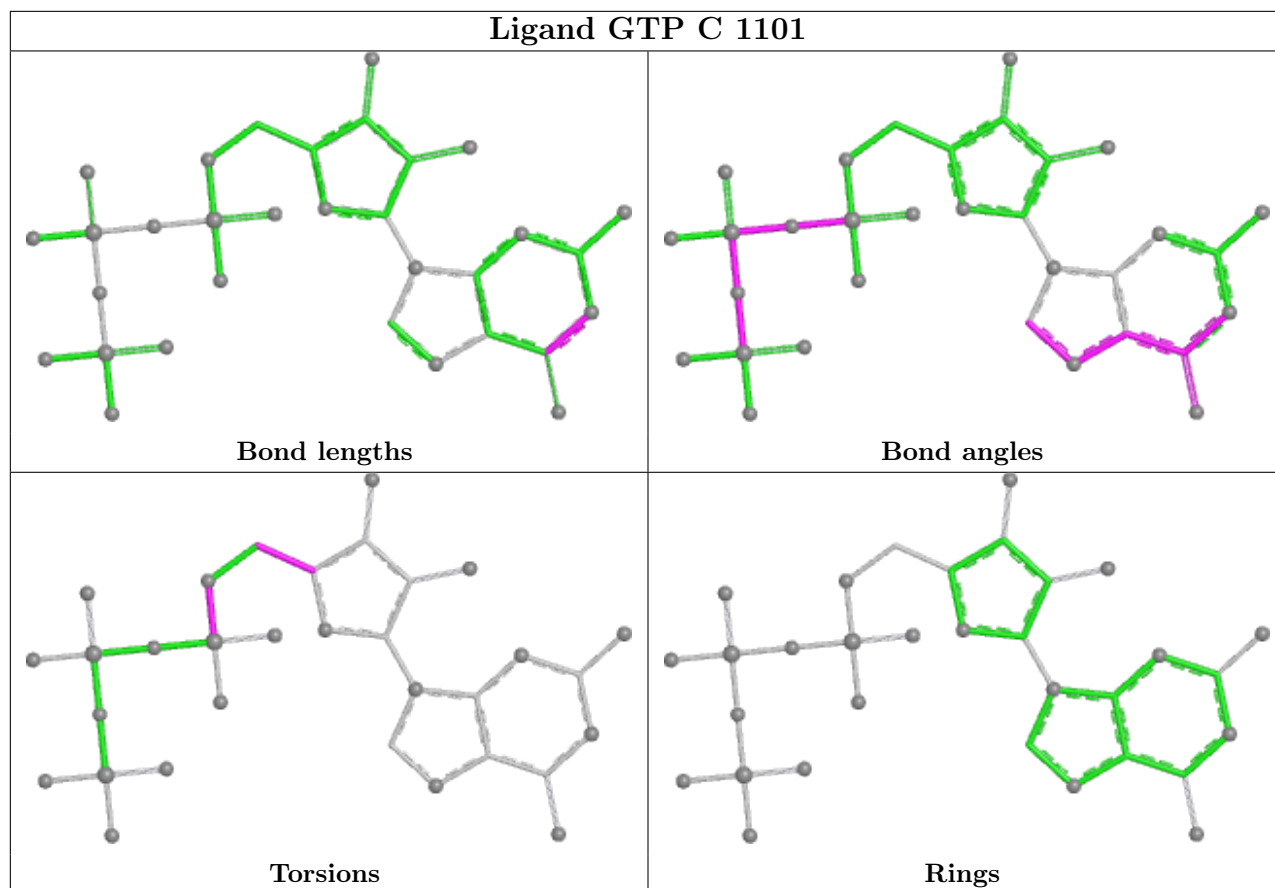
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	C	1101	GTP	C5'-O5'-PA-O1A
29	C	1101	GTP	O4'-C4'-C5'-O5'
29	C	1101	GTP	C3'-C4'-C5'-O5'
29	C	1101	GTP	C5'-O5'-PA-O3A

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
18	E	13
10	x	2
3	A	1
19	U	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	x	120:UNK	C	201:UNK	N	117.38
1	x	62:UNK	C	101:UNK	N	54.41
1	E	132:UNK	C	150:UNK	N	36.51

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	170:UNK	C	180:UNK	N	34.13
1	E	102:UNK	C	120:UNK	N	31.43
1	E	226:UNK	C	240:UNK	N	25.24
1	E	250:UNK	C	270:UNK	N	25.14
1	E	420:UNK	C	487:UNK	N	24.41
1	E	280:UNK	C	310:UNK	N	16.17
1	E	194:UNK	C	210:UNK	N	13.89
1	E	318:UNK	C	330:UNK	N	13.76
1	E	57:UNK	C	70:UNK	N	11.67
1	E	25:UNK	C	40:UNK	N	8.61
1	E	91:UNK	C	96:UNK	N	7.62
1	E	79:UNK	C	82:UNK	N	5.98
1	A	1860:VAL	C	1861:THR	N	4.45
1	U	166:U	O3'	167:A	P	3.43

