



Full wwPDB EM Validation Report ⓘ

Aug 9, 2026 – 06:51 AM JST

PDB ID : 9XU3 / pdb_00009xu3
EMDB ID : EMD-67263
Title : Human minor spliceosome exon-ligation-ready C* complex (prior to step-II)
Authors : Wan, R.; Bai, R.
Deposited on : 2025-11-24
Resolution : 3.00 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:

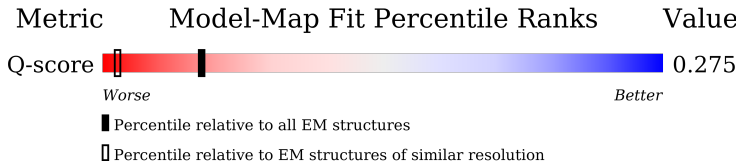
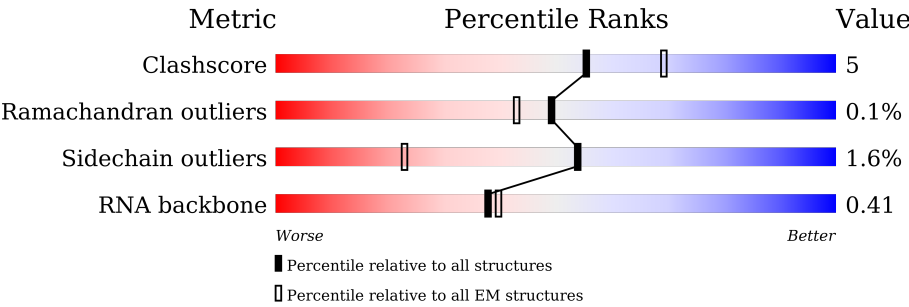
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 3.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	0	57	
2	1	277	
3	2	150	

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Mol	Chain	Length	Quality of chain
4	4	646	
5	5	117	
6	6	125	
7	A	2335	
8	B	972	
9	C	2136	
10	D	357	
11	E	802	
12	F	855	
13	G	848	
14	H	166	
15	I	285	
16	J	536	
17	K	514	
18	L	367	
19	L2	95	
20	L3	102	
21	L4	139	
22	L5	91	
23	L6	80	
24	L7	103	
25	L8	96	
26	M	198	
27	N	229	
28	O	166	

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Mol	Chain	Length	Quality of chain
29	P	301	
30	Q	1485	
31	R	161	
32	S	586	
33	T	1220	
34	U	2752	
35	V	908	
36	W	544	
37	X	758	
38	Y	112	
39	Z	415	
40	a	240	
40	h	240	
41	b	119	
41	i	119	
42	c	118	
42	j	118	
43	d	126	
43	k	126	
44	e	92	
44	l	92	
45	f	86	
45	m	86	
46	g	76	
46	n	76	

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Mol	Chain	Length	Quality of chain
47	p	476	
48	q	504	
48	r	504	
48	s	504	
48	t	504	
49	u	225	
50	v	411	
51	w	146	
52	x	174	
53	y	413	
54	z	233	

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 123688 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 MSE-U12_5 exon.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	25	Total	C	N	O	P	0	0
			533	238	98	172	25		

- Molecule 2 is a RNA chain called MSE-U12_intron-3 exon.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	55	Total	C	N	O	P	0	0
			1155	518	190	392	55		

- Molecule 3 is a RNA chain called U12 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	42	Total	C	N	O	P	0	0
			898	403	163	290	42		

- Molecule 4 is a protein called Peptidylprolyl isomerase domain and WD repeat-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	407	Total	C	N	O	S	0	0
			3283	2095	559	606	23		

- Molecule 5 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	109	Total	C	N	O	P	0	0
			2296	1028	383	776	109		

- Molecule 6 is a RNA chain called U6atac snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	115	Total	C	N	O	P	0	0
			2439	1085	432	805	117		

- Molecule 7 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	2283	Total	C	N	O	S	0	0
			18932	12179	3305	3366	82		

- Molecule 8 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	900	Total	C	N	O	S	0	0
			7122	4556	1185	1347	34		

- Molecule 9 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	1923	Total	C	N	O	S	0	0
			15118	9637	2604	2804	73		

- Molecule 10 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	308	Total	C	N	O	S	0	0
			2406	1509	424	459	14		

- Molecule 11 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	608	Total	C	N	O	S	0	0
			3925	2408	752	757	8		

- Molecule 12 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	741	Total	C	N	O	S	0	0
			4897	3044	900	935	18		

- Molecule 13 is a protein called Crooked neck-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	639	Total	C	N	O	S	0	0
			4412	2762	819	825	6		

- Molecule 14 is a protein called Coiled-coil domain-containing protein 12.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	H	44	Total	C	N	O	0	0
			320	201	65	54		

- Molecule 15 is a protein called Pre-mRNA-splicing factor ISY1 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	I	48	Total	C	N	O	0	0
			238	142	48	48		

- Molecule 16 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	J	245	Total	C	N	O	P	S	0	0
			1815	1133	322	348	2	10		

- Molecule 17 is a protein called Pleiotropic regulator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	K	406	Total	C	N	O	S	0	0
			3014	1897	550	558	9		

- Molecule 18 is a protein called RNA-binding protein 48.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	L	141	Total	C	N	O	S	0	0
			1139	727	197	210	5		

- Molecule 19 is a protein called U6 snRNA-associated Sm-like protein LSm2.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	L2	95	Total	C	N	O	0	0
			472	282	95	95		

- Molecule 20 is a protein called U6 snRNA-associated Sm-like protein LSm3.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	L3	85	Total	C	N	O	0	0
			421	251	85	85		

- Molecule 21 is a protein called U6 snRNA-associated Sm-like protein LSm4.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	L4	80	Total	C	N	O	0	0
			396	236	80	80		

- Molecule 22 is a protein called U6 snRNA-associated Sm-like protein LSm5.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	L5	82	Total	C	N	O	0	0
			402	238	82	82		

- Molecule 23 is a protein called U6 snRNA-associated Sm-like protein LSm6.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	L6	75	Total	C	N	O	0	0
			368	218	75	75		

- Molecule 24 is a protein called U6 snRNA-associated Sm-like protein LSm7.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	L7	89	Total	C	N	O	0	0
			437	259	89	89		

- Molecule 25 is a protein called U6 snRNA-associated Sm-like protein LSm8.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	L8	96	Total	C	N	O	0	0
			472	280	96	96		

- Molecule 26 is a protein called Armadillo repeat-containing protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	M	173	Total	C	N	O	S	0	0
			1292	815	218	253	6		

- Molecule 27 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	N	98	Total	C	N	O	S	0	0
			845	517	167	159	2		

- Molecule 28 is a protein called Peptidyl-prolyl cis-trans isomerase-like 1.

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

- Molecule 29 is a protein called Peptidyl-prolyl cis-trans isomerase E.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	P	79	Total	C	N	O	0	0
			390	232	79	79		

- Molecule 30 is a protein called RNA helicase aquarius.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	Q	1327	Total	C	N	O	0	0
			6579	3925	1327	1327		

- Molecule 31 is a protein called Peptidyl-prolyl cis-trans isomerase-like 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	R	161	Total	C	N	O	0	0
			791	468	161	162		

- Molecule 32 is a protein called Pre-mRNA-splicing factor SLU7.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	S	272	Total	C	N	O	S	0	0
			2249	1413	402	426	8		

- Molecule 33 is a protein called ATP-dependent RNA helicase DHX8.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	T	780	Total	C	N	O	S	0	0
			6236	3955	1058	1182	41		

- Molecule 34 is a protein called Serine/arginine repetitive matrix protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	U	132	Total	C	N	O	S	0	0
			874	530	174	169	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	V	464	Total	C	N	O	S	0	0
			3768	2415	642	689	22		

- Molecule 36 is a protein called WD repeat-containing protein 25.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	W	348	Total	C	N	O	S	0	0
			2764	1753	500	493	18		

- Molecule 37 is a protein called Splicing factor Cactin.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	X	142	Total	C	N	O	S	0	0
			1243	815	220	205	3		

- Molecule 38 is a protein called Protein FAM32A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Y	59	Total	C	N	O	S	0	0
			494	308	94	90	2		

- Molecule 39 is a protein called NF-kappa-B-activating protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Z	31	Total	C	N	O	S	0	0
			234	142	44	46	2		

- Molecule 40 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	a	73	Total	C	N	O	S	0	0
			591	376	105	103	7		
40	h	73	Total	C	N	O		0	0
			360	214	73	73			

- Molecule 41 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	b	82	Total	C	N	O	S	0	0
			649	413	113	119	4		

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Mol	Chain	Residues	Atoms				AltConf	Trace
41	i	81	Total	C	N	O	0	0
			401	239	81	81		

- Molecule 42 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	c	98	Total	C	N	O	S	0	0
			796	498	144	148	6		
42	j	98	Total	C	N	O		0	0
			487	291	98	98			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	d	85	Total	C	N	O	S	0	0
			663	415	117	125	6		
43	k	81	Total	C	N	O		0	0
			399	237	81	81			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
44	e	77	Total	C	N	O	S	0	0
			638	405	113	115	5		
44	l	77	Total	C	N	O		0	0
			381	227	77	77			

- Molecule 45 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	f	73	Total	C	N	O	S	0	0
			567	367	94	101	5		
45	m	73	Total	C	N	O		0	0
			356	210	73	73			

- Molecule 46 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	g	74	Total	C	N	O	S	0	0
			577	364	104	103	6		
46	n	74	Total	C	N	O		0	0
			364	215	74	75			

- Molecule 47 is a protein called Splicing factor ESS-2 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	p	52	Total	C	N	O	0	0
			265	161	52	52		

- Molecule 48 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	q	137	Total	C	N	O	0	0
			684	410	137	137		
48	r	135	Total	C	N	O	0	0
			674	404	135	135		
48	s	138	Total	C	N	O	0	0
			689	413	138	138		
48	t	136	Total	C	N	O	0	0
			679	407	136	136		

- Molecule 49 is a protein called Pre-mRNA-splicing factor SPF27.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	u	225	Total	C	N	O	0	0
			1117	666	225	226		

- Molecule 50 is a protein called Eukaryotic initiation factor 4A-III.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	v	390	Total	C	N	O	S	0	0
			3130	1976	546	589	19		

- Molecule 51 is a protein called Protein mago nashi homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	w	144	Total	C	N	O	S	0	0
			1196	772	200	221	3		

- Molecule 52 is a protein called RNA-binding protein 8A.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	x	91	Total	C	N	O	S	0	0
			730	463	122	142	3		

- Molecule 53 is a protein called RNA-binding protein 41.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	y	147	Total	C	N	O	0	0
			751	452	149	150		

- Molecule 54 is a protein called Protein FAM204A.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	z	114	Total	C	N	O	S	0	0
			933	588	169	173	3		

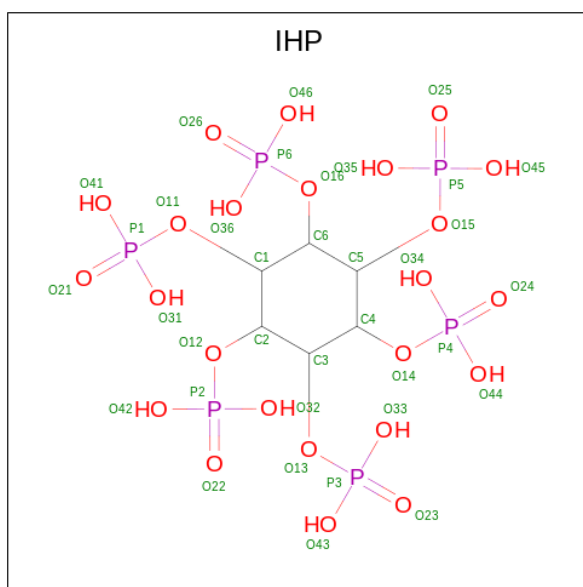
- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
55	1	2	Total	Mg	0
			2	2	
55	6	4	Total	Mg	0
			4	4	
55	B	1	Total	Mg	0
			1	1	
55	C	1	Total	Mg	0
			1	1	
55	v	1	Total	Mg	0
			1	1	

- Molecule 56 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

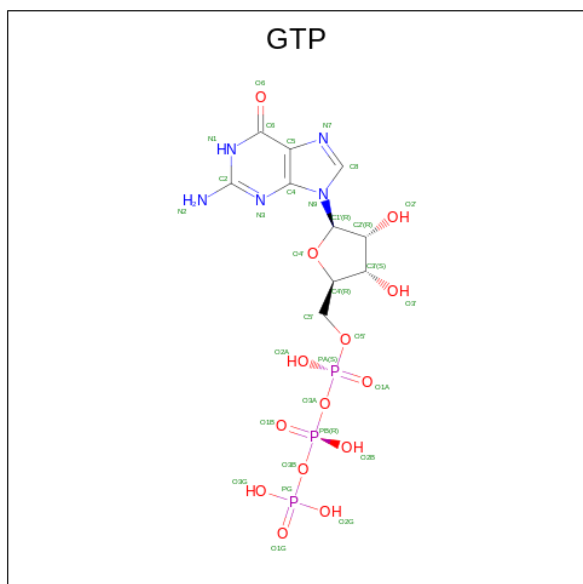
Mol	Chain	Residues	Atoms		AltConf
56	6	2	Total	K	0
			2	2	

- Molecule 57 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: C₆H₁₈O₂₄P₆) (labeled as "Ligand of Interest" by depositor).



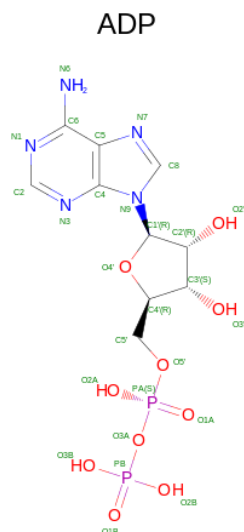
Mol	Chain	Residues	Atoms				AltConf
57	A	1	Total	C	O	P	0
			36	6	24	6	

- Molecule 58 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 59 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

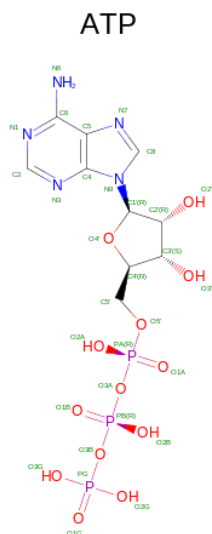


Mol	Chain	Residues	Atoms					AltConf
59	C	1	Total 27	C 10	N 5	O 10	P 2	0
59	C	1	Total 27	C 10	N 5	O 10	P 2	0

- Molecule 60 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
60	S	1	Total Zn 1 1	0

- Molecule 61 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$) (labeled as "Ligand of Interest" by depositor).

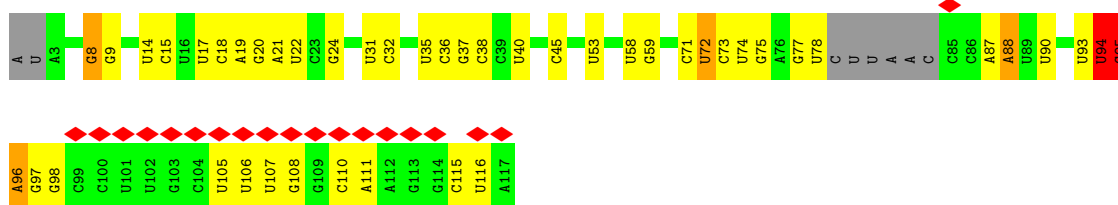
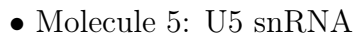


Mol	Chain	Residues	Atoms					AltConf
61	v	1	Total 31	C 10	N 5	O 13	P 3	0

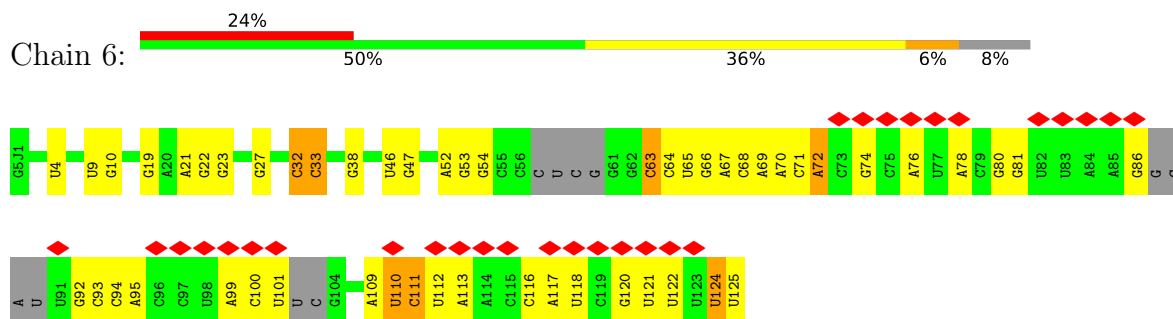
- Molecule 62 is water.