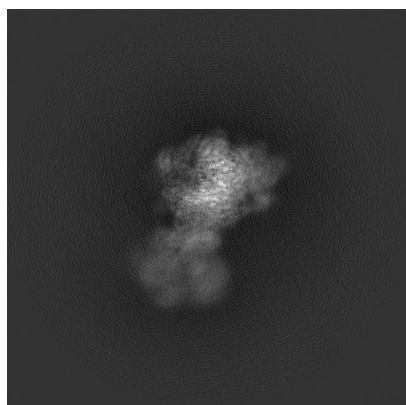
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8012. These allow visual inspection of the internal detail of the map and identification of artifacts.

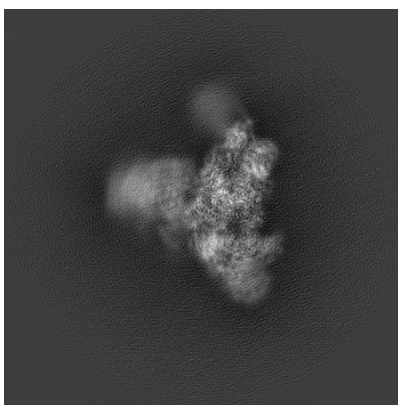
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

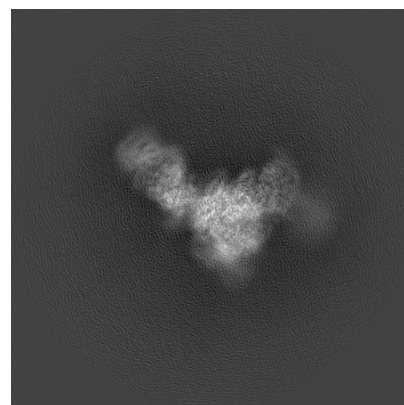
6.1.1 Primary map



X



Y

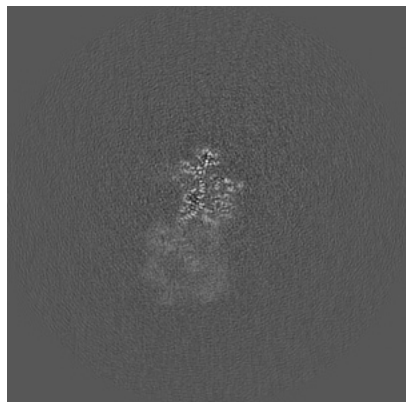


Z

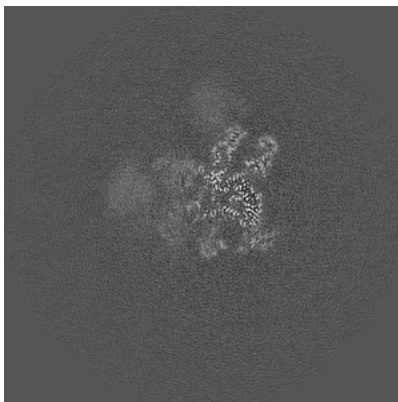
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

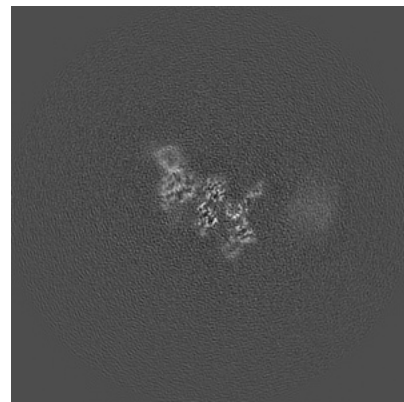
6.2.1 Primary map



X Index: 190



Y Index: 190

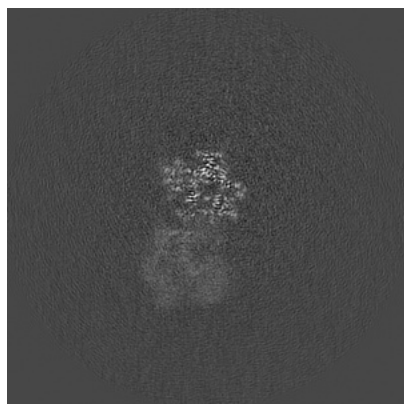


Z Index: 190

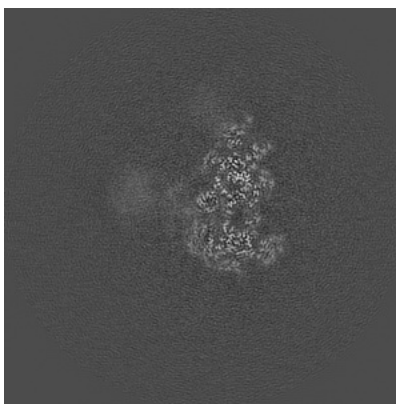
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

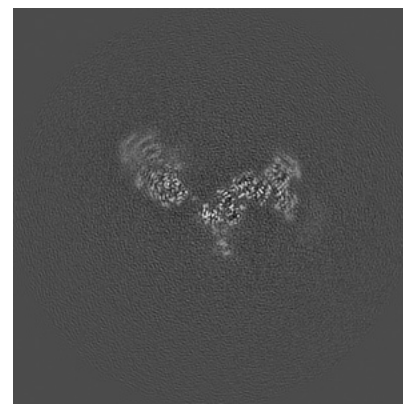
6.3.1 Primary map



X Index: 196



Y Index: 202



Z Index: 221

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

6.4 Orthogonal surface views [i](#)

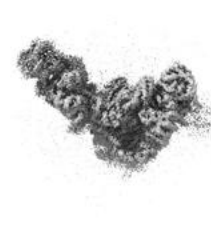
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.036. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

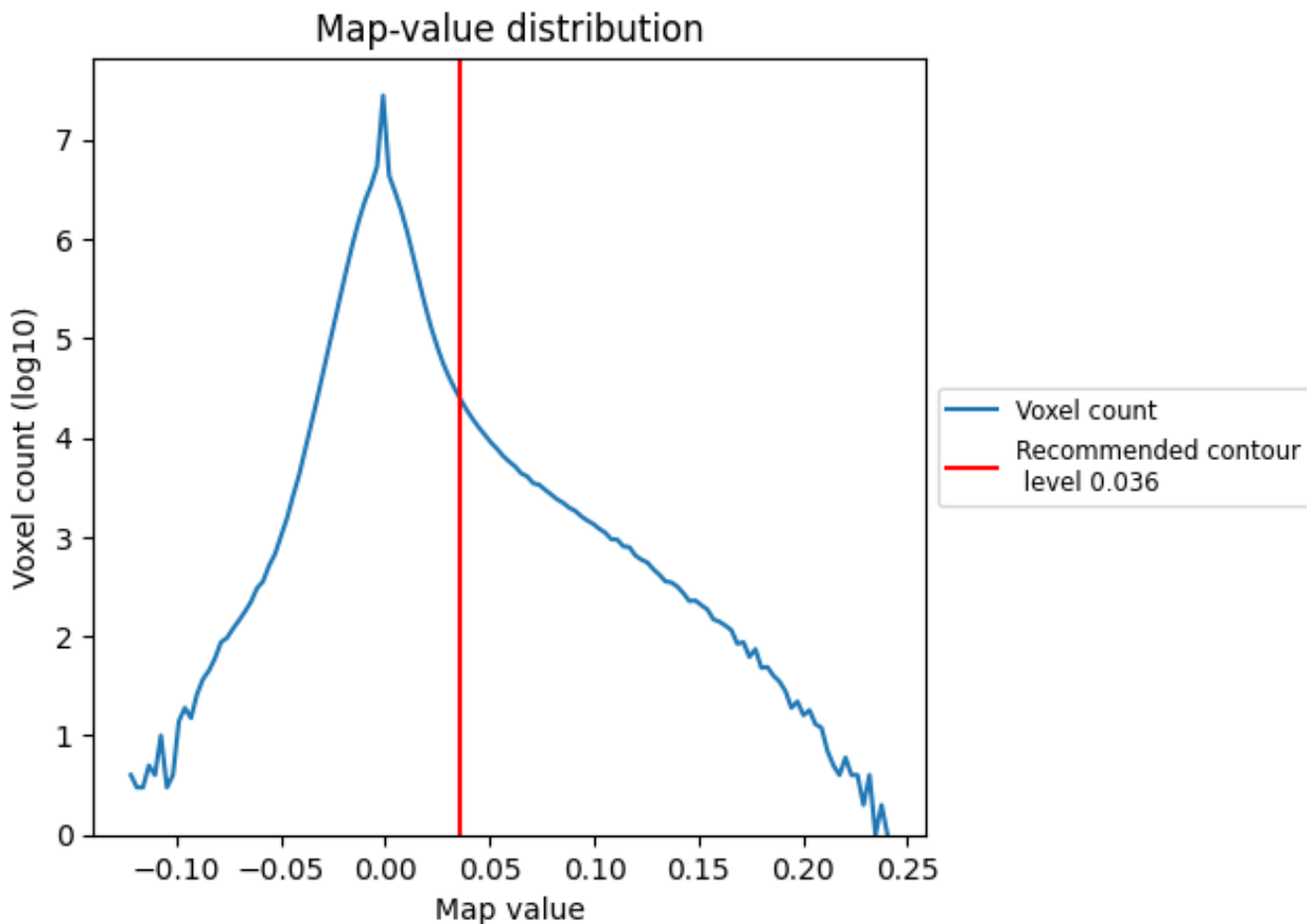
6.5 Mask visualisation

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

7 Map analysis [i](#)

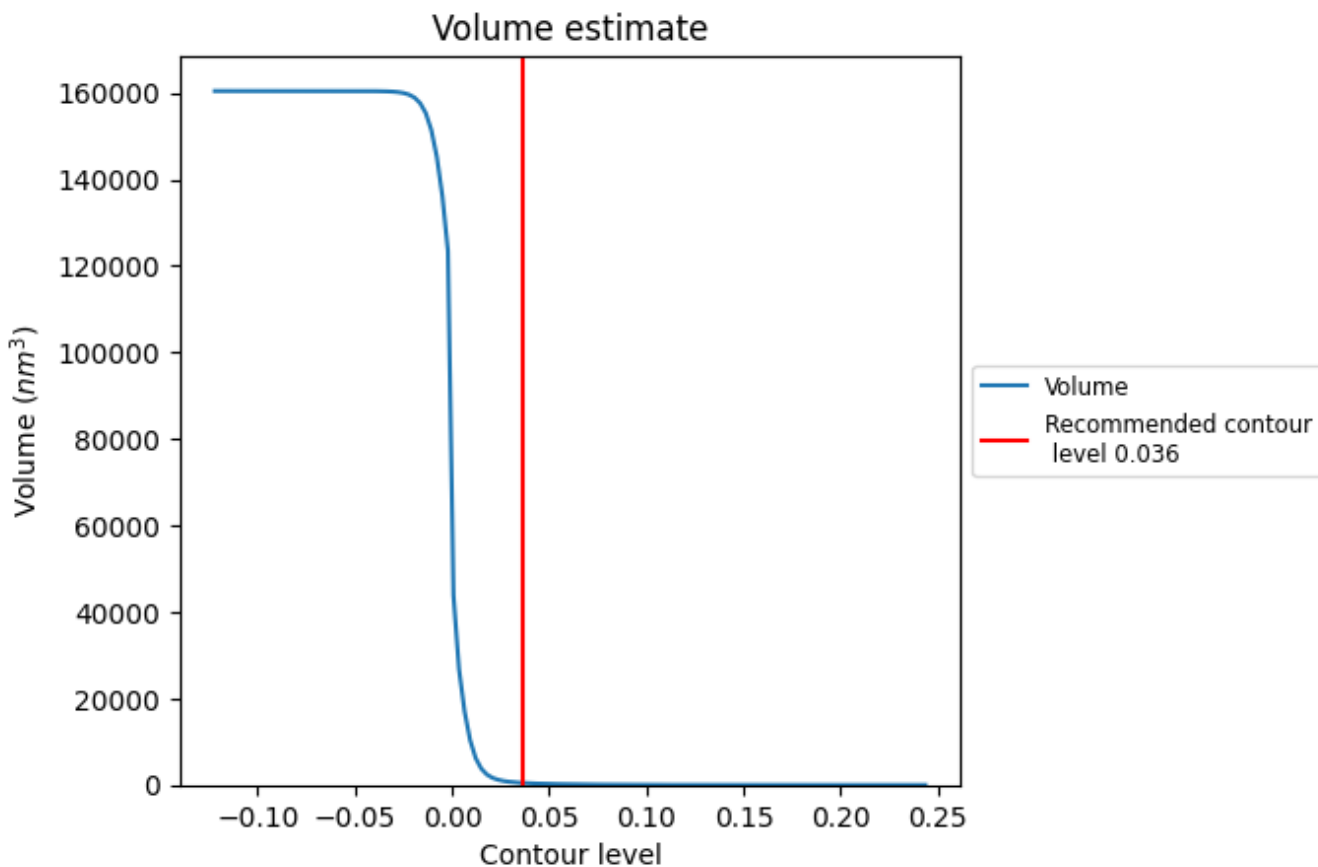
This section contains the results of statistical analysis of the map.

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.