Mol	Chain	Residues	Atoms	AltConf
62	6	1	Total O 1 1	0

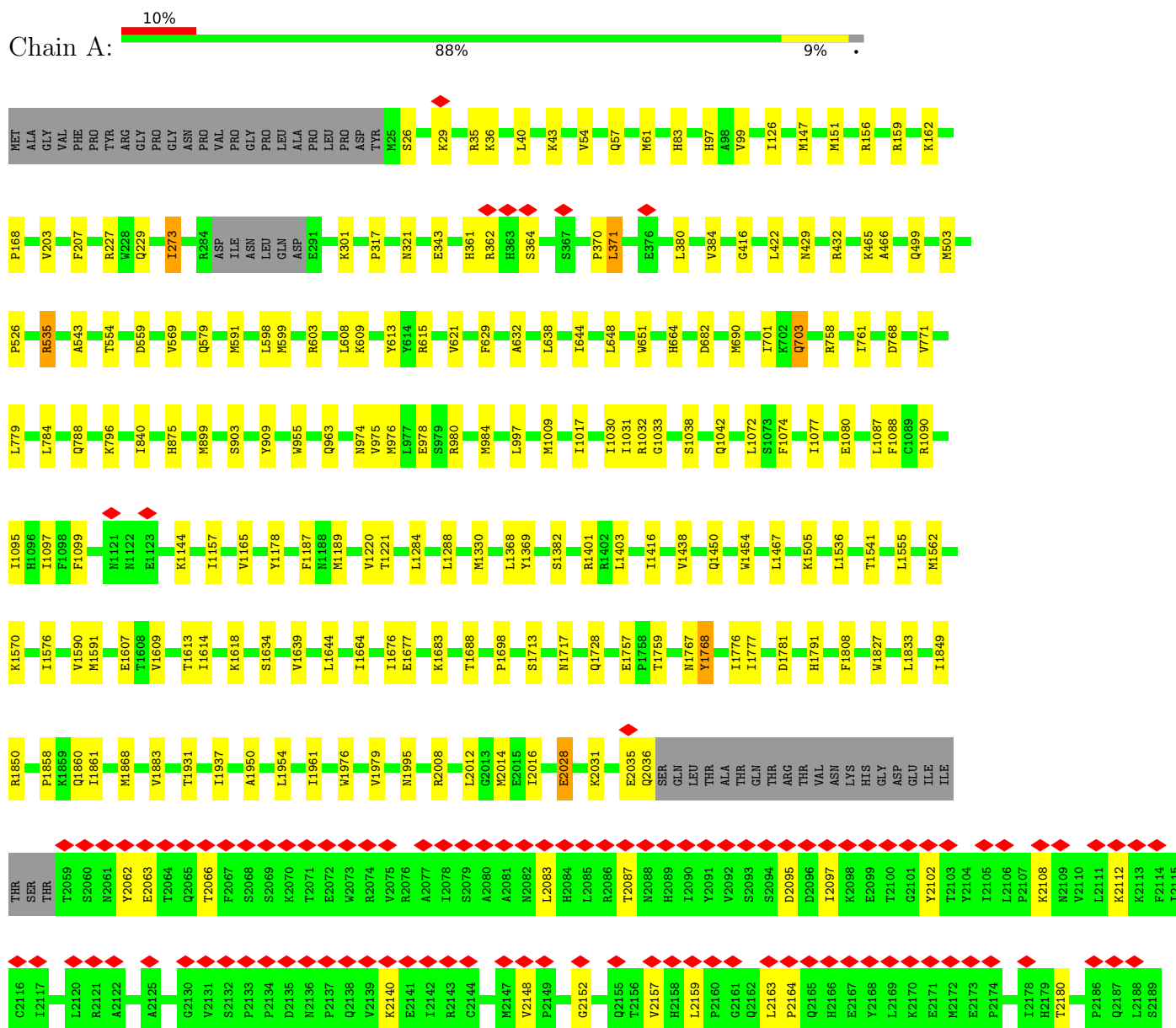
- Chain 4:



- Molecule 6: U6atac snRNA

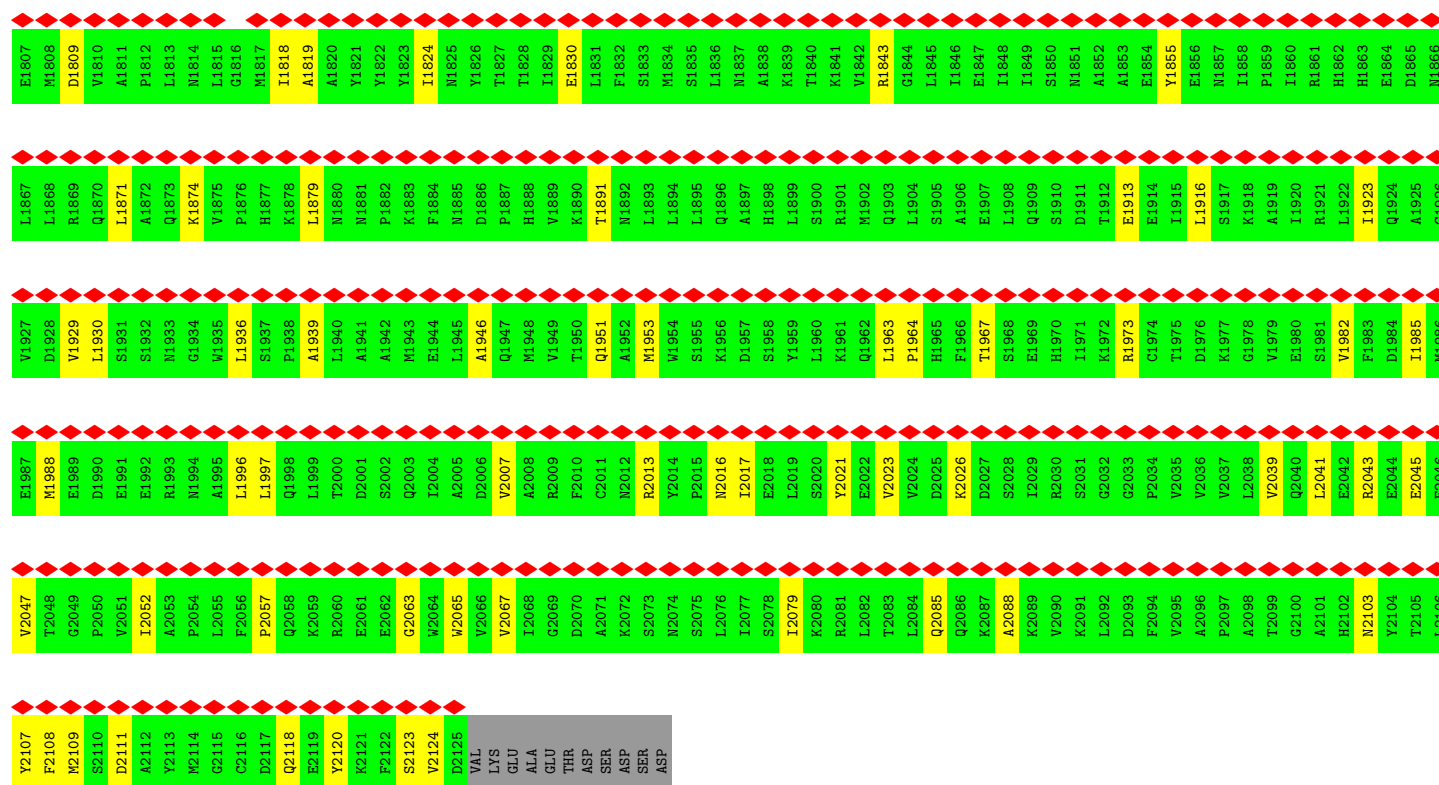


- Molecule 7: Pre-mRNA-processing-splicing factor 8

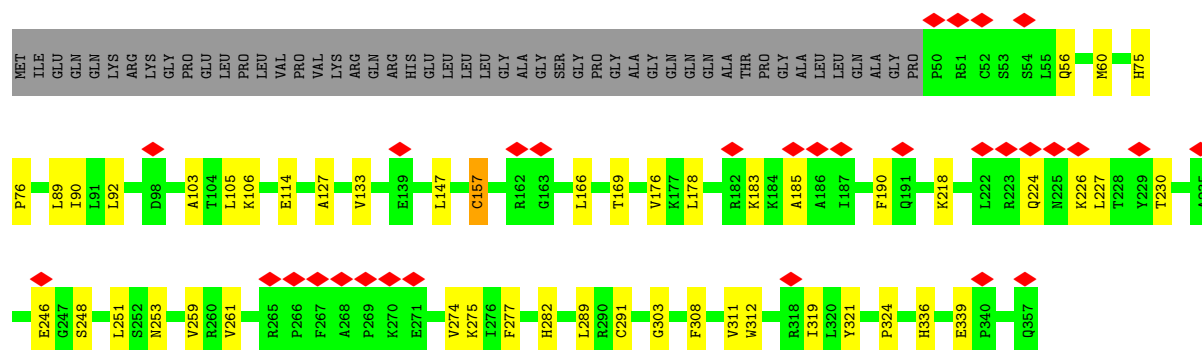
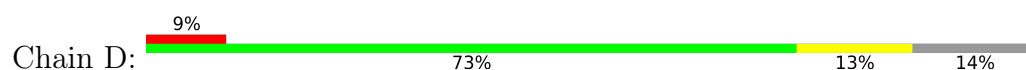


A961	L962	M963	L964	D965	K966	N967	N968	L969	V970	K971	Y972	D973	K974	D975	A976	G977	N978	F979	Q980	Y981	T982	E983	L984	G985	R986	I987	A988	S989	H990	Y991	Y992	N993	T994	N995	D996	N997	Y998	Q999	T1000	Y1001	N1002	Q1003	L1004	G1005	K1006	P1007	T1008	L1009	S1010	E1011	I1012	E1013	L1014	F1015	R1016	V1017	F1018	S1019	L1020						
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G781	F782	A783	T784	H785	H786	L787	G788	M789	T790	R791	V792	D793	R794	T795	L796	V797	E798	D799	L800	F801	A802	D803	K804	H805	L806	Q807	L808	L809	V810	S811	T812	A813	T814	L815	A816	H817	L818	V819	N820	L821	A822	H823	T824	V825	V826	I827	T828	K829	G830	T831	Q832	H833	Y834	S835	P836	E837	K838	G839	R840						
V721	L722	V723	F724	V725	H726	S727	R728	M729	E730	T731	G732	K733	T734	A735	R736	A737	I738	R739	D740	M741	C742	L743	E744	K745	D746	T747	L748	G749	L750	F751	L752	R753	E754	G755	S756	A757	S758	T759	E760	V761	R762	R763	T764	E765	V766	E767	Q768	C769	K770	N771	L772	E773	L774	K775	D776	L777	P778	Y779	V780						
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Y361	Q362	L363	H364	E365	T366	GLU	LYS	GLU	ASP	LEU	ILE	ARG	GLU	GLU	SER	ARG	ARG	GLU	VAL	ARG	GLN	SER	ARG	MET	ASP	THR	ASP	LEU	GLU	THR	ASP	LEU	GLN	C331	T332	L333	L334	A335	S336	A337	I280	V281	S339	E340	Q283	K284	K285	A286	D287	E288	V289	L290	E291	K349	Q418	L293	K294	T295	A296	S297	D298	D299	R300		
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SER	ALA	ASN	LEU	VAL	ALA	SER	GLY	GLU	LEU	M251	S252	S253	K254	K255	K256	D257	L258	T259	P260	R261	ARG	R262	GLN	PHE	SER	SER	ASP	GLU	VAL	L271	L272	TYR	GLY	GLY	VAL	ARG	GLU	GLU	ALA	SER	ASP	ASP	ASP	MET	GLU	GLY	ASP	GLU	ALA	VAL	VAL	ARG	CYS	THR	LEU										
D181	Y182	G183	G184	ASP	LYS	GLY	ILE	GLN	ASN	ASN	MET	ASP	ASP	ASN	ASP	ILE	ASP	THR	TYR	GLY	VAL	ASN	VAL	GLN	PHE	SER	SER	ASP	GLU	VAL	TYR	GLY	VAL	ARG	GLU	GLU	ALA	SER	ASP	ASP	ASP	MET	GLU	GLY	ASP	GLU	ALA	VAL	VAL	ARG	CYS	THR	LEU												

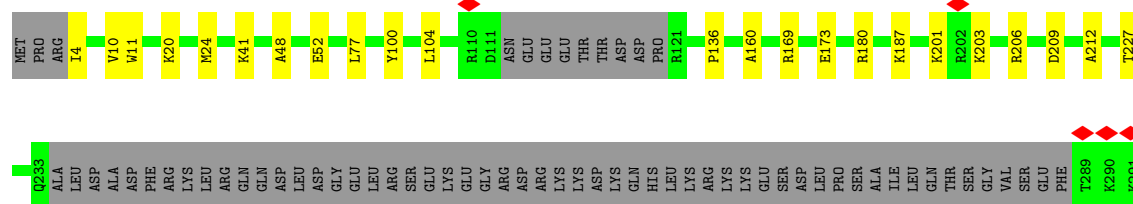
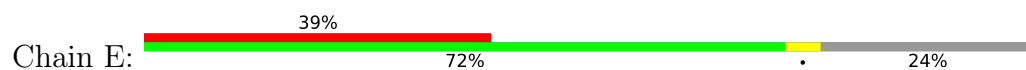
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D1753	M1692	V1632	T1572	F1512	V1452	D1392	Q1332	S1272	E1212	E1151	L1091
L1754	R1693	E1633	A1573	M1513	V1453	W1393	T1333	D1273	K1213	R1152	M1092
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W1757	Q1696	F1636	I1576	P1516	V1456	K1396	F1336	L1276	G1216	D1155	I1095
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L1760	D1698	S1638	T1578	V1518	L1458	Q1398	T1338	C1278	E1218	N1157	E1097
Y1761	E1699	G1639	T1579	R1519	I1459	D1399	V1339	E1279	S1219	H1158	I1098
R1762	G1700	A1640	C1580	P1520	G1460	R1400	Y1340	T1280	A1220	N1159	V1099
C1763	R1701	I1641	C1580	V1521	G1461	L1401	N1341	Q1281	F1221	E1160	L1100
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T1765	V1703	V1643	D1583	L1523	N1463	K1403	D1343	P1283	I1223	G1162	E1042
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M1767	G1706	V1645	Q1585	L1525	P1465	V1405	N1345	S1285	V1225	L1164	W1044
	Q1707	A1646	R1586	H1526	V1466	V1406	V1346	F1286	E1226	I1165	A1105
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M1772	G1708	R1648	R1588	Q1528	E1468	L1408	V1348	L1288	V1228	M1167	L1107
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R1779	K1715	L1655	K1595	T1535	R1475	D1415	G1355	Y1295	H1235	I1174	N1113
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L1781	F1717	A1657	L1597	T1537	I1477	K1417	T1357	P1297	E1237	K1176	C1115
S1782	L1718	A1658	I1598	R1538	S1478	L1418	I1358	P1298	Y1238	V1177	K1116
D1783	Y1719	H1659	P1599	L1539	S1479	L1419	C1359	T1299	F1239	V1178	K1058
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L1785	P1721	V1661	L1601	M1541	I1481	K1421	E1361	L1301	L1241	L1180	K1120
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V1788		M1664	L1604	K1544	P1484	I1424	I1364	Q1305	Y1245	K1183	W1123
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L1728	L1728	T1666	D1606	V1546	R1486	I1426	R1366	L1307	Q1247	L1185	S1125
D1729	T1729	Q1667	S1607	Y1547	I1487	S1427	M1367	P1308	L1248	M1126	F1066
H1730	H1730	Y1668	T1608	H1548	V1488	T1428	L1368	V1309	E1248	S1187	I1067
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M1732	M1732	N1670	K1610	I1550	L1490	E1430	Q1370	S1310	H1250	H1189	Q1069
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L1734	D1734	K1672	T1612	H1552	S1492	W1432	S1372	L1312	I1252		K1071
E1735	H1735	L1673	L1613	H1553	S1493	D1433	E1373	R1313	T1253		
F1736	F1736	H1674	L1614	S1554	L1494	I1434	G1374	M1314	F1254	R1193	F1132
M1737	M1737	A1675	N1615	P1555	S1495	L1435	R1375	S1315	F1255	R1194	E1073
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E1739	E1739	V1677	V1617	L1557	A1497	R1437	V1377	F1317	P1257	S1196	G1074
S1803	S1803	D1678	G1618	P1558	K1498	R1438	I1378	E1318	V1258	T1197	F1075
I1804	V1741	Y1679	Y1619	V1559	D1499	W1439	Y1379	S1319	F1259	L1198	A1076
E1805	T1742	P1680	L1620	I1560	V1500	K1440	T1380	E1260	L1320	V1200	M1078
D1806	K1743	I1681	H1621	F1561	A1501	Q1441	P1381	Y1321	P1261	E1201	A1079
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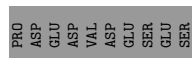


• Molecule 10: U5 small nuclear ribonucleoprotein 40 kDa protein

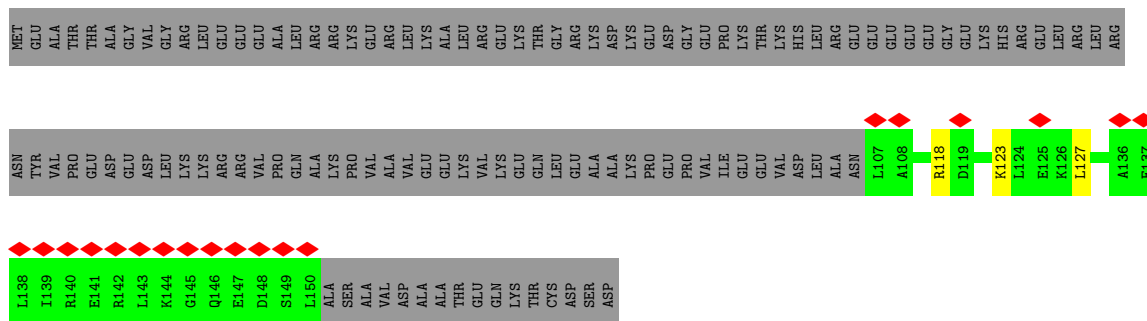


• Molecule 11: Cell division cycle 5-like protein

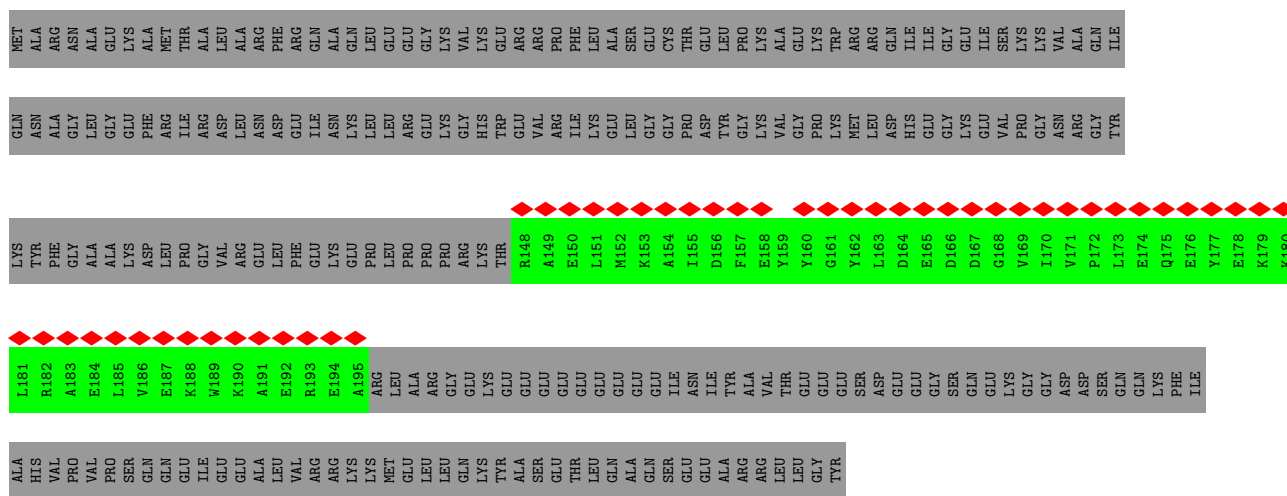




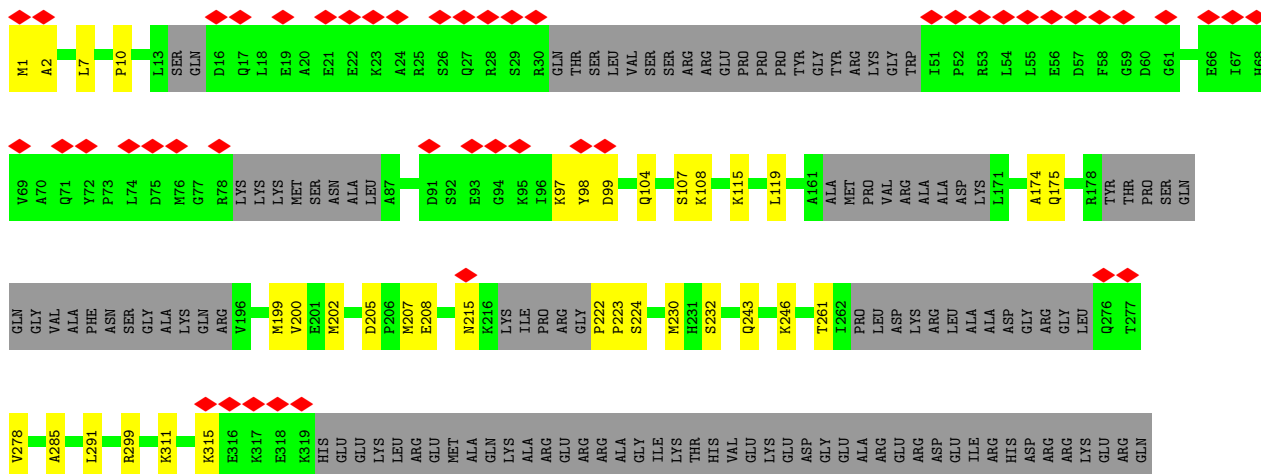
Chain H: 11% 25% 73%



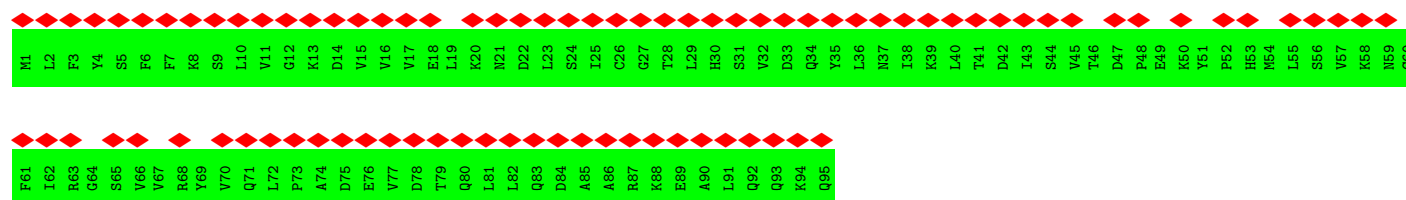
Chain I:



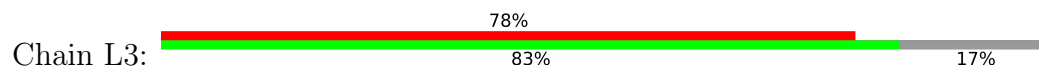
Chain J: 9% 39% 7% 45%



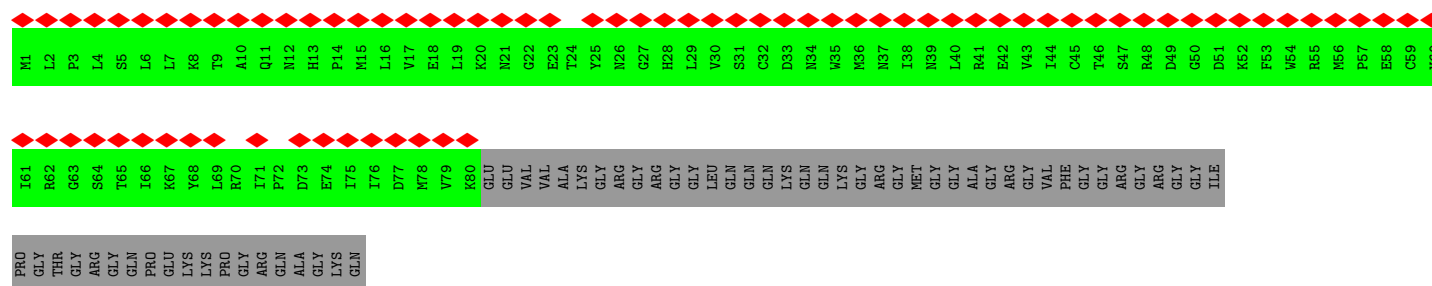




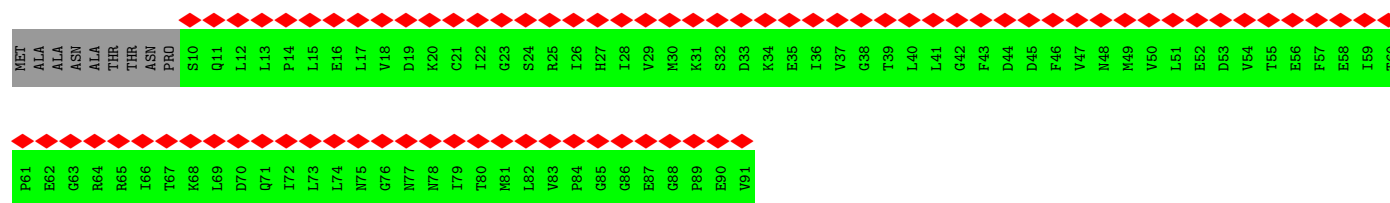
• Molecule 20: U6 snRNA-associated Sm-like protein LSm3



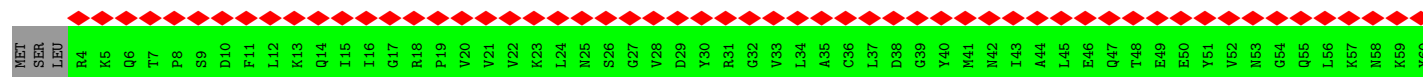
• Molecule 21: U6 snRNA-associated Sm-like protein LSm4



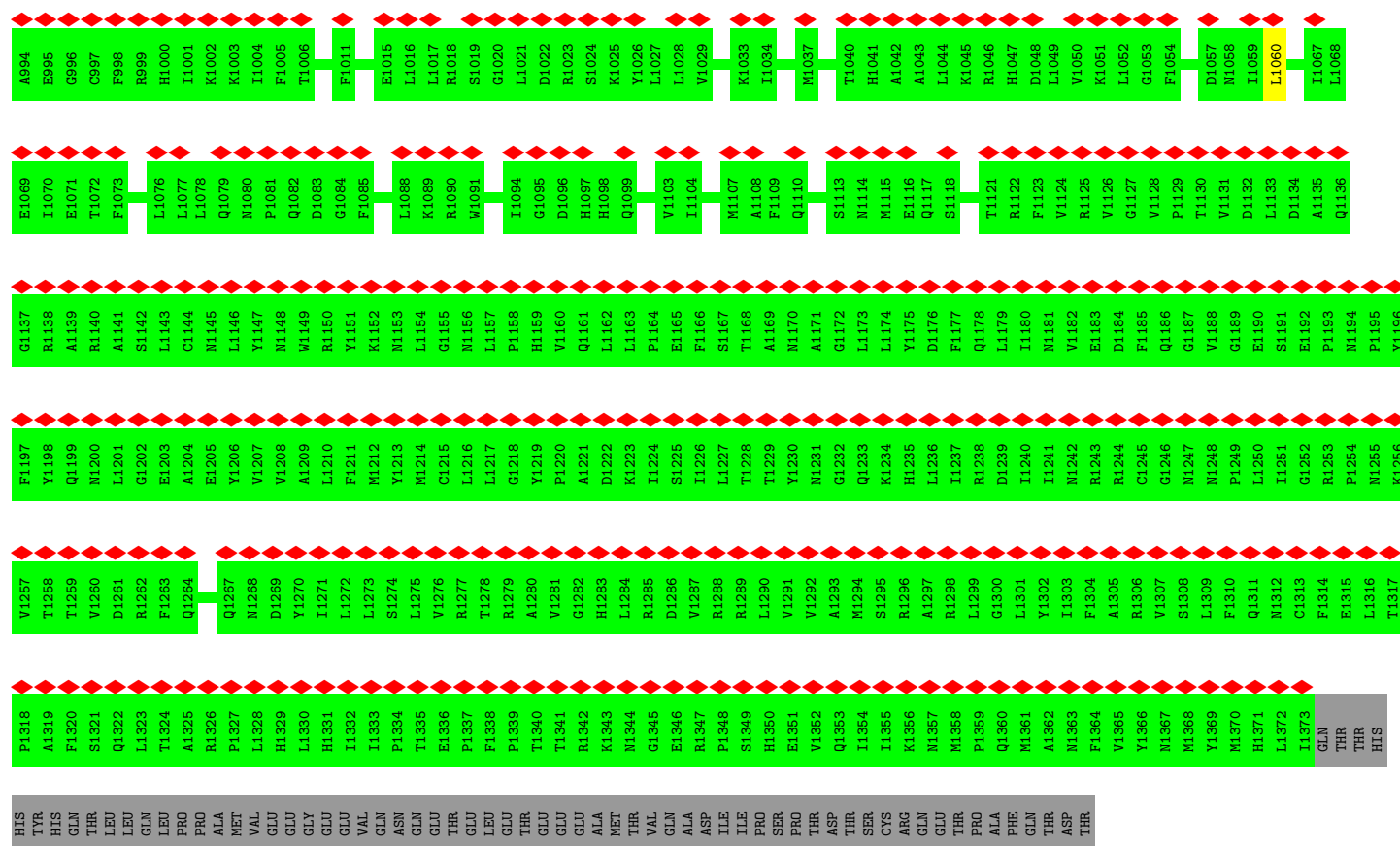
• Molecule 22: U6 snRNA-associated Sm-like protein LSm5



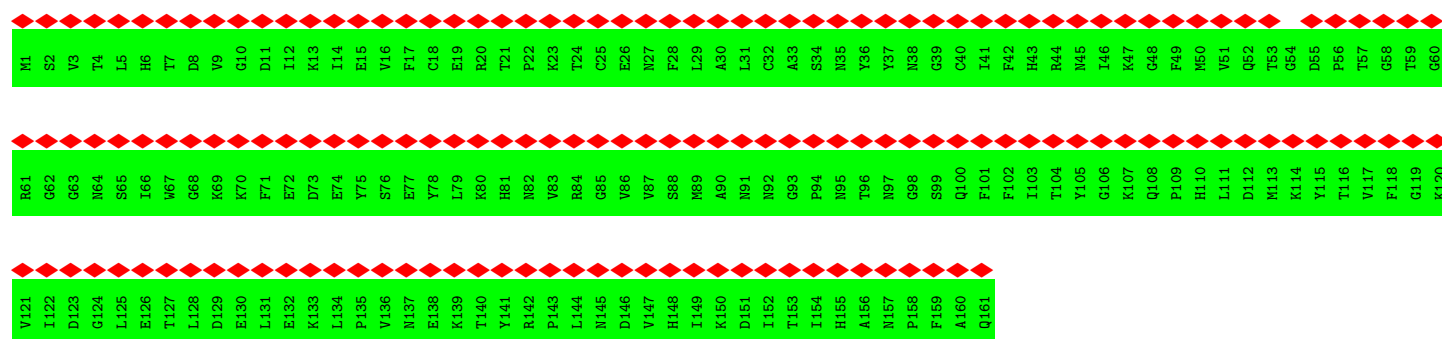
• Molecule 23: U6 snRNA-associated Sm-like protein LSm6



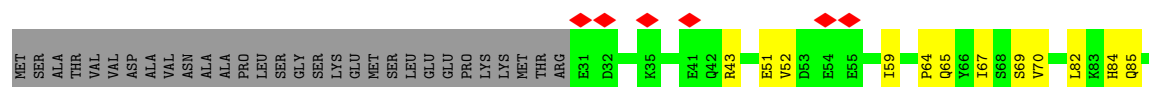
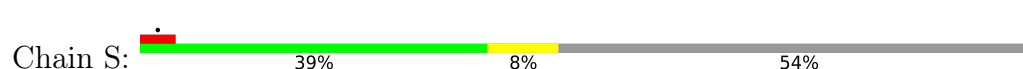




• Molecule 31: Peptidyl-prolyl cis-trans isomerase-like 3



• Molecule 32: Pre-mRNA-splicing factor SLU7

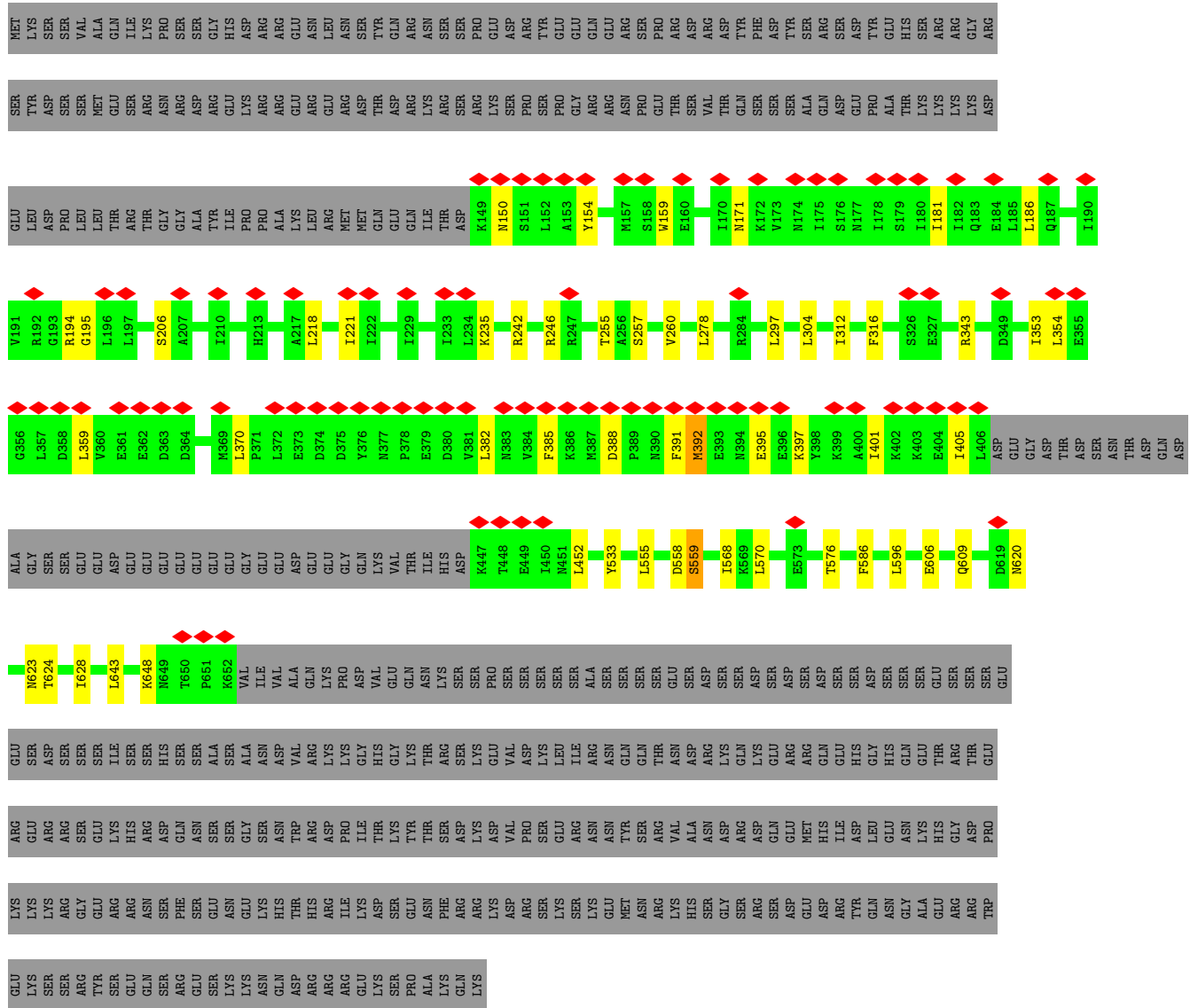




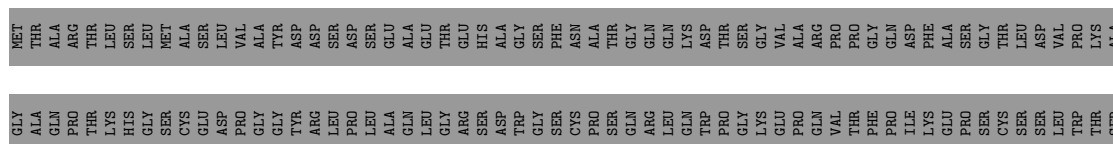


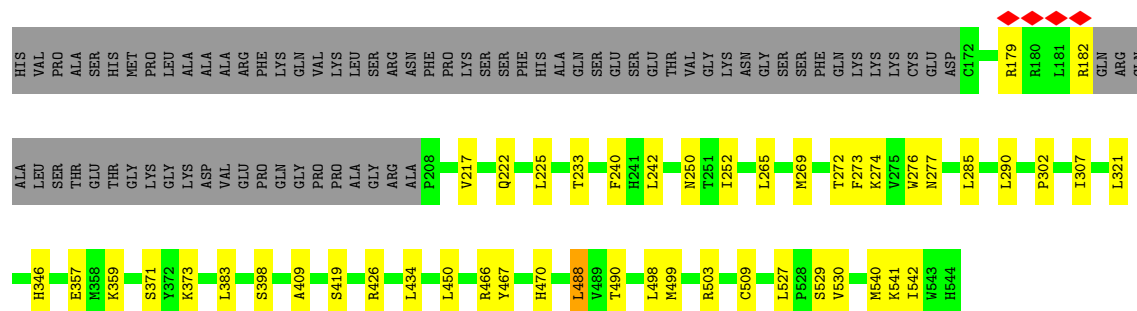


Chain V:

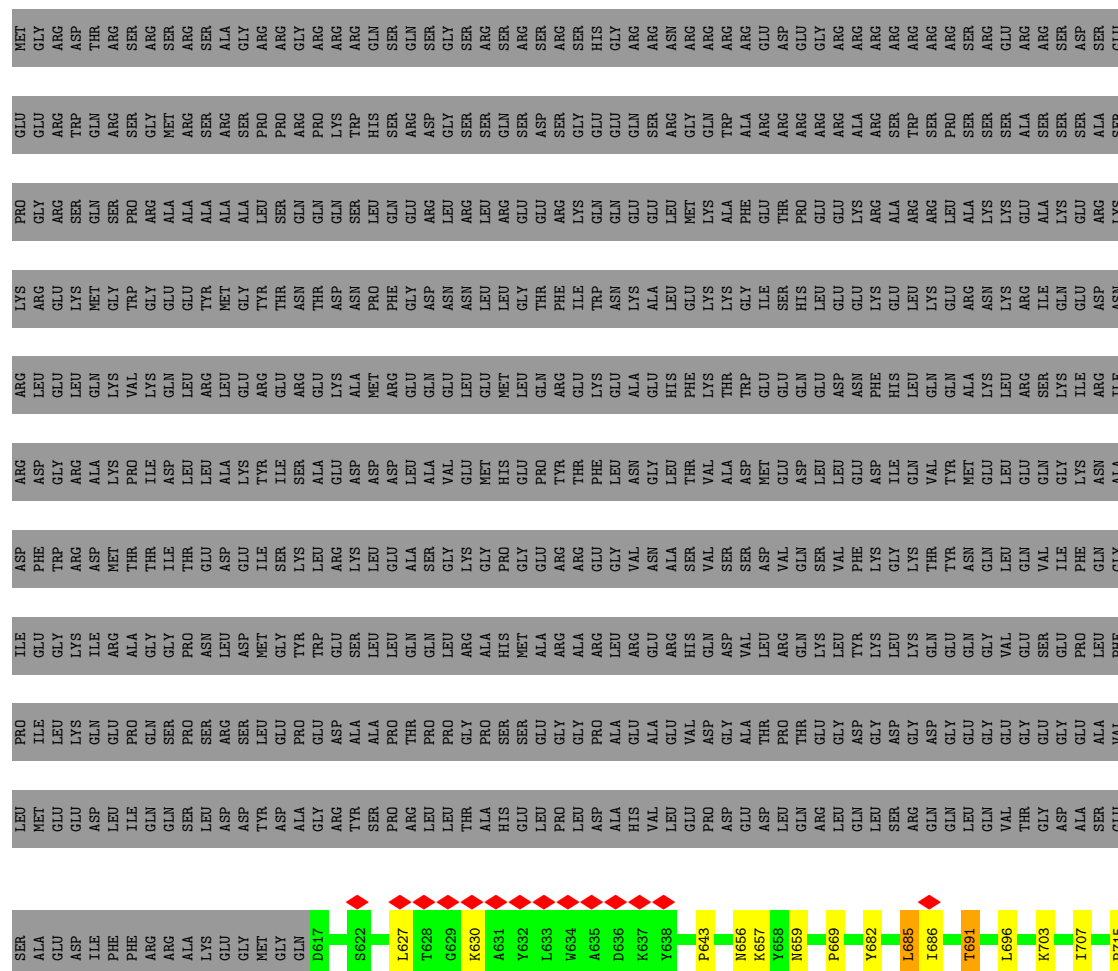


Chain W: 55% 9% 36%





- Molecule 37: Splicing factor Cactin

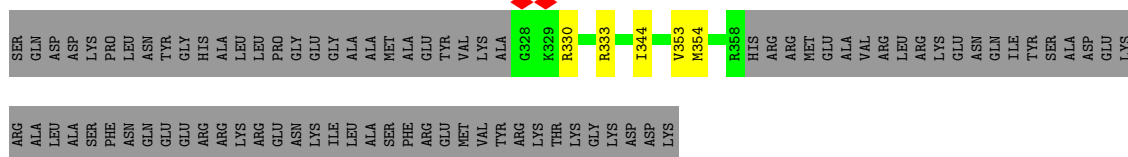


- Molecule 38: Protein FAM32A

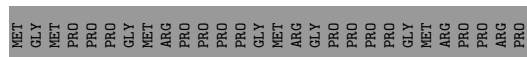




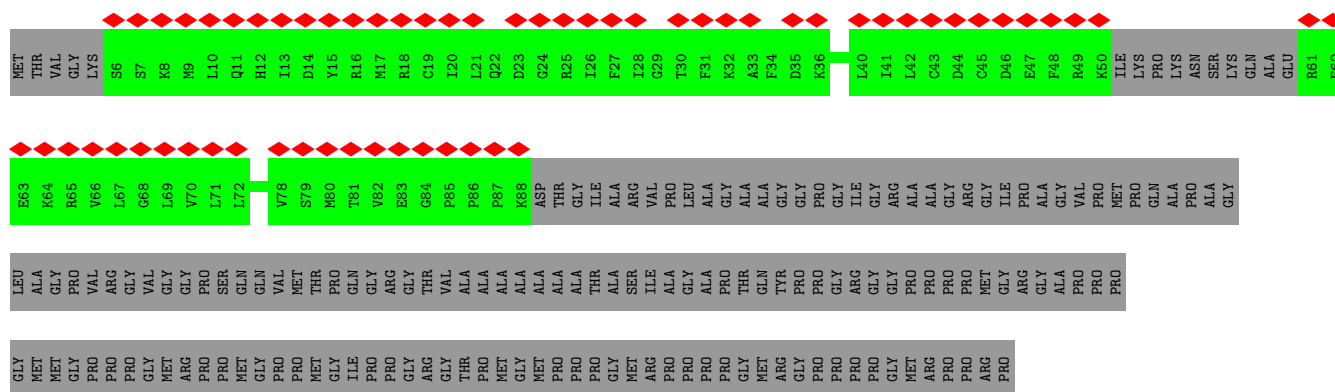
Chain Z: 6% 93%



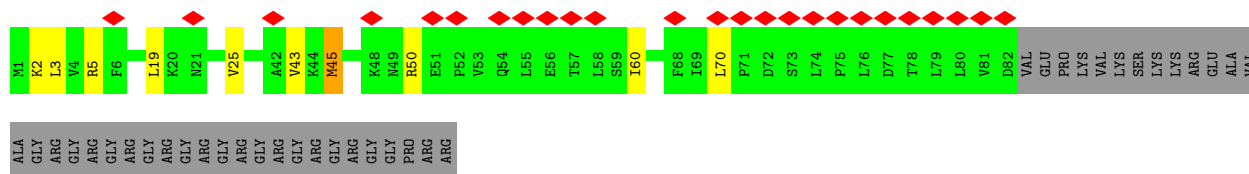
Chain a:



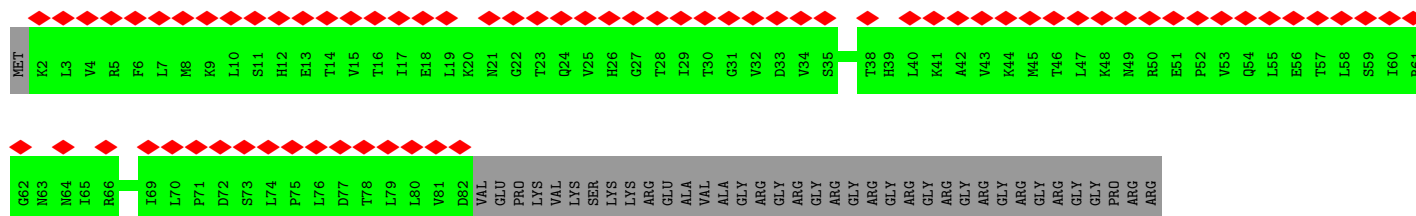
Chain h:



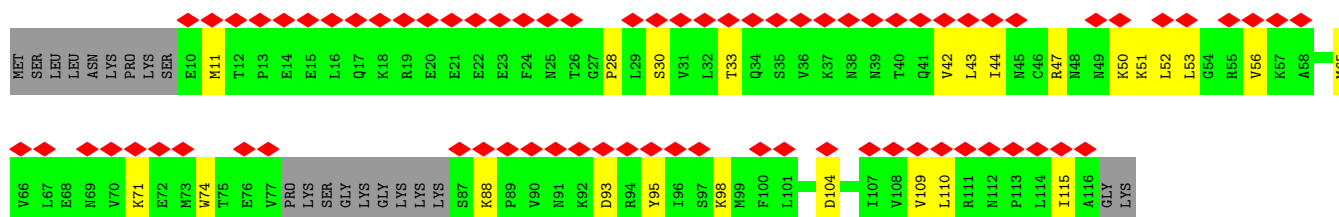
• Molecule 41: Small nuclear ribonucleoprotein Sm D1



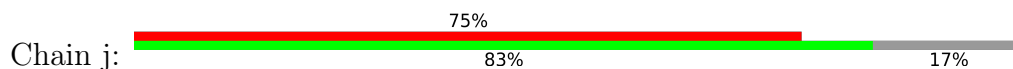
• Molecule 41: Small nuclear ribonucleoprotein Sm D1

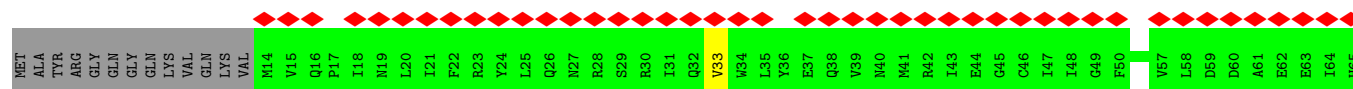


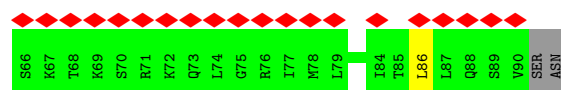
• Molecule 42: Small nuclear ribonucleoprotein Sm D2



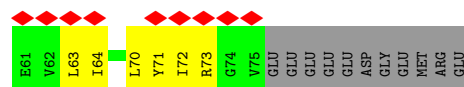
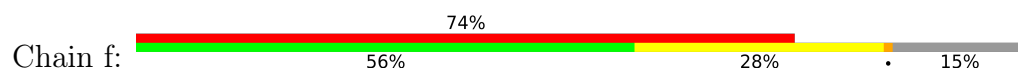
• Molecule 42: Small nuclear ribonucleoprotein Sm D2



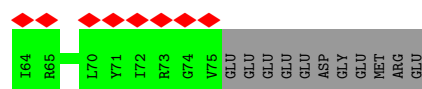
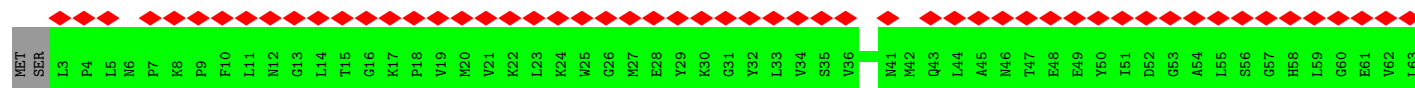
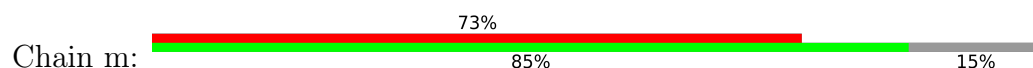




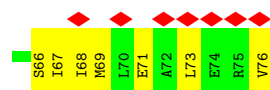
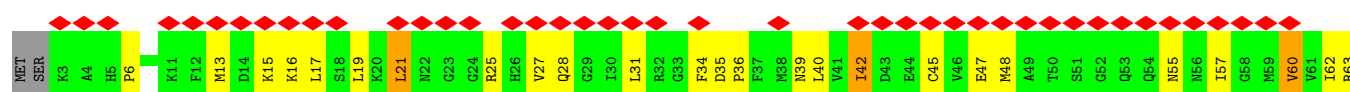
- Molecule 45: Small nuclear ribonucleoprotein F



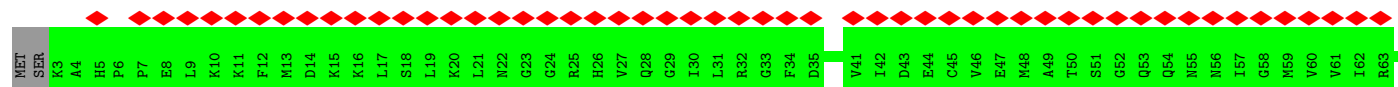
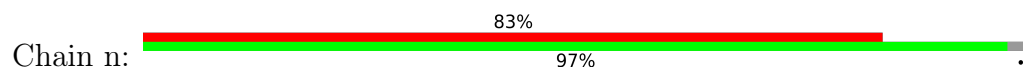
- Molecule 45: Small nuclear ribonucleoprotein F



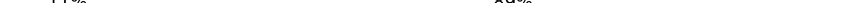
- Molecule 46: Small nuclear ribonucleoprotein G

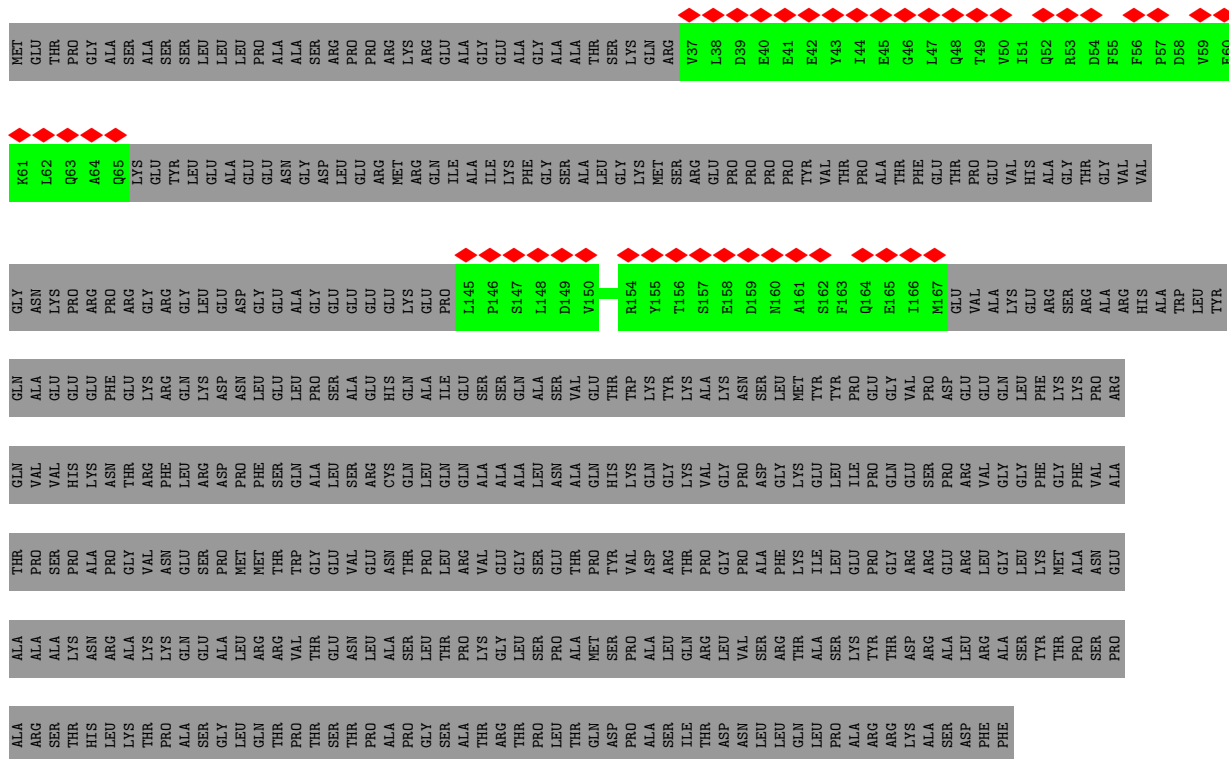


- Molecule 46: Small nuclear ribonucleoprotein G

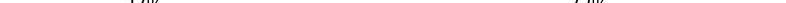


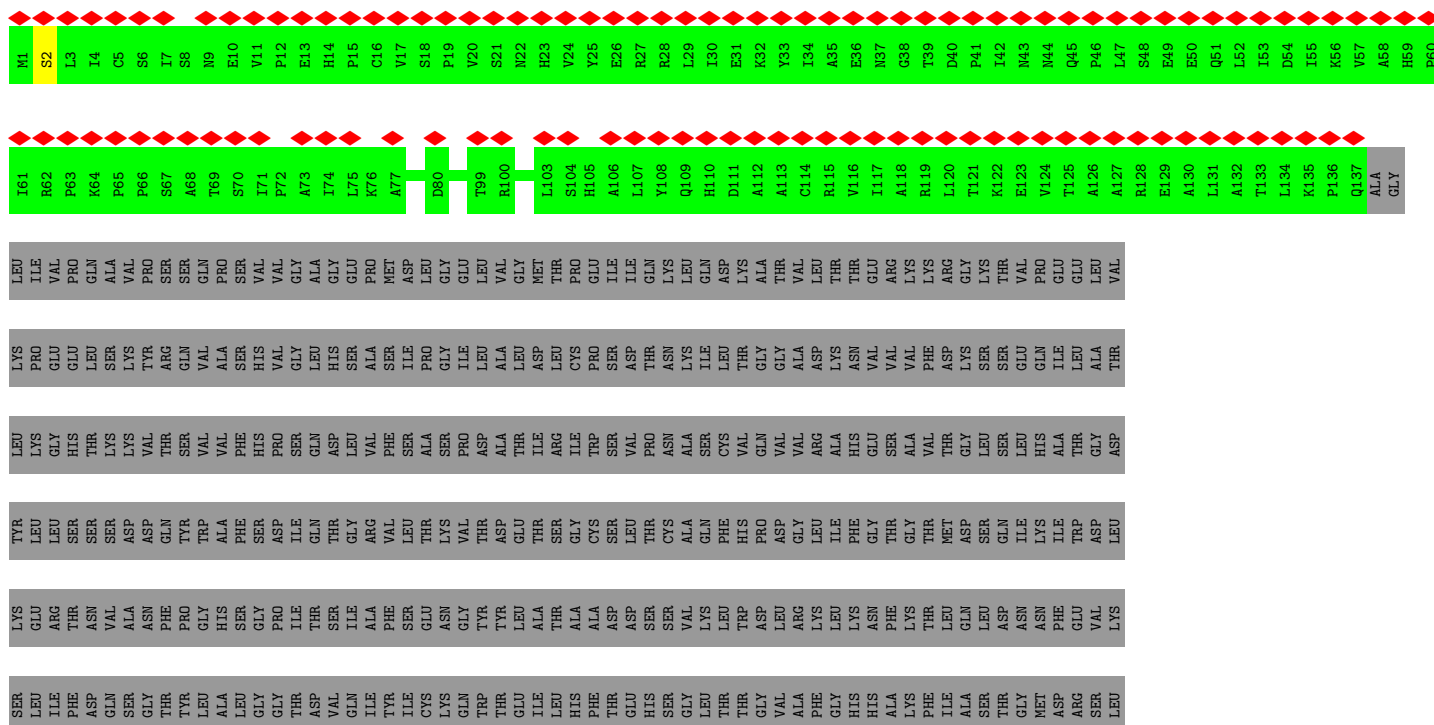
- Molecule 47: Splicing factor ESS-2 homolog

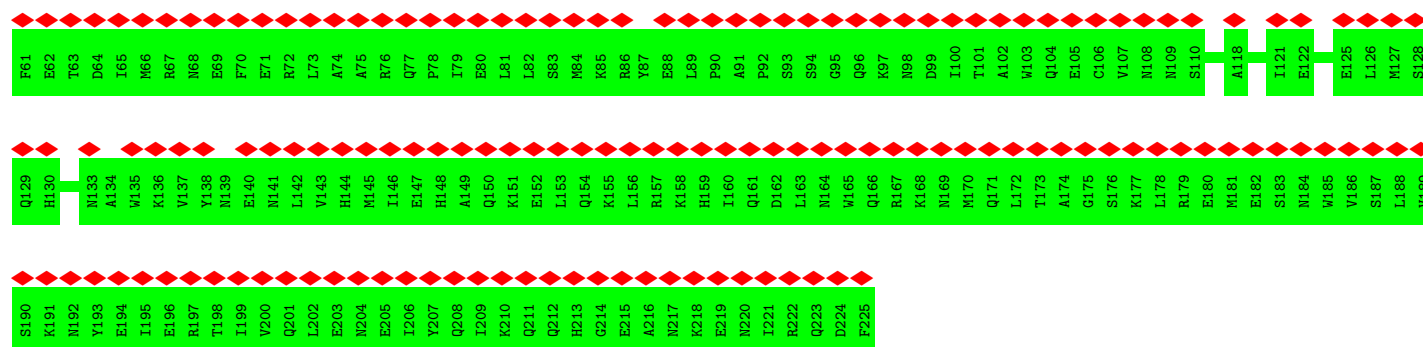
Chain p:  9% 11% 89%



- Molecule 48: Pre-mRNA-processing factor 19

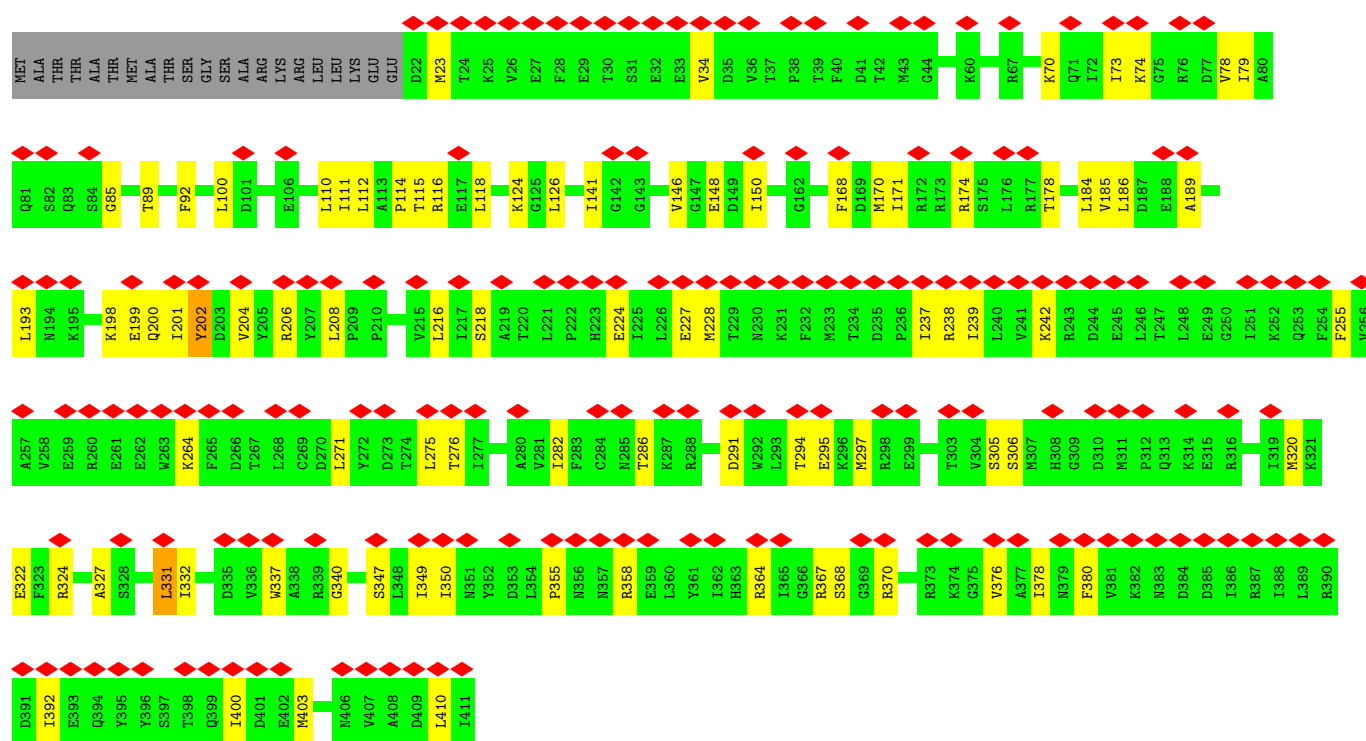
Chain q: 





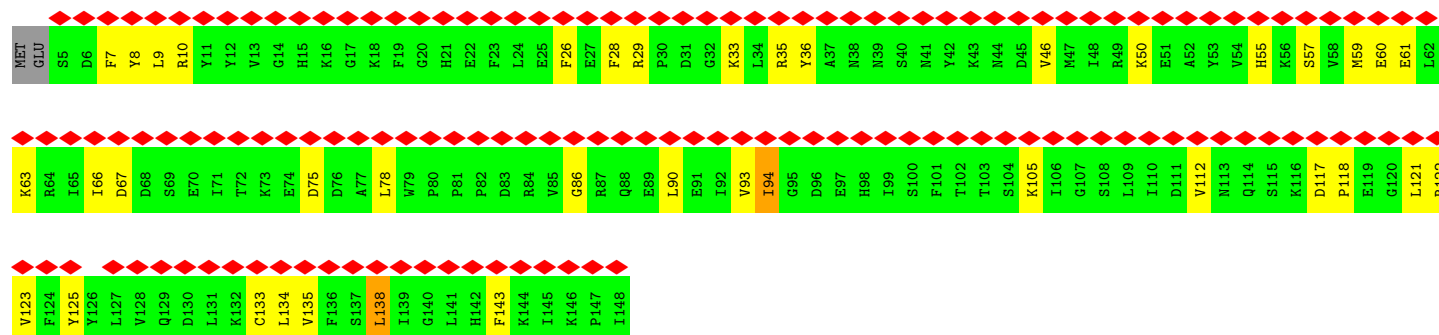
• Molecule 50: Eukaryotic initiation factor 4A-III

Chain v:

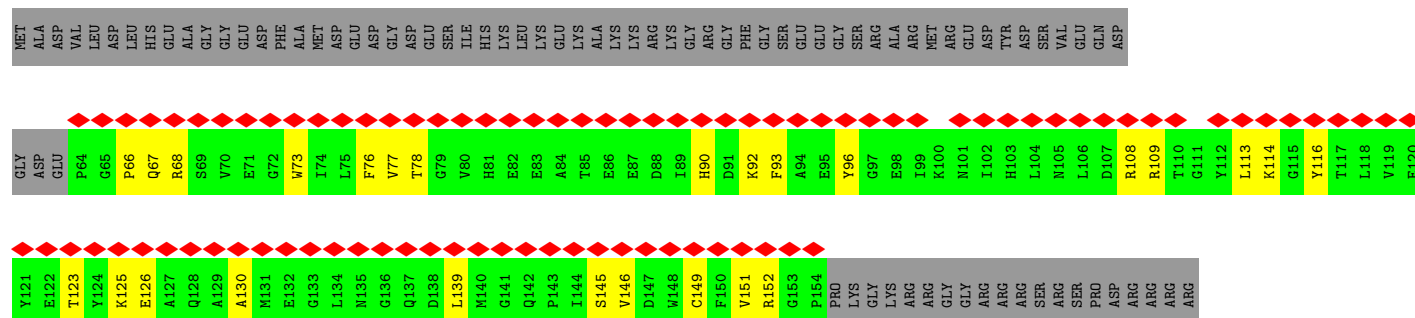


• Molecule 51: Protein mago nashi homolog

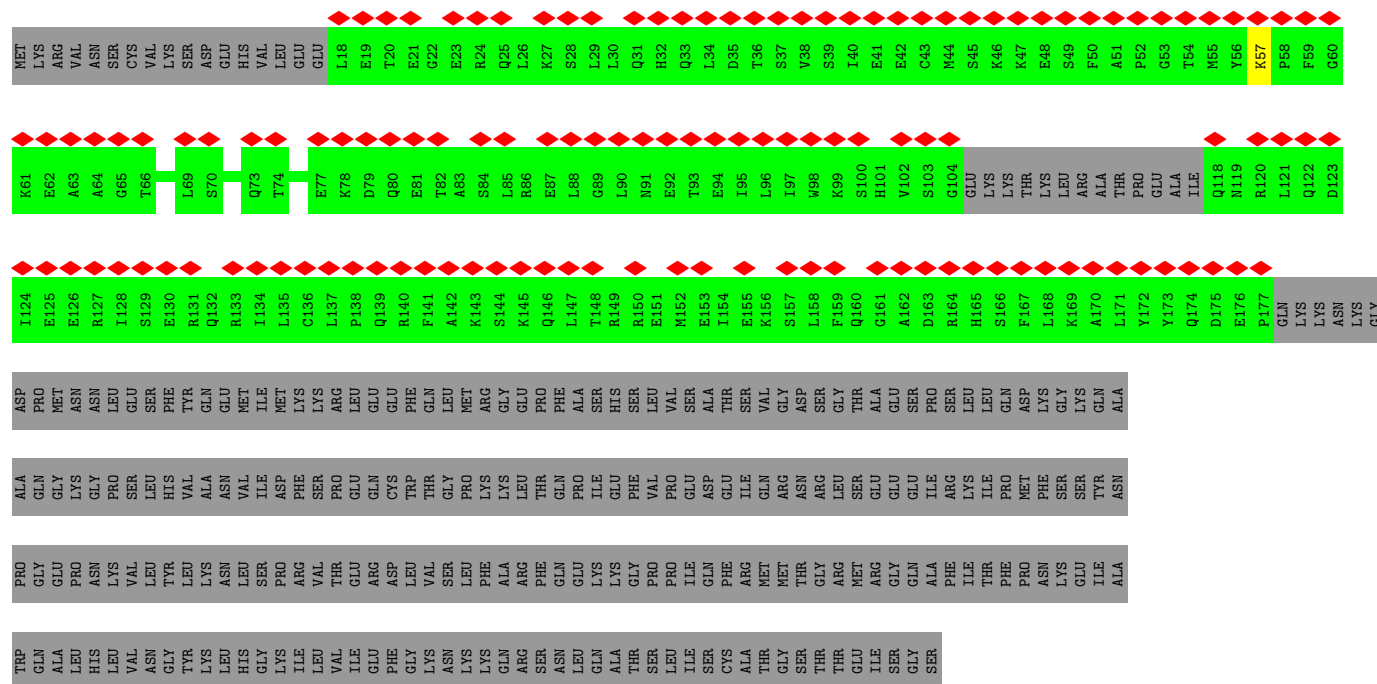
Chain w:



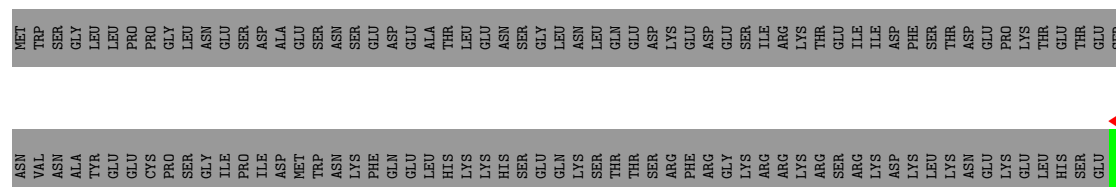
Chain x:



Chain v:



Chain z:





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	145908	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.879	Depositor
Minimum map value	-1.241	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.059	Depositor
Recommended contour level	0.36	Depositor
Map size (Å)	689.472, 689.472, 689.472	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0773, 1.0773, 1.0773	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: G5J, GTP, ZN, ATP, IHP, SEP, ADP, K, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	0.27	0/595	0.58	2/925 (0.2%)
2	1	0.29	0/1285	0.50	2/1991 (0.1%)
3	2	0.24	0/1005	0.29	0/1561
4	4	0.16	0/3354	0.39	0/4515
5	5	0.31	0/2559	0.45	4/3977 (0.1%)
6	6	0.27	0/2687	0.38	1/4178 (0.0%)
7	A	0.31	0/19453	0.42	1/26385 (0.0%)
8	B	0.32	0/7283	0.49	0/9895
9	C	0.16	0/15420	0.41	0/20908
10	D	0.14	0/2461	0.35	0/3334
11	E	0.21	0/3959	0.39	0/5392
12	F	0.17	0/4968	0.45	0/6796
13	G	0.19	0/4487	0.42	0/6122
14	H	0.18	0/323	0.59	0/433
15	I	0.14	0/237	0.53	0/329
16	J	0.28	0/1817	0.55	0/2446
17	K	0.35	0/3089	0.47	0/4223
18	L	0.24	0/1160	0.39	1/1559 (0.1%)
19	L2	0.15	0/471	0.51	0/656
20	L3	0.15	0/420	0.40	0/584
21	L4	0.14	0/395	0.38	0/549
22	L5	0.12	0/401	0.40	0/555
23	L6	0.12	0/367	0.37	0/508
24	L7	0.13	0/436	0.38	0/604
25	L8	0.13	0/471	0.37	0/653
26	M	0.21	0/1314	0.56	0/1793
27	N	0.25	0/857	0.41	0/1138
28	O	0.15	0/775	0.37	0/1070
29	P	0.13	0/389	0.41	0/540
30	Q	0.14	0/6575	0.38	0/9165
31	R	0.12	0/790	0.35	0/1094
32	S	0.26	0/2303	0.48	0/3097

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	T	0.23	0/6355	0.54	0/8596
34	U	0.29	0/883	0.53	0/1198
35	V	0.22	0/3835	0.46	0/5164
36	W	0.26	0/2841	0.47	0/3851
37	X	0.20	0/1293	0.46	0/1749
38	Y	0.22	0/503	0.38	0/672
39	Z	0.21	0/236	0.39	0/312
40	a	0.16	0/599	0.49	0/798
40	h	0.14	0/358	0.44	0/495
41	b	0.24	0/657	0.54	0/888
41	i	0.19	0/400	0.48	0/556
42	c	0.19	0/805	0.48	0/1081
42	j	0.15	0/485	0.49	0/674
43	d	0.22	0/671	0.55	0/904
43	k	0.13	0/398	0.35	0/552
44	e	0.29	0/646	0.77	0/867
44	l	0.15	0/380	0.47	0/528
45	f	0.28	0/579	0.71	0/783
45	m	0.14	0/355	0.41	0/490
46	g	0.35	0/584	0.73	0/779
46	n	0.16	0/363	0.42	0/501
47	p	0.12	0/264	0.37	0/365
48	q	0.14	0/683	0.32	0/954
48	r	0.18	0/673	0.33	0/940
48	s	0.15	0/688	0.39	0/961
48	t	0.15	0/678	0.35	0/947
49	u	0.15	0/1116	0.33	0/1554
50	v	0.23	0/3179	0.48	0/4291
51	w	0.26	0/1225	0.61	1/1648 (0.1%)
52	x	0.28	0/748	0.55	0/1012
53	y	0.11	0/752	0.36	0/1044
54	z	0.21	0/950	0.48	0/1267
All	All	0.24	0/126288	0.45	12/173396 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	14	G	P-O3'-C3'	-7.64	108.74	120.20
5	5	95	G	P-O3'-C3'	-6.89	109.87	120.20
5	5	96	A	P-O3'-C3'	-6.64	110.23	120.20
1	0	-8	C	P-O3'-C3'	-6.34	110.69	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	w	94	ILE	N-CA-C	-6.24	106.24	112.17
6	6	32	C	P-O3'-C3'	-6.02	111.17	120.20
1	0	-7	C	P-O3'-C3'	-5.83	111.46	120.20
5	5	94	U	P-O3'-C3'	-5.66	111.71	120.20
7	A	903	SER	N-CA-C	-5.56	107.04	113.88
18	L	56	VAL	N-CA-C	-5.46	107.96	113.20
5	5	38	C	P-O3'-C3'	-5.11	112.53	120.20
2	1	13	A	P-O3'-C3'	-5.09	112.56	120.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	533	0	272	6	0
2	1	1155	0	586	13	0
3	2	898	0	451	9	0
4	4	3283	0	3269	33	0
5	5	2296	0	1163	25	0
6	6	2439	0	1216	21	0
7	A	18932	0	18817	138	0
8	B	7122	0	7132	84	0
9	C	15118	0	14962	195	0
10	D	2406	0	2342	27	0
11	E	3925	0	3079	18	0
12	F	4897	0	3855	56	0
13	G	4412	0	3489	24	0
14	H	320	0	312	2	0
15	I	238	0	111	0	0
16	J	1815	0	1723	21	0
17	K	3014	0	2792	20	0
18	L	1139	0	1136	18	0
19	L2	472	0	204	0	0
20	L3	421	0	175	0	0
21	L4	396	0	165	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	L5	402	0	167	0	0
23	L6	368	0	163	0	0
24	L7	437	0	186	1	0
25	L8	472	0	219	0	0
26	M	1292	0	1233	32	0
27	N	845	0	829	5	0
28	O	776	0	358	1	0
29	P	390	0	190	2	0
30	Q	6579	0	2831	1	0
31	R	791	0	347	0	0
32	S	2249	0	2193	27	0
33	T	6236	0	6292	125	0
34	U	874	0	702	31	0
35	V	3768	0	3833	34	0
36	W	2764	0	2717	29	0
37	X	1243	0	1165	14	0
38	Y	494	0	496	6	0
39	Z	234	0	232	2	0
40	a	591	0	613	7	0
40	h	360	0	149	0	0
41	b	649	0	693	8	0
41	i	401	0	165	0	0
42	c	796	0	821	25	0
42	j	487	0	199	0	0
43	d	663	0	680	11	0
43	k	399	0	176	0	0
44	e	638	0	657	19	0
44	l	381	0	159	1	0
45	f	567	0	575	25	0
45	m	356	0	156	0	0
46	g	577	0	603	23	0
46	n	364	0	160	0	0
47	p	265	0	114	0	0
48	q	684	0	308	1	0
48	r	674	0	305	0	0
48	s	689	0	313	0	0
48	t	679	0	306	1	0
49	u	1117	0	514	0	0
50	v	3130	0	3173	67	0
51	w	1196	0	1182	26	0
52	x	730	0	690	18	0
53	y	751	0	350	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	z	933	0	947	15	0
55	1	2	0	0	0	0
55	6	4	0	0	0	0
55	B	1	0	0	0	0
55	C	1	0	0	0	0
55	v	1	0	0	0	0
56	6	2	0	0	0	0
57	A	36	0	6	0	0
58	B	32	0	12	1	0
59	C	54	0	24	0	0
60	S	1	0	0	0	0
61	v	31	0	12	0	0
62	6	1	0	0	0	0
All	All	123688	0	105466	1152	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 5.

All (1152) 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)
32:S:65:GLN:O	32:S:69:SER:HB2	1.61	0.99
33:T:1151:TYR:HB3	33:T:1162:MET:HG2	1.44	0.97
9:C:1001:TYR:O	9:C:1005:LEU:HB2	1.70	0.91
46:g:45:CYS:HB3	46:g:57:ILE:HG13	1.59	0.84
7:A:362:ARG:HG3	7:A:364:SER:H	1.45	0.81
33:T:786:ILE:HG12	33:T:837:ILE:HG12	1.65	0.79
33:T:989:LEU:HD21	33:T:1152:HIS:HE1	1.46	0.79
33:T:980:MET:HE2	33:T:994:ILE:HD12	1.65	0.78
9:C:486:SER:HA	9:C:489:TYR:CE1	2.20	0.77
33:T:1151:TYR:HB3	33:T:1162:MET:CG	2.14	0.77
34:U:139:PHE:HB3	50:v:198:LYS:HD3	1.67	0.76
46:g:35:ASP:HB2	46:g:36:PRO:HD2	1.66	0.76
36:W:527:LEU:HD22	36:W:530:VAL:HG23	1.68	0.76
5:5:110:C:H2'	5:5:111:A:H8	1.50	0.75
9:C:1558:PRO:HG2	9:C:1693:ARG:HH12	1.50	0.75
45:f:49:GLU:HB2	45:f:59:LEU:HD11	1.69	0.74
54:z:149:VAL:HG12	54:z:150:GLU:HG3	1.69	0.74
5:5:110:C:H2'	5:5:111:A:C8	2.23	0.74
5:5:95:G:H5''	45:f:25:TRP:HH2	1.52	0.74
44:e:48:ILE:HG13	44:e:57:VAL:HG13	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:1606:ASP:HB3	9:C:1609:LEU:HB2	1.69	0.73
33:T:495:GLU:O	33:T:498:MET:HG2	1.89	0.73
12:F:736:THR:OG1	12:F:739:ASN:HB2	1.88	0.72
50:v:294:THR:HG21	50:v:306:SER:HB3	1.70	0.72
33:T:879:ILE:HG13	33:T:912:MET:HE1	1.73	0.70
33:T:495:GLU:HA	33:T:498:MET:HE3	1.73	0.69
34:U:139:PHE:HB2	50:v:202:TYR:CZ	2.27	0.69
12:F:460:THR:HG21	12:F:490:LEU:HD22	1.75	0.69
9:C:1662:ILE:HA	9:C:1703:VAL:O	1.93	0.69
54:z:141:ASP:HB2	54:z:146:ARG:HH22	1.58	0.69
8:B:731:SER:HB2	8:B:747:ASP:HB3	1.74	0.68
9:C:738:ILE:HD12	9:C:741:MET:HE3	1.75	0.68
7:A:2087:THR:HB	7:A:2112:LYS:HG2	1.74	0.68
7:A:1032:ARG:HH12	27:N:229:LYS:HG2	1.59	0.68
13:G:431:ARG:HE	16:J:7:LEU:HD12	1.57	0.68
16:J:175:GLN:HG2	16:J:199:MET:HE1	1.76	0.67
6:6:22:G:H2'	6:6:23:G:C8	2.29	0.67
11:E:136:PRO:HD3	54:z:145:LYS:HE2	1.75	0.67
33:T:1149:VAL:HG23	33:T:1165:VAL:HG13	1.77	0.67
33:T:1189:LEU:HD13	33:T:1190:SER:H	1.59	0.67
33:T:449:LEU:HB3	33:T:453:THR:HG23	1.76	0.67
46:g:21:LEU:O	46:g:68:ILE:HD12	1.94	0.67
18:L:132:ARG:HG2	26:M:162:ILE:HD12	1.76	0.67
35:V:194:ARG:HD3	35:V:382:LEU:HD13	1.77	0.66
7:A:2062:TYR:O	7:A:2066:THR:HG23	1.94	0.66
50:v:331:LEU:HG	50:v:337:TRP:HZ3	1.61	0.66
44:e:32:GLN:HB2	44:e:88:GLN:HB3	1.75	0.66
9:C:933:PRO:HG3	9:C:943:LEU:HD22	1.77	0.66
35:V:297:LEU:HD11	35:V:312:ILE:HD11	1.78	0.66
26:M:116:LEU:HD22	26:M:159:LEU:HD12	1.77	0.66
33:T:1162:MET:SD	33:T:1165:VAL:HG22	2.36	0.65
9:C:1843:ARG:HH22	9:C:1879:LEU:HG	1.62	0.65
45:f:21:VAL:HG22	45:f:72:ILE:HG23	1.79	0.65
33:T:818:SER:HA	33:T:821:GLN:HB2	1.79	0.65
34:U:132:ASN:HD21	34:U:136:ARG:HH21	1.44	0.65
43:d:22:THR:HG21	46:g:69:MET:HE1	1.79	0.65
8:B:564:THR:HG21	8:B:577:PHE:H	1.62	0.65
9:C:1561:VAL:HG22	9:C:1662:ILE:HB	1.78	0.65
11:E:227:THR:HG22	13:G:293:ASN:HB3	1.78	0.65
2:1:205:G:H3'	2:1:206:C:H4'	1.78	0.65
4:4:159:VAL:HB	4:4:169:ASN:HB3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:688:THR:HB	9:C:868:ILE:HG13	1.79	0.64
12:F:474:GLU:HB3	12:F:478:ASN:HD22	1.62	0.64
9:C:1459:ILE:HD12	9:C:1468:GLU:HG3	1.80	0.64
36:W:357:GLU:HG2	36:W:373:LYS:HG3	1.78	0.64
33:T:918:PRO:HB2	33:T:920:ILE:HG12	1.80	0.64
18:L:65:ARG:HH21	18:L:107:MET:HE1	1.62	0.64
12:F:437:CYS:HA	12:F:489:MET:HE2	1.79	0.64
32:S:112:ILE:HG22	32:S:113:THR:HG23	1.79	0.63
39:Z:344:ILE:HG23	39:Z:354:MET:HE3	1.81	0.63
34:U:138:ALA:HB1	50:v:228:MET:HE1	1.80	0.63
12:F:697:PRO:HG2	12:F:731:GLN:HG3	1.79	0.63
50:v:305:SER:HB3	50:v:331:LEU:HD22	1.80	0.63
44:e:28:ARG:HH12	44:e:48:ILE:HG23	1.64	0.63
52:x:76:PHE:HB2	52:x:149:CYS:HB2	1.81	0.63
7:A:371:LEU:HD11	8:B:358:LYS:HD3	1.80	0.63
50:v:201:ILE:O	50:v:204:VAL:HG22	2.00	0.62
7:A:2316:ASN:HA	7:A:2319:LEU:HD12	1.82	0.62
8:B:501:ILE:HG22	8:B:530:LEU:HD11	1.81	0.62
26:M:100:VAL:HB	26:M:101:PRO:HD3	1.80	0.62
9:C:1450:LEU:HD22	9:C:1486:ARG:HB3	1.80	0.62
44:e:54:MET:HE2	46:g:63:ARG:HH11	1.65	0.62
3:2:16:G:H21	37:X:755:ARG:HH22	1.48	0.62
51:w:60:GLU:HA	51:w:63:LYS:HG2	1.80	0.62
7:A:535:ARG:HD2	38:Y:106:PRO:HB2	1.81	0.62
45:f:28:GLU:HG2	45:f:50:TYR:HB2	1.80	0.62
26:M:11:VAL:HG12	26:M:13:ARG:H	1.64	0.62
7:A:664:HIS:HA	16:J:215:ASN:HB3	1.82	0.61
9:C:1604:LEU:HD11	9:C:1609:LEU:HD13	1.82	0.61
9:C:509:LYS:HB3	9:C:651:LEU:HD13	1.82	0.61
9:C:619:LEU:HD21	9:C:624:ARG:HB2	1.82	0.61
17:K:356:LEU:HD13	17:K:366:VAL:HB	1.82	0.61
9:C:1361:GLU:HA	9:C:1364:ILE:HD12	1.83	0.61
9:C:1561:VAL:HA	9:C:1662:ILE:O	2.00	0.61
16:J:174:ALA:HB3	16:J:200:VAL:HG12	1.82	0.61
41:b:2:LYS:HD2	41:b:5:ARG:HE	1.66	0.61
46:g:42:ILE:HG22	46:g:60:VAL:HG22	1.82	0.61
7:A:701:ILE:HG22	7:A:703:GLN:H	1.65	0.61
38:Y:55:LEU:HD13	38:Y:58:ARG:HH22	1.65	0.61
4:4:286:VAL:HG22	4:4:297:THR:HG22	1.82	0.61
2:1:13:A:H3'	2:1:14:G:H8	1.64	0.61
9:C:1561:VAL:HB	9:C:1645:VAL:HG12	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:w:75:ASP:HB3	51:w:78:LEU:HD12	1.83	0.61
7:A:768:ASP:HB3	7:A:771:VAL:HG12	1.83	0.61
8:B:798:GLN:HB3	8:B:800:PRO:HD2	1.83	0.61
33:T:1149:VAL:CG2	33:T:1165:VAL:HG13	2.31	0.61
46:g:62:ILE:HD12	46:g:67:ILE:HD11	1.83	0.60
9:C:538:ILE:HD12	9:C:611:LEU:HB3	1.83	0.60
7:A:1781:ASP:HB3	7:A:1808:PHE:HB3	1.82	0.60
40:a:17:MET:HG3	40:a:31:PHE:HB2	1.83	0.60
33:T:463:LYS:HE2	33:T:466:LYS:HG2	1.83	0.60
9:C:488:LEU:HD21	9:C:501:LEU:HD13	1.84	0.60
1:0:-6:U:H2'	1:0:-6:U:O2	2.00	0.60
4:4:445:LYS:HG3	4:4:447:ARG:H	1.65	0.60
9:C:1604:LEU:HD21	9:C:1609:LEU:HB3	1.83	0.60
9:C:2041:LEU:HB2	9:C:2088:ALA:HB3	1.84	0.60
50:v:79:ILE:HD11	50:v:238:ARG:HG2	1.83	0.60
10:D:166:LEU:HB3	10:D:178:LEU:HD11	1.82	0.60
33:T:933:LYS:HB3	33:T:973:LEU:HD22	1.84	0.60
4:4:84:GLU:HA	4:4:456:PRO:HB3	1.83	0.60
34:U:135:LEU:HD23	50:v:206:ARG:NH1	2.17	0.60
11:E:378:PRO:HA	16:J:299:ARG:HG3	1.83	0.59
43:d:22:THR:HA	43:d:68:ILE:HA	1.82	0.59
32:S:64:PRO:HG2	32:S:67:ILE:HD12	1.84	0.59
26:M:27:THR:HG21	26:M:33:LYS:HD3	1.83	0.59
12:F:736:THR:HG23	54:z:182:LEU:HD22	1.83	0.59
34:U:135:LEU:HD23	50:v:206:ARG:HH12	1.67	0.59
43:d:16:HIS:HB2	43:d:74:PRO:HG2	1.84	0.59
1:0:-1:G:H1	5:5:40:U:H3	1.50	0.59
33:T:1032:LYS:O	33:T:1036:HIS:HB2	2.03	0.59
51:w:59:MET:O	51:w:63:LYS:HG2	2.02	0.59
44:e:34:TRP:HA	44:e:42:ARG:HG2	1.84	0.59
8:B:673:LYS:HE3	8:B:792:LEU:HD12	1.85	0.59
7:A:40:LEU:HD12	18:L:79:ASP:HB2	1.84	0.59
9:C:1375:ARG:HH12	9:C:1423:ASN:HA	1.68	0.59
7:A:156:ARG:HD2	32:S:153:GLU:HG2	1.84	0.59
9:C:2067:VAL:HB	9:C:2107:TYR:HB2	1.85	0.59
12:F:747:LYS:HD2	12:F:775:ARG:HB2	1.85	0.59
36:W:499:MET:HB2	36:W:509:CYS:HB3	1.84	0.59
42:c:53:LEU:HD12	42:c:71:LYS:HZ1	1.67	0.59
9:C:1913:GLU:HG2	9:C:2057:PRO:HG3	1.84	0.58
44:e:76:ARG:HH22	45:f:5:LEU:HD23	1.68	0.58
8:B:500:THR:HG22	8:B:545:PRO:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:a:17:MET:O	40:a:28:ILE:HA	2.03	0.58
8:B:319:THR:H	8:B:322:SER:HB3	1.69	0.58
9:C:849:ILE:HD12	9:C:852:MET:HB2	1.85	0.58
33:T:764:VAL:HG22	33:T:776:ILE:HG21	1.84	0.58
50:v:23:MET:HB2	50:v:227:GLU:HB2	1.86	0.58
5:5:96:A:C2	45:f:25:TRP:HB3	2.38	0.58
7:A:35:ARG:HH22	7:A:36:LYS:HG2	1.67	0.58
33:T:642:VAL:HG12	33:T:658:ILE:HB	1.84	0.58
6:6:80:G:H2'	6:6:81:G:H8	1.68	0.58
7:A:1590:VAL:HG22	7:A:1664:ILE:HD13	1.84	0.58
16:J:205:ASP:HB3	16:J:208:GLU:HB2	1.84	0.58
32:S:107:LYS:HG2	32:S:108:GLU:H	1.68	0.58
46:g:16:LYS:HG3	46:g:73:LEU:HD13	1.84	0.58
33:T:851:ILE:HG21	33:T:893:ARG:HH22	1.68	0.58
12:F:467:ALA:HB2	12:F:474:GLU:HB2	1.86	0.58
3:2:15:U:H2'	3:2:16:G:H8	1.67	0.58
12:F:623:VAL:HG21	12:F:631:MET:HG3	1.86	0.58
35:V:206:SER:HA	35:V:255:THR:HG21	1.86	0.58
7:A:2102:TYR:HB3	7:A:2140:LYS:HG3	1.86	0.58
8:B:475:MET:HE3	8:B:566:THR:HB	1.85	0.58
9:C:1348:VAL:HA	9:C:1512:PHE:HB2	1.86	0.58
9:C:1416:LEU:HD22	9:C:1444:ASN:HD21	1.68	0.58
12:F:741:MET:HE2	12:F:745:MET:HE2	1.86	0.58
13:G:473:VAL:HA	13:G:500:LEU:HD11	1.85	0.58
50:v:201:ILE:HA	50:v:204:VAL:HG22	1.85	0.58
12:F:542:GLU:HG3	13:G:460:LYS:HB3	1.86	0.57
13:G:501:VAL:HG13	13:G:505:ALA:HB3	1.85	0.57
33:T:652:THR:HG21	33:T:659:LYS:HE3	1.86	0.57
50:v:174:ARG:HH12	50:v:178:THR:H	1.52	0.57
17:K:346:ILE:HD13	17:K:380:LEU:HD11	1.86	0.57
50:v:378:ILE:HG23	50:v:403:MET:HE1	1.85	0.57
5:5:93:U:H1'	42:c:104:ASP:HB3	1.84	0.57
12:F:623:VAL:HG11	12:F:631:MET:HE3	1.87	0.57
10:D:274:VAL:HG12	10:D:275:LYS:HG3	1.87	0.57
33:T:1114:ASN:HB3	33:T:1151:TYR:CZ	2.39	0.57
9:C:1336:PHE:HA	9:C:1339:VAL:HG12	1.85	0.57
33:T:683:MET:HB3	33:T:714:ILE:HB	1.87	0.57
41:b:25:VAL:HG22	41:b:45:MET:HB3	1.87	0.57
7:A:1591:MET:HE1	32:S:268:ARG:HD2	1.86	0.57
50:v:78:VAL:HG22	50:v:237:ILE:HB	1.86	0.57
51:w:50:LYS:HZ1	51:w:143:PHE:HD1	1.51	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:K:396:LYS:HB3	17:K:405:PHE:HE1	1.69	0.57
33:T:993:LEU:HD13	33:T:1005:MET:HE1	1.85	0.57
42:c:43:LEU:HD23	42:c:110:LEU:HD12	1.86	0.57
8:B:476:CYS:SG	8:B:496:VAL:HG22	2.45	0.57
18:L:70:GLY:HA3	18:L:99:SER:HB3	1.86	0.57
7:A:526:PRO:HG3	38:Y:106:PRO:HD3	1.86	0.57
33:T:1104:GLN:HE22	33:T:1172:TRP:CD1	2.23	0.57
45:f:30:LYS:O	45:f:47:THR:HA	2.05	0.57
9:C:1281:GLN:HG3	9:C:1283:PRO:HD3	1.86	0.57
7:A:1931:THR:HG23	32:S:347:PRO:HB2	1.87	0.56
10:D:114:GLU:HB3	10:D:127:ALA:HB3	1.87	0.56
9:C:785:HIS:HB2	9:C:809:LEU:HD11	1.85	0.56
9:C:1546:VAL:HG23	9:C:1662:ILE:HG21	1.88	0.56
26:M:104:ILE:HD11	26:M:141:VAL:HG11	1.88	0.56
7:A:2063:GLU:HA	7:A:2066:THR:OG1	2.05	0.56
9:C:1679:TYR:CE2	9:C:1687:MET:HE1	2.40	0.56
50:v:271:LEU:O	50:v:275:LEU:HB2	2.05	0.56
7:A:2028:GLU:HA	7:A:2031:LYS:HD3	1.88	0.56
17:K:195:LYS:HZ1	17:K:490:ARG:HH21	1.52	0.56
35:V:628:ILE:HD11	35:V:643:LEU:HG	1.88	0.56
1:O:-17:A:H1'	50:v:146:VAL:HB	1.88	0.56
5:5:8:G:H22	5:5:72:U:H2'	1.68	0.56
8:B:474:LEU:HD21	8:B:501:ILE:HD13	1.88	0.56
9:C:1381:PRO:HG2	9:C:1458:LEU:HD12	1.88	0.56
50:v:110:LEU:HB3	50:v:184:LEU:HD12	1.88	0.56
52:x:123:THR:HG22	52:x:126:GLU:HG2	1.87	0.56
9:C:1799:SER:HA	9:C:1830:GLU:HG3	1.88	0.56
9:C:1923:ILE:HD12	9:C:1946:ALA:HA	1.87	0.56
7:A:2212:ILE:HG22	7:A:2229:LYS:HB3	1.86	0.56
9:C:603:ARG:HB3	9:C:1540:LEU:HD12	1.88	0.56
45:f:8:LYS:HD3	45:f:40:MET:HE1	1.87	0.56
9:C:620:LEU:HA	9:C:625:GLY:HA3	1.87	0.56
51:w:123:VAL:HG22	52:x:109:ARG:HH12	1.71	0.56
8:B:181:ILE:HG22	8:B:182:LYS:HG2	1.87	0.55
9:C:2107:TYR:HB3	9:C:2109:MET:HE2	1.86	0.55
33:T:954:LEU:O	33:T:958:MET:HG2	2.06	0.55
34:U:136:ARG:HD3	50:v:206:ARG:NH2	2.21	0.55
9:C:725:VAL:HB	9:C:731:THR:HG22	1.89	0.55
12:F:494:GLU:HA	12:F:498:GLY:H	1.71	0.55
33:T:1104:GLN:HE22	33:T:1172:TRP:NE1	2.04	0.55
37:X:627:LEU:HD21	37:X:630:LYS:HD2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:c:43:LEU:O	42:c:110:LEU:HB2	2.05	0.55
8:B:692:LEU:HD23	8:B:693:GLU:H	1.70	0.55
9:C:848:ASP:O	9:C:852:MET:HG2	2.07	0.55
9:C:1565:SER:HB3	9:C:1568:GLN:HB2	1.89	0.55
34:U:135:LEU:O	34:U:136:ARG:C	2.48	0.55
5:5:95:G:H4'	5:5:96:A:O5'	2.07	0.55
45:f:11:LEU:HA	45:f:14:LEU:HG	1.89	0.55
48:q:2:SER:HA	48:t:3:LEU:H	1.71	0.55
6:6:94:C:H2'	6:6:95:A:H8	1.72	0.55
5:5:74:U:H2'	5:5:75:G:C8	2.42	0.55
9:C:2108:PHE:HB3	9:C:2118:GLN:HB2	1.89	0.55
50:v:322:GLU:HG3	50:v:327:ALA:HB3	1.88	0.55
52:x:92:LYS:HE2	52:x:139:LEU:HD11	1.89	0.55
2:1:13:A:C4	2:1:14:G:C8	2.94	0.55
8:B:876:PRO:HG2	8:B:879:ASP:HB2	1.87	0.55
9:C:732:GLY:HA2	9:C:784:ILE:HD13	1.89	0.55
9:C:2017:ILE:HB	9:C:2043:ARG:HG3	1.89	0.55
36:W:409:ALA:HB3	36:W:419:SER:HB3	1.89	0.55
46:g:34:PHE:HB3	46:g:40:LEU:HD22	1.89	0.55
52:x:76:PHE:HE2	52:x:116:TYR:HB2	1.72	0.55
4:4:78:PRO:HG2	4:4:438:ILE:HG12	1.89	0.55
7:A:147:MET:O	7:A:151:MET:HG3	2.07	0.55
33:T:641:GLU:HA	33:T:656:THR:HA	1.88	0.55
51:w:118:PRO:O	51:w:122:ARG:HG2	2.06	0.55
33:T:1108:CYS:HB2	33:T:1168:ILE:HD13	1.89	0.55
5:5:95:G:H2'	5:5:95:G:N3	2.21	0.54
7:A:168:PRO:HG2	7:A:559:ASP:HB3	1.90	0.54
10:D:311:VAL:HB	10:D:321:TYR:HB2	1.90	0.54
33:T:447:PRO:HG2	33:T:969:ASP:HA	1.89	0.54
36:W:240:PHE:HB2	36:W:542:ILE:HB	1.90	0.54
35:V:278:LEU:HD11	35:V:297:LEU:HD13	1.89	0.54
36:W:450:LEU:HD13	36:W:488:LEU:HD21	1.90	0.54
43:d:19:THR:HB	43:d:72:ILE:HB	1.90	0.54
46:g:21:LEU:HG	46:g:25:ARG:HH21	1.72	0.54
5:5:110:C:O5'	5:5:110:C:H6	1.89	0.54
33:T:1124:TYR:HE1	33:T:1135:ILE:HD11	1.72	0.54
9:C:1051:SER:HB2	9:C:1057:ALA:HB2	1.88	0.54
43:d:18:VAL:HG12	43:d:74:PRO:HD3	1.89	0.54
4:4:250:TRP:HA	4:4:260:PRO:HD3	1.90	0.54
9:C:1375:ARG:HB2	9:C:1448:ILE:HA	1.90	0.54
43:d:40:ASN:HA	43:d:63:ILE:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:183:LYS:HG3	10:D:185:ALA:H	1.73	0.54
13:G:306:LEU:HD12	13:G:312:PHE:HE2	1.71	0.54
33:T:570:LEU:HB3	33:T:573:GLN:HB3	1.90	0.54
43:d:48:VAL:O	43:d:55:VAL:HA	2.08	0.54
12:F:456:LEU:HD11	12:F:493:LEU:HD22	1.90	0.54
2:1:195:U:H2'	2:1:196:U:C6	2.43	0.54
7:A:997:LEU:HD13	7:A:1009:MET:HE3	1.89	0.54
9:C:982:THR:HG22	9:C:984:LEU:H	1.73	0.54
10:D:218:LYS:HG2	10:D:230:THR:HG22	1.89	0.53
13:G:433:ARG:HH12	13:G:463:GLY:HA2	1.73	0.53
9:C:1356:LYS:HB3	9:C:1490:LEU:HG	1.89	0.53
33:T:824:ILE:HD13	33:T:836:VAL:HG21	1.91	0.53
50:v:116:ARG:HB3	50:v:141:ILE:HD12	1.90	0.53
7:A:758:ARG:HH21	7:A:761:ILE:HG21	1.73	0.53
33:T:442:VAL:HG22	33:T:1182:LYS:HG2	1.89	0.53
33:T:677:THR:HA	33:T:708:ARG:HH22	1.74	0.53
33:T:687:ALA:HB3	33:T:717:SER:HA	1.90	0.53
51:w:7:PHE:HA	51:w:93:VAL:O	2.09	0.53
8:B:696:LEU:HD21	8:B:718:PHE:HE1	1.71	0.53
18:L:142:VAL:HG11	26:M:86:PRO:HB2	1.91	0.53
26:M:58:VAL:HG23	26:M:61:LEU:HD13	1.90	0.53
33:T:683:MET:HA	33:T:714:ILE:O	2.09	0.53
7:A:758:ARG:HD2	7:A:779:LEU:HD11	1.91	0.53
9:C:602:GLU:HA	9:C:605:TYR:HD2	1.73	0.53
12:F:82:VAL:HA	12:F:91:ALA:HB1	1.91	0.53
12:F:638:ARG:HA	12:F:641:GLU:HG2	1.90	0.53
33:T:387:GLU:HB3	33:T:390:ARG:HB2	1.91	0.53
50:v:282:ILE:HG23	50:v:350:ILE:HB	1.90	0.53
8:B:129:ILE:HG22	8:B:199:LEU:HB3	1.91	0.53
8:B:224:GLY:HA3	8:B:438:ILE:HD12	1.90	0.53
9:C:562:TYR:HB2	9:C:564:ILE:HG22	1.91	0.53
10:D:90:ILE:HB	10:D:105:LEU:HB2	1.90	0.53
2:1:205:G:C6	2:1:206:C:H1'	2.43	0.53
9:C:1819:ALA:HA	9:C:1824:ILE:HG22	1.91	0.53
9:C:2026:LYS:HE2	9:C:2124:VAL:HA	1.91	0.53
9:C:482:ASN:HB2	9:C:485:GLN:HB3	1.90	0.53
9:C:720:GLN:HB3	9:C:823:ALA:HB1	1.91	0.53
9:C:1545:PRO:HA	9:C:1548:HIS:HB2	1.90	0.53
12:F:451:GLU:HA	12:F:454:ARG:HB3	1.91	0.53
7:A:1536:LEU:HD21	7:A:1576:ILE:HD11	1.91	0.53
9:C:726:HIS:HD2	9:C:833:VAL:HG23	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:T:1113:ARG:HG2	33:T:1180:PHE:CE1	2.44	0.53
50:v:264:LYS:HE2	50:v:380:PHE:HB3	1.91	0.53
4:4:139:ILE:HB	4:4:148:PHE:HE1	1.74	0.52
5:5:58:U:H2'	5:5:59:G:H8	1.74	0.52
7:A:2095:ASP:HB2	7:A:2258:ARG:HD2	1.91	0.52
9:C:827:ILE:HG22	9:C:868:ILE:HB	1.90	0.52
10:D:133:VAL:HG21	10:D:169:THR:HG21	1.91	0.52
33:T:464:ILE:HG23	33:T:465:VAL:HG23	1.91	0.52
36:W:466:ARG:HH21	54:z:214:LEU:HB3	1.74	0.52
2:1:15:C:H2'	2:1:15:C:O2	2.09	0.52
7:A:909:TYR:HB2	7:A:1033:GLY:HA3	1.91	0.52
9:C:1041:LEU:HD12	9:C:1061:VAL:HG21	1.91	0.52
9:C:1951:GLN:HB2	9:C:1953:MET:HE2	1.91	0.52
11:E:209:ASP:HA	11:E:212:ALA:HB3	1.91	0.52
11:E:311:VAL:O	11:E:315:GLN:HG2	2.09	0.52
7:A:35:ARG:NH2	7:A:36:LYS:HG2	2.24	0.52
27:N:51:PRO:HA	27:N:54:VAL:HG22	1.91	0.52
50:v:34:VAL:HG11	50:v:239:ILE:HD11	1.90	0.52
26:M:143:GLN:HE21	26:M:147:ARG:HH22	1.56	0.52
34:U:55:PRO:HA	34:U:58:LEU:HG	1.92	0.52
43:d:5:VAL:O	43:d:9:VAL:HG23	2.09	0.52
9:C:2047:VAL:HG21	9:C:2085:GLN:HA	1.91	0.52
33:T:1041:ASP:HB2	33:T:1164:GLU:OE2	2.10	0.52
34:U:55:PRO:O	34:U:58:LEU:HG	2.10	0.52
35:V:150:ASN:HA	35:V:154:TYR:HB3	1.90	0.52
7:A:1860:GLN:HG2	7:A:1883:VAL:HB	1.92	0.52
12:F:172:PHE:O	12:F:176:SER:CB	2.57	0.52
51:w:78:LEU:HB3	51:w:117:ASP:HB2	1.92	0.52
4:4:102:ASP:HB3	4:4:118:LYS:HB3	1.92	0.52
36:W:359:LYS:HD3	36:W:371:SER:HB3	1.92	0.52
7:A:1995:ASN:HD22	37:X:656:ASN:ND2	2.07	0.52
9:C:846:ALA:HA	9:C:882:LEU:HD21	1.91	0.52
12:F:627:GLN:O	12:F:631:MET:HG2	2.10	0.52
33:T:783:GLN:HA	33:T:786:ILE:HB	1.91	0.52
33:T:992:MET:HE2	33:T:1107:ILE:HA	1.92	0.52
36:W:470:HIS:HB3	36:W:498:LEU:HD13	1.92	0.52
7:A:899:MET:HE2	7:A:1450:GLN:HG3	1.92	0.52
34:U:62:ARG:HE	34:U:62:ARG:HA	1.75	0.52
50:v:150:ILE:HG13	50:v:170:MET:HE1	1.92	0.52
51:w:86:GLY:HA3	51:w:105:LYS:HD2	1.92	0.52
5:5:97:G:H1	5:5:116:U:H3	1.57	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1995:ASN:HD22	37:X:656:ASN:HD22	1.57	0.51
18:L:135:LEU:HD12	26:M:162:ILE:HD13	1.92	0.51
33:T:851:ILE:HG12	33:T:891:ALA:HA	1.91	0.51
45:f:24:LYS:HA	45:f:70:LEU:HD13	1.92	0.51
4:4:247:ILE:HB	4:4:273:LEU:HD12	1.92	0.51
5:5:88:A:H61	45:f:40:MET:HG2	1.74	0.51
7:A:2226:THR:HA	7:A:2261:MET:HE1	1.92	0.51
8:B:135:CYS:HB2	8:B:242:LEU:HD13	1.92	0.51
34:U:55:PRO:HA	34:U:58:LEU:CD2	2.40	0.51
4:4:438:ILE:HB	4:4:451:PHE:HB2	1.92	0.51
6:6:22:G:H2'	6:6:23:G:H8	1.73	0.51
4:4:157:MET:HE2	4:4:193:VAL:HG11	1.93	0.51
7:A:26:SER:HB3	7:A:29:LYS:HD2	1.93	0.51
9:C:902:ASN:HB2	9:C:964:LEU:HD21	1.91	0.51
9:C:1122:MET:HE1	9:C:1130:ARG:HH21	1.74	0.51
37:X:686:ILE:HG12	37:X:715:PRO:HB3	1.91	0.51
26:M:115:VAL:O	26:M:119:ILE:HG12	2.10	0.51
7:A:361:HIS:O	7:A:362:ARG:HB3	2.11	0.51
9:C:1223:ILE:HG22	9:C:1270:VAL:HG22	1.92	0.51
12:F:463:PRO:HD2	12:F:481:TYR:HB3	1.92	0.51
50:v:184:LEU:HD13	50:v:208:LEU:HD21	1.93	0.51
33:T:1148:TRP:HB2	33:T:1168:ILE:O	2.11	0.51
36:W:307:ILE:HD13	36:W:321:LEU:HD21	1.93	0.51
37:X:707:ILE:HD11	37:X:722:LYS:HD2	1.92	0.51
7:A:2163:LEU:HD13	7:A:2164:PRO:HD2	1.92	0.51
13:G:214:ILE:HG21	13:G:220:LEU:HD13	1.91	0.51
35:V:354:LEU:H	35:V:354:LEU:HD23	1.75	0.51
7:A:1639:VAL:HG13	7:A:1717:ASN:HB3	1.91	0.51
33:T:996:SER:HA	33:T:999:LEU:HB2	1.91	0.51
54:z:168:GLU:O	54:z:172:GLU:HG2	2.11	0.51
7:A:2328:ALA:HB2	9:C:1078:MET:HE1	1.93	0.51
9:C:115:VAL:HG12	9:C:175:LEU:HD21	1.93	0.51
35:V:194:ARG:HD2	35:V:195:GLY:H	1.76	0.51
2:1:188:G:H5'	36:W:503:ARG:HD3	1.93	0.50
33:T:648:PHE:HB3	33:T:1081:GLN:HE22	1.76	0.50
33:T:861:LYS:HD3	33:T:874:LEU:HD21	1.93	0.50
33:T:1039:GLU:HB2	33:T:1043:LEU:HD12	1.92	0.50
9:C:1190:LEU:HD23	9:C:1200:VAL:HG22	1.93	0.50
40:a:9:MET:HE1	40:a:38:MET:HG3	1.94	0.50
3:2:15:U:H2'	3:2:16:G:C8	2.46	0.50
7:A:384:VAL:HG21	8:B:334:ILE:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:1379:ILE:HB	9:C:1453:VAL:HG13	1.94	0.50
9:C:1397:PHE:HB3	9:C:1403:LYS:HB2	1.93	0.50
9:C:1465:PRO:HD3	9:C:1727:HIS:HB3	1.94	0.50
9:C:1855:TYR:HB3	9:C:1891:THR:HG21	1.92	0.50
42:c:110:LEU:HD11	45:f:59:LEU:HD23	1.93	0.50
5:5:110:C:H5'	41:b:50:ARG:NH2	2.26	0.50
43:d:16:HIS:CE1	43:d:76:MET:HE2	2.46	0.50
34:U:135:LEU:HG	50:v:202:TYR:HE1	1.76	0.50
44:l:33:VAL:HA	44:l:86:LEU:O	2.11	0.50
51:w:60:GLU:HA	51:w:63:LYS:CG	2.42	0.50
52:x:76:PHE:CE2	52:x:116:TYR:HB2	2.47	0.50
9:C:486:SER:HA	9:C:489:TYR:CZ	2.47	0.50
35:V:558:ASP:O	35:V:559:SER:C	2.54	0.50
7:A:1368:LEU:HD11	7:A:1467:LEU:HD13	1.92	0.50
9:C:1453:VAL:HG11	9:C:1467:LEU:HD11	1.93	0.50
17:K:287:HIS:CE1	17:K:313:ARG:HD2	2.47	0.50
50:v:358:ARG:HG2	50:v:392:ILE:HG22	1.93	0.50
6:6:112:U:H2'	6:6:113:A:H8	1.76	0.50
33:T:841:ILE:HG12	33:T:846:LEU:HD23	1.93	0.50
40:a:67:LEU:HB3	43:d:72:ILE:HD12	1.93	0.50
51:w:26:PHE:CE1	51:w:135:VAL:HG21	2.47	0.50
7:A:83:HIS:CD2	18:L:111:SER:HB2	2.46	0.50
7:A:2008:ARG:HG2	32:S:344:GLN:HG2	1.94	0.50
8:B:678:THR:HA	8:B:811:THR:HG21	1.94	0.50
9:C:538:ILE:HG23	9:C:611:LEU:HB3	1.93	0.50
52:x:66:PRO:HA	52:x:151:VAL:HA	1.94	0.50
4:4:89:HIS:HA	4:4:114:LYS:HZ1	1.76	0.49
9:C:1564:PRO:HA	9:C:1648:ARG:HB3	1.94	0.49
11:E:100:TYR:HE1	11:E:369:LEU:HD13	1.77	0.49
18:L:56:VAL:HG23	18:L:58:VAL:HG13	1.92	0.49
4:4:96:VAL:HG23	4:4:106:THR:HG22	1.95	0.49
7:A:126:ILE:HG21	16:J:207:MET:HE2	1.93	0.49
46:g:47:GLU:HG3	46:g:55:ASN:HB2	1.93	0.49
54:z:157:ARG:HA	54:z:160:GLN:HG3	1.93	0.49
54:z:160:GLN:O	54:z:164:GLU:HG3	2.12	0.49
42:c:30:SER:HA	42:c:33:THR:HG22	1.95	0.49
9:C:1001:TYR:O	9:C:1005:LEU:CB	2.54	0.49
37:X:682:TYR:HB3	37:X:685:LEU:HD21	1.94	0.49
6:6:110:U:H1'	6:6:111:C:H5'	1.94	0.49
7:A:955:TRP:CG	7:A:1189:MET:HE1	2.47	0.49
9:C:1376:CYS:HB2	9:C:1450:LEU:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:2067:VAL:HG22	9:C:2079:ILE:HG13	1.93	0.49
35:V:624:THR:HG23	35:V:643:LEU:HD11	1.94	0.49
51:w:9:LEU:HB3	51:w:28:PHE:HD1	1.78	0.49
7:A:301:LYS:HG2	8:B:939:ARG:HG2	1.95	0.49
8:B:335:ASN:HB3	8:B:338:GLU:HB2	1.95	0.49
8:B:343:LEU:HD13	8:B:373:ILE:HD11	1.95	0.49
10:D:133:VAL:HB	10:D:147:LEU:HB2	1.94	0.49
33:T:1096:CYS:HB2	33:T:1099:SER:HB3	1.95	0.49
33:T:1171:ARG:HD2	33:T:1171:ARG:N	2.28	0.49
6:6:94:C:H2'	6:6:95:A:C8	2.48	0.49
10:D:289:LEU:HB3	10:D:303:GLY:HA3	1.94	0.49
46:g:19:LEU:HD11	46:g:67:ILE:HD12	1.95	0.49
8:B:736:GLY:HA3	8:B:741:GLY:HA3	1.95	0.49
9:C:849:ILE:HG12	9:C:879:TYR:HE1	1.78	0.49
33:T:583:ILE:HD11	33:T:715:VAL:HG22	1.94	0.49
33:T:884:ALA:HB1	33:T:901:ARG:HH21	1.77	0.49
36:W:527:LEU:HD23	36:W:529:SER:H	1.78	0.49
51:w:57:SER:O	51:w:61:GLU:HG2	2.12	0.49
52:x:77:VAL:HG21	52:x:93:PHE:HZ	1.77	0.49
26:M:70:ASN:HB3	26:M:73:LEU:HB2	1.95	0.49
12:F:67:SER:HA	29:P:58:GLU:HA	1.95	0.48
12:F:669:LEU:HD21	12:F:703:PHE:HD1	1.77	0.48
35:V:555:LEU:HD12	35:V:586:PHE:HZ	1.78	0.48
50:v:70:LYS:O	50:v:74:LYS:HG2	2.12	0.48
50:v:116:ARG:HG2	50:v:141:ILE:HB	1.95	0.48
7:A:422:LEU:HD21	7:A:638:LEU:HD12	1.95	0.48
7:A:2230:LEU:HA	7:A:2256:TYR:HA	1.96	0.48
17:K:117:MET:HE3	17:K:117:MET:HA	1.95	0.48
7:A:370:PRO:HG3	8:B:304:LEU:HG	1.95	0.48
33:T:1136:HIS:CD2	33:T:1163:ARG:HE	2.31	0.48
44:e:31:ILE:O	44:e:44:GLU:HA	2.14	0.48
16:J:97:LYS:O	16:J:99:ASP:N	2.43	0.48
33:T:1153:GLU:OE1	33:T:1163:ARG:HB3	2.13	0.48
35:V:620:ASN:HB3	35:V:623:ASN:HB2	1.96	0.48
8:B:948:SER:H	8:B:951:LYS:HE2	1.78	0.48
9:C:617:ILE:HB	9:C:652:SER:HB3	1.94	0.48
7:A:429:ASN:HA	7:A:432:ARG:HB2	1.95	0.48
8:B:677:GLU:HB2	8:B:682:LYS:HA	1.94	0.48
8:B:742:PRO:HG2	8:B:785:ARG:HG2	1.95	0.48
9:C:964:LEU:HG	9:C:969:LEU:HB3	1.95	0.48
36:W:252:ILE:HA	36:W:265:LEU:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:159:ARG:HG3	38:Y:56:ASP:HB2	1.95	0.48
33:T:842:ALA:HA	33:T:846:LEU:HG	1.96	0.48
6:6:4:U:H5'	18:L:30:GLY:HA2	1.96	0.48
6:6:52:A:H2'	6:6:53:G:C8	2.48	0.48
9:C:737:ALA:O	9:C:741:MET:HG2	2.14	0.48
16:J:315:LYS:HD3	16:J:315:LYS:HA	1.66	0.48
50:v:89:THR:HA	50:v:92:PHE:CE2	2.49	0.48
50:v:282:ILE:HD12	50:v:332:ILE:HG12	1.95	0.48
50:v:291:ASP:O	50:v:295:GLU:HG2	2.13	0.48
52:x:77:VAL:HG21	52:x:93:PHE:CZ	2.49	0.48
52:x:77:VAL:HG22	52:x:146:VAL:HG12	1.96	0.48
7:A:499:GLN:O	7:A:503:MET:HG3	2.14	0.48
7:A:875:HIS:CD2	33:T:1193:LYS:HB3	2.49	0.48
7:A:2035:GLU:HA	32:S:322:ILE:HG23	1.94	0.48
11:E:160:ALA:HB2	13:G:198:ALA:HB1	1.95	0.48
11:E:169:ARG:O	11:E:173:GLU:HG2	2.14	0.48
33:T:841:ILE:O	33:T:845:SER:HB3	2.14	0.48
51:w:7:PHE:HZ	51:w:66:ILE:HD12	1.79	0.48
7:A:1403:LEU:HD12	7:A:1403:LEU:H	1.79	0.47
8:B:313:GLN:HB2	58:B:1501:GTP:C6	2.49	0.47
9:C:1679:TYR:CD2	9:C:1687:MET:HE1	2.49	0.47
41:b:19:LEU:HD11	41:b:60:ILE:HD13	1.96	0.47
46:g:40:LEU:HB2	46:g:62:ILE:HD11	1.95	0.47
9:C:1139:VAL:O	9:C:1143:ILE:HG13	2.13	0.47
11:E:180:ARG:HG2	36:W:398:SER:HB2	1.96	0.47
12:F:716:ASN:O	12:F:720:ILE:HG13	2.13	0.47
36:W:274:LYS:HB2	36:W:276:TRP:NE1	2.29	0.47
7:A:701:ILE:HG22	7:A:703:GLN:N	2.28	0.47
9:C:1587:GLN:HB2	9:C:1590:LEU:HB3	1.97	0.47
12:F:469:TYR:HB2	12:F:482:LYS:HD3	1.95	0.47
17:K:370:ASN:HB3	17:K:396:LYS:HE2	1.97	0.47
26:M:99:GLY:O	26:M:103:ILE:HG23	2.14	0.47
33:T:1113:ARG:HG2	33:T:1180:PHE:HE1	1.80	0.47
7:A:974:ASN:HB2	7:A:1178:TYR:HB3	1.96	0.47
7:A:1698:PRO:HG3	32:S:185:TYR:HB2	1.96	0.47
8:B:850:LEU:HB3	8:B:855:GLY:HA3	1.96	0.47
9:C:1681:ILE:HG12	9:C:1722:LEU:HD13	1.95	0.47
34:U:53:PRO:HG3	34:U:126:GLU:HG3	1.95	0.47
42:c:28:PRO:HA	45:f:43:GLN:HB2	1.96	0.47
7:A:975:VAL:HB	7:A:1099:PHE:HB2	1.97	0.47
7:A:2097:ILE:HG23	7:A:2260:GLN:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:846:VAL:HG22	8:B:887:LEU:HD21	1.95	0.47
9:C:721:VAL:HG23	9:C:825:THR:HG23	1.95	0.47
9:C:836:PRO:HG3	9:C:1079:ALA:HB1	1.96	0.47
9:C:1930:LEU:HD13	9:C:1939:ALA:HA	1.97	0.47
10:D:282:HIS:CE1	10:D:289:LEU:HD12	2.49	0.47
5:5:19:A:C8	7:A:466:ALA:HB1	2.50	0.47
7:A:317:PRO:O	7:A:321:ASN:HB2	2.15	0.47
7:A:963:GLN:HG3	7:A:1077:ILE:HG23	1.95	0.47
8:B:481:MET:HE2	8:B:612:LYS:HE3	1.97	0.47
8:B:617:LEU:HD13	8:B:640:VAL:HG21	1.97	0.47
9:C:139:VAL:HG21	9:C:161:LEU:HD11	1.95	0.47
9:C:409:LEU:HD21	9:C:956:LEU:HD22	1.97	0.47
9:C:525:ILE:HA	9:C:531:ILE:HG13	1.97	0.47
9:C:1307:LEU:HD12	9:C:1308:PRO:HD2	1.96	0.47
12:F:553:VAL:HG13	12:F:554:SER:H	1.79	0.47
12:F:553:VAL:HG23	12:F:556:ILE:HB	1.97	0.47
17:K:250:ARG:HD3	17:K:266:GLU:HG3	1.96	0.47
45:f:7:PRO:O	45:f:11:LEU:HD23	2.15	0.47
51:w:57:SER:O	51:w:60:GLU:HG3	2.14	0.47
51:w:125:TYR:HE1	52:x:108:ARG:HH22	1.62	0.47
4:4:442:SER:HB3	4:4:445:LYS:HB3	1.96	0.47
10:D:224:GLN:HG3	10:D:226:LYS:HB3	1.96	0.47
18:L:137:MET:HE3	18:L:137:MET:O	2.15	0.47
50:v:271:LEU:O	50:v:275:LEU:CB	2.63	0.47
7:A:1728:GLN:HG3	32:S:278:LEU:HD23	1.96	0.47
7:A:2148:VAL:HG21	7:A:2159:LEU:HD23	1.95	0.47
10:D:75:HIS:CD2	10:D:76:PRO:HD2	2.50	0.47
17:K:343:PRO:HG3	17:K:356:LEU:HD23	1.97	0.47
36:W:242:LEU:HB2	36:W:540:MET:HB2	1.96	0.47
42:c:42:VAL:HA	42:c:110:LEU:O	2.14	0.47
13:G:429:PHE:O	13:G:433:ARG:HG2	2.14	0.47
7:A:1401:ARG:HE	7:A:1401:ARG:HB3	1.56	0.46
9:C:1415:ASP:HB3	9:C:1435:LEU:HD11	1.97	0.46
9:C:1620:LEU:HD23	9:C:1629:ARG:HG3	1.96	0.46
35:V:401:ILE:O	35:V:405:ILE:HG12	2.15	0.46
36:W:217:VAL:HG12	36:W:222:GLN:HG2	1.96	0.46
7:A:2180:THR:HG22	7:A:2216:CYS:HB3	1.97	0.46
24:L7:23:ILE:HA	24:L7:87:GLN:H	1.80	0.46
33:T:793:LEU:O	33:T:797:MET:HG3	2.15	0.46
36:W:179:ARG:HA	36:W:182:ARG:HG2	1.96	0.46
40:a:65:ARG:HE	40:a:67:LEU:HD21	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:92:G:H1'	6:6:111:C:H4'	1.97	0.46
7:A:1849:ILE:HD11	7:A:1861:ILE:HD11	1.98	0.46
8:B:166:CYS:HB3	8:B:169:ASP:HB2	1.98	0.46
35:V:388:ASP:HB3	35:V:391:PHE:HB2	1.98	0.46
40:a:72:LEU:HD21	40:a:77:LEU:HB2	1.98	0.46
44:e:54:MET:HE3	44:e:84:ILE:HD12	1.96	0.46
4:4:295:ILE:HD11	4:4:309:PHE:HD1	1.80	0.46
7:A:1220:VAL:HG13	7:A:1221:THR:HG23	1.97	0.46
9:C:832:GLN:HG2	9:C:841:TRP:HB3	1.98	0.46
9:C:1062:LEU:HD21	9:C:1077:LEU:HD11	1.97	0.46
9:C:1195:ARG:HA	9:C:1291:LEU:HD12	1.98	0.46
12:F:619:ALA:O	12:F:623:VAL:HG13	2.15	0.46
26:M:22:THR:O	26:M:26:GLU:HG2	2.16	0.46
33:T:1008:ILE:HD12	33:T:1042:HIS:HB3	1.97	0.46
42:c:51:LYS:HE3	42:c:51:LYS:HB3	1.82	0.46
11:E:20:LYS:O	11:E:24:MET:HG2	2.15	0.46
12:F:452:ALA:O	12:F:456:LEU:HG	2.15	0.46
33:T:1135:ILE:HG23	33:T:1165:VAL:HG21	1.97	0.46
4:4:151:VAL:HB	4:4:177:PRO:HG2	1.98	0.46
4:4:401:MET:HE3	4:4:401:MET:HB3	1.69	0.46
8:B:531:TRP:CD1	8:B:540:GLU:HG3	2.50	0.46
9:C:466:LYS:HA	9:C:466:LYS:HD3	1.72	0.46
9:C:1428:THR:H	9:C:1431:LYS:HE2	1.81	0.46
9:C:2065:TRP:HB2	9:C:2109:MET:HB2	1.98	0.46
17:K:187:LYS:HD3	17:K:187:LYS:HA	1.75	0.46
33:T:854:VAL:HG23	33:T:891:ALA:HB2	1.97	0.46
46:g:15:LYS:HG3	46:g:76:VAL:HG12	1.97	0.46
50:v:114:PRO:HD2	50:v:118:LEU:HD23	1.98	0.46
50:v:320:MET:HE1	50:v:324:ARG:HE	1.81	0.46
7:A:1688:THR:HG22	32:S:181:ILE:HD13	1.97	0.46
8:B:508:LYS:HE2	8:B:510:LEU:HD21	1.98	0.46
8:B:726:LEU:HD12	8:B:726:LEU:H	1.81	0.46
8:B:830:PRO:HG2	8:B:877:ALA:HB3	1.97	0.46
9:C:1558:PRO:HD2	9:C:1693:ARG:HH22	1.80	0.46
9:C:1805:GLU:HG2	9:C:1809:ASP:HB3	1.98	0.46
26:M:53:LEU:HD22	26:M:58:VAL:HG11	1.97	0.46
26:M:126:SER:HB3	26:M:133:LEU:HD23	1.97	0.46
33:T:786:ILE:HG23	33:T:837:ILE:HG23	1.97	0.46
36:W:541:LYS:HE3	36:W:541:LYS:HB2	1.81	0.46
42:c:88:LYS:HA	42:c:88:LYS:HD3	1.78	0.46
45:f:14:LEU:HD13	45:f:19:VAL:HG11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:w:29:ARG:HH12	51:w:35:ARG:HG3	1.80	0.46
5:5:94:U:H5''	42:c:104:ASP:HB2	1.97	0.46
7:A:1088:PHE:HD1	7:A:1097:ILE:HG12	1.81	0.46
7:A:1868:MET:HE3	7:A:1868:MET:HB3	1.78	0.46
7:A:2307:GLU:HG2	9:C:1124:GLN:HB2	1.97	0.46
8:B:500:THR:HG21	8:B:543:ARG:HH12	1.81	0.46
8:B:802:HIS:H	8:B:802:HIS:CD2	2.32	0.46
32:S:292:MET:HE3	32:S:292:MET:HB2	1.76	0.46
33:T:648:PHE:HB3	33:T:1081:GLN:NE2	2.31	0.46
33:T:807:LEU:HG	33:T:835:VAL:HG23	1.98	0.46
33:T:958:MET:HE3	33:T:967:LEU:HD11	1.98	0.46
34:U:136:ARG:HD3	50:v:206:ARG:HH21	1.81	0.46
39:Z:330:ARG:NH2	39:Z:333:ARG:HH21	2.13	0.46
46:g:13:MET:HA	46:g:31:LEU:HD23	1.97	0.46
4:4:344:MET:O	4:4:348:ARG:HG2	2.16	0.45
7:A:796:LYS:HE2	7:A:796:LYS:HB3	1.77	0.45
8:B:792:LEU:HD22	34:U:60:HIS:CE1	2.51	0.45
9:C:1228:VAL:HG11	9:C:1264:PRO:HD2	1.98	0.45
9:C:1470:ILE:O	9:C:1474:MET:HG2	2.15	0.45
50:v:92:PHE:HE1	50:v:111:ILE:HD13	1.81	0.45
50:v:347:SER:HA	50:v:368:SER:HB2	1.97	0.45
7:A:227:ARG:HA	7:A:416:GLY:O	2.16	0.45
7:A:343:GLU:HB2	32:S:144:PHE:HZ	1.80	0.45
9:C:849:ILE:HG12	9:C:879:TYR:CE1	2.51	0.45
9:C:1487:ILE:HG21	9:C:1504:LEU:HD22	1.98	0.45
17:K:294:LEU:HD12	17:K:303:LEU:HD11	1.97	0.45
26:M:30:GLN:HE21	26:M:30:GLN:CA	2.29	0.45
33:T:446:PRO:HG2	33:T:449:LEU:HB2	1.99	0.45
52:x:123:THR:HG23	52:x:125:LYS:H	1.81	0.45
9:C:1963:LEU:HD23	9:C:2007:VAL:HB	1.99	0.45
26:M:119:ILE:HG21	26:M:159:LEU:HB3	1.98	0.45
33:T:980:MET:HE1	33:T:991:LYS:HA	1.98	0.45
34:U:150:SER:HA	50:v:199:GLU:CD	2.42	0.45
42:c:50:LYS:HG2	42:c:74:TRP:HB3	1.97	0.45
44:e:19:ASN:O	44:e:23:ARG:HG2	2.16	0.45
51:w:134:LEU:O	51:w:138:LEU:HD22	2.17	0.45
7:A:2016:ILE:HG13	37:X:657:LYS:NZ	2.31	0.45
9:C:993:ILE:HD12	9:C:1091:LEU:HD23	1.98	0.45
9:C:1225:VAL:HG12	9:C:1268:ILE:HG22	1.97	0.45
10:D:246:GLU:HG2	10:D:248:SER:H	1.82	0.45
33:T:668:ARG:HA	33:T:671:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:U:135:LEU:HA	34:U:138:ALA:HB3	1.97	0.45
43:d:43:MET:HB3	43:d:46:ILE:HD11	1.98	0.45
46:g:39:ASN:HA	46:g:62:ILE:O	2.17	0.45
53:y:57:LYS:HE3	53:y:57:LYS:HB2	1.83	0.45
7:A:784:LEU:O	7:A:788:GLN:HG3	2.17	0.45
8:B:754:VAL:HG13	8:B:756:LYS:HD2	1.98	0.45
9:C:1534:HIS:HB3	9:C:1537:THR:HB	1.97	0.45
9:C:1763:ARG:HA	9:C:1766:GLN:HB2	1.99	0.45
9:C:2016:ASN:H	9:C:2045:GLU:HG2	1.80	0.45
11:E:203:LYS:HD3	11:E:203:LYS:HA	1.80	0.45
33:T:1171:ARG:HD2	33:T:1171:ARG:H	1.81	0.45
35:V:606:GLU:HA	35:V:609:GLN:HG2	1.98	0.45
42:c:53:LEU:HD23	42:c:53:LEU:HA	1.83	0.45
44:e:31:ILE:HD12	44:e:87:LEU:HG	1.98	0.45
50:v:376:VAL:HG21	50:v:410:LEU:HD22	1.98	0.45
7:A:99:VAL:HG13	7:A:554:THR:HG21	1.98	0.45
9:C:723:VAL:HG22	9:C:827:ILE:HD11	1.99	0.45
17:K:213:GLU:HG2	17:K:214:PRO:HD2	1.98	0.45
18:L:128:VAL:HG21	26:M:161:GLN:HB2	1.98	0.45
50:v:349:ILE:HG12	50:v:368:SER:HB3	1.98	0.45
6:6:63:C:H2'	6:6:64:C:C6	2.52	0.45
7:A:875:HIS:CE1	33:T:1193:LYS:HD2	2.52	0.45
8:B:359:LYS:HE3	8:B:359:LYS:HB3	1.79	0.45
9:C:439:ARG:HG3	9:C:440:LYS:HG2	1.97	0.45
34:U:54:ASN:HB3	34:U:57:