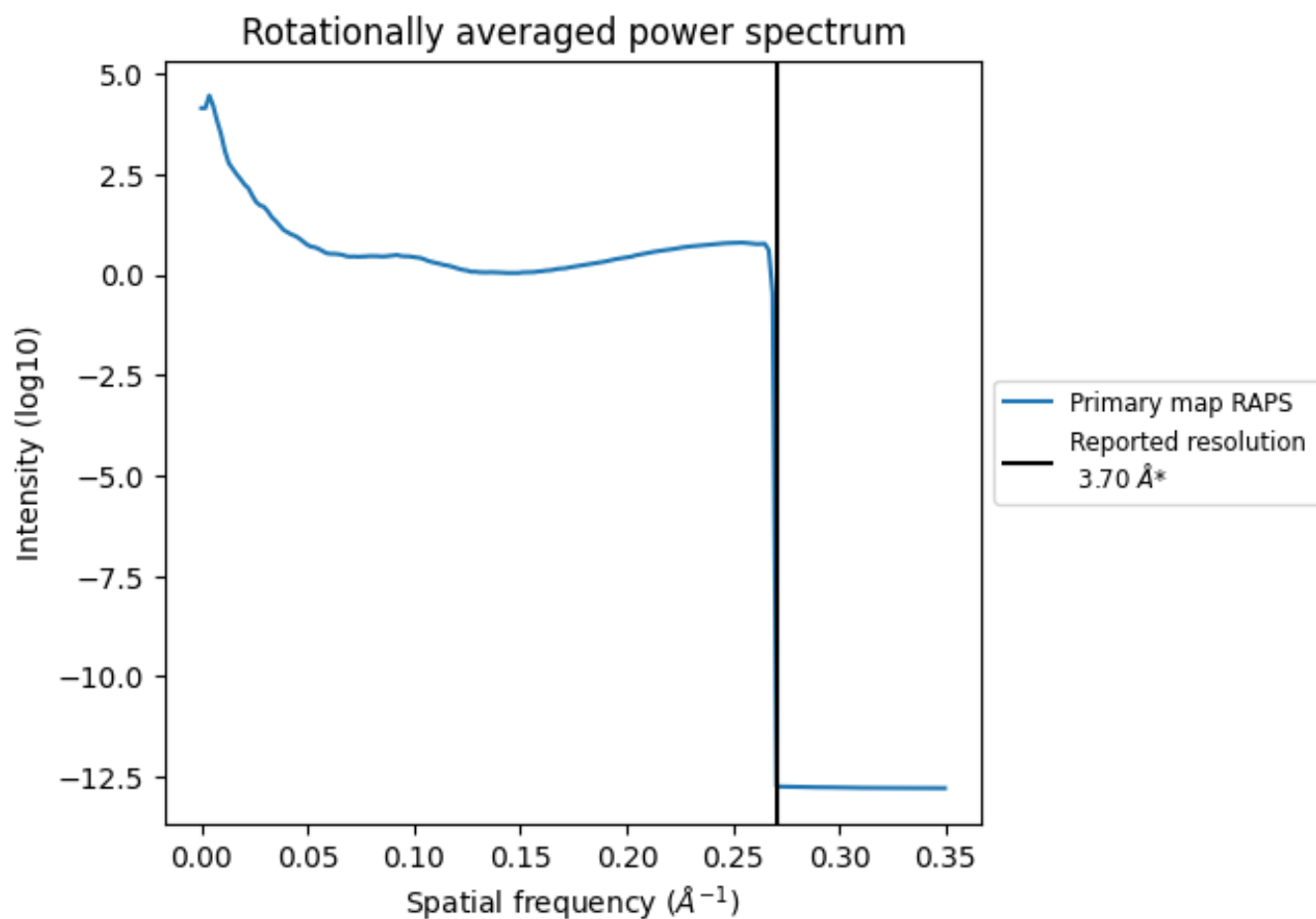
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 478 nm^3 ; this corresponds to an approximate mass of 432 kDa.

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

7.3 Rotationally averaged power spectrum i

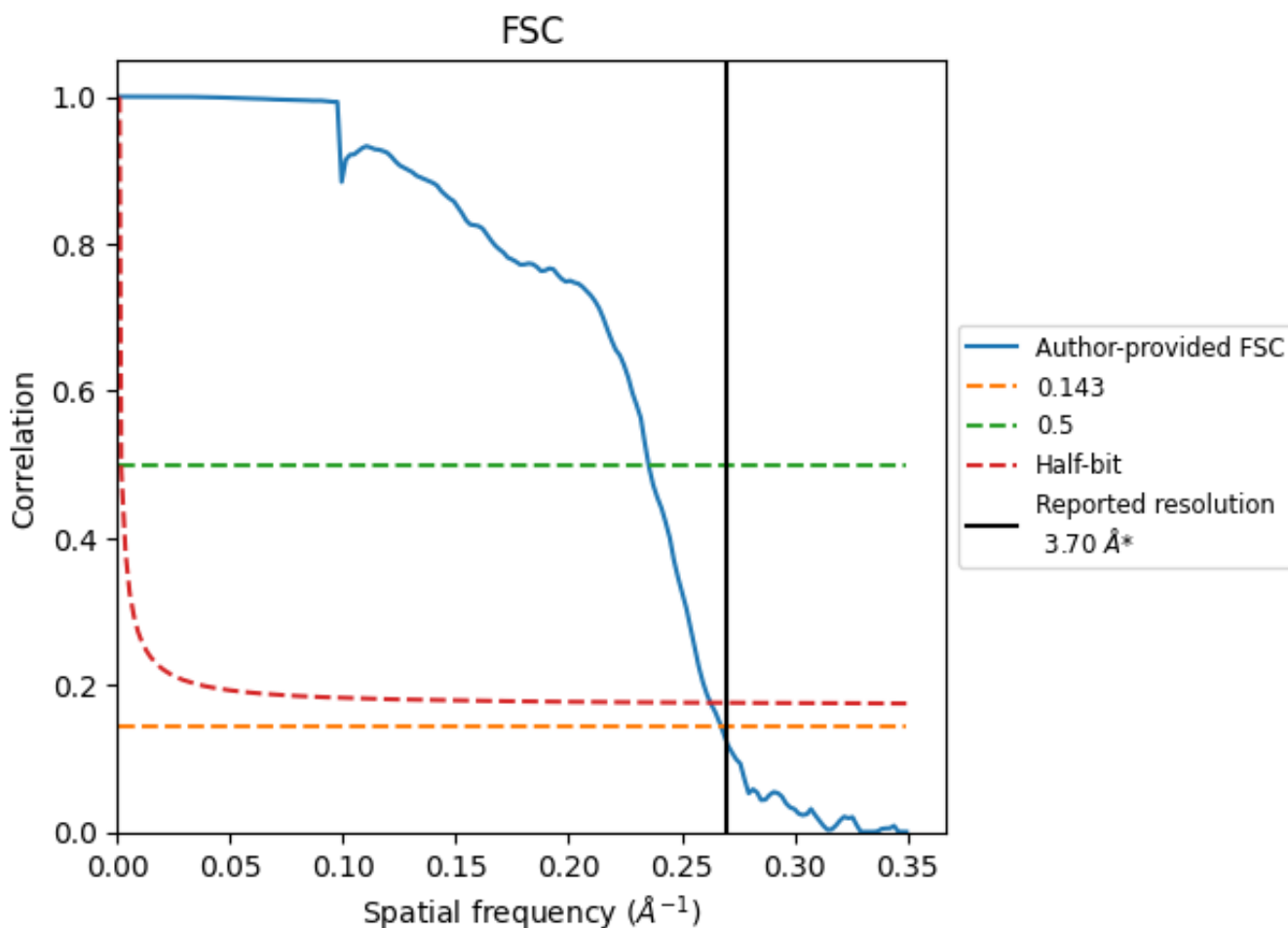


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

8.2 Resolution estimates [i](#)

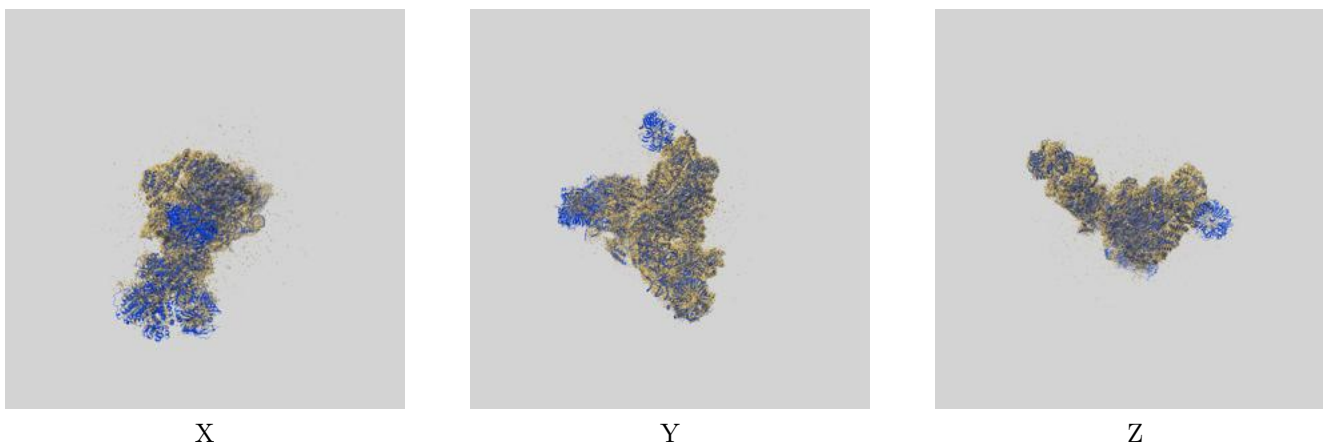
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.74	4.25	3.81
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

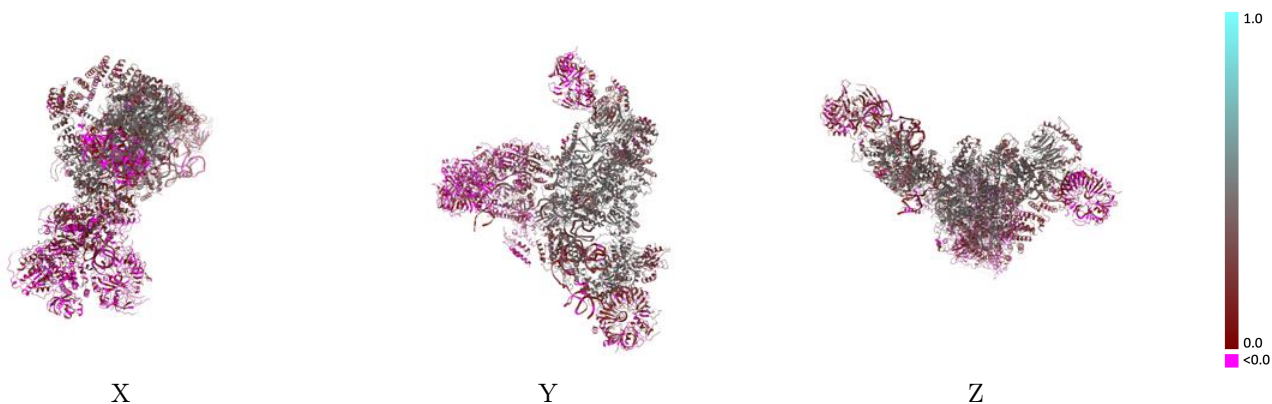
This section contains information regarding the fit between EMDB map EMD-8012 and PDB model 5GAN. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



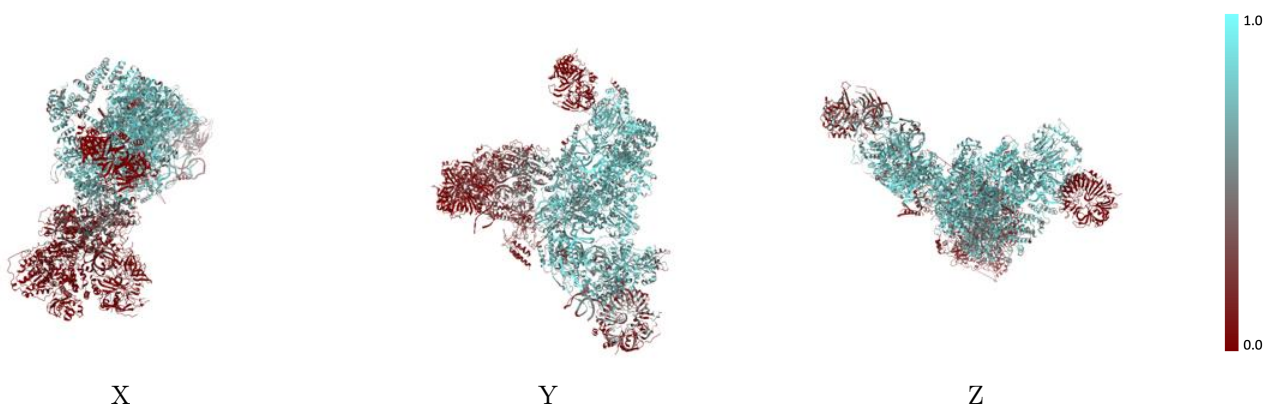
The images above show the 3D surface view of the map at the recommended contour level 0.036 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



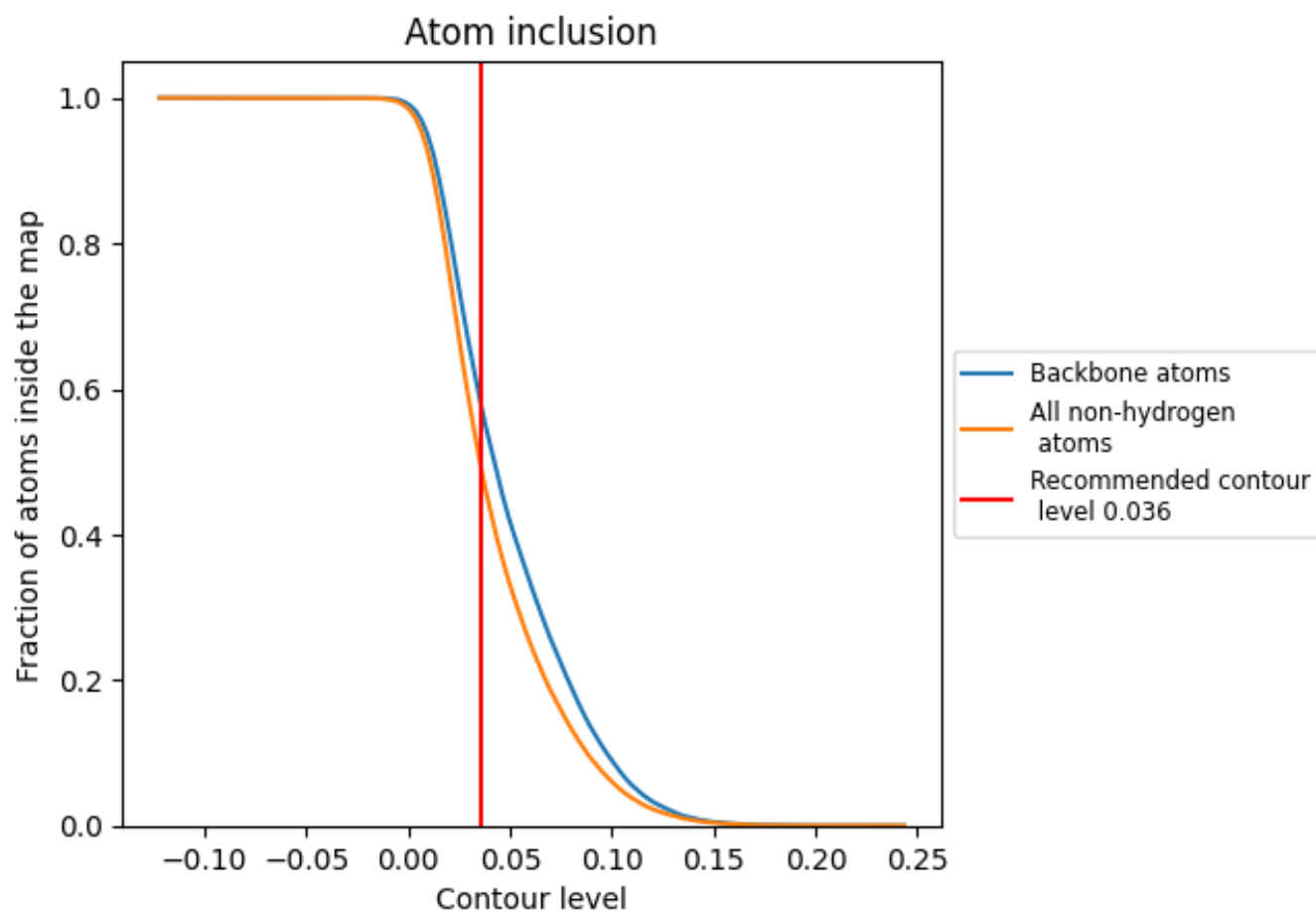
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.036).









































































9.4 Atom inclusion [i](#)



At the recommended contour level, 58% of all backbone atoms, 49% 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 (0.036) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4890	 0.2540
2	 0.0222	 0.0760
3	 0.0084	 0.0640
4	 0.0189	 0.0770
5	 0.0000	 0.0550
6	 0.0035	 0.0430
7	 0.0101	 0.0630
8	 0.0102	 0.0400
A	 0.6815	 0.3630
B	 0.1815	 0.1170
C	 0.7241	 0.3730
D	 0.7458	 0.4020
E	 0.0848	 0.0850
F	 0.7667	 0.4080
G	 0.6913	 0.3490
H	 0.7421	 0.3860
J	 0.6790	 0.3010
K	 0.7998	 0.4520
U	 0.6445	 0.2000
V	 0.5712	 0.2740
W	 0.7071	 0.2760
b	 0.3306	 0.1900
d	 0.4320	 0.2390
e	 0.2378	 0.1230
f	 0.2313	 0.0880
g	 0.3301	 0.1810
h	 0.2893	 0.1520
j	 0.2058	 0.1110
k	 0.0308	 0.0540
l	 0.0339	 0.0340
m	 0.0375	 0.0270
n	 0.0097	 0.0140
p	 0.0070	 0.0770
q	 0.0178	 0.0120
r	 0.0077	 0.0270
x	 0.7280	 0.3730

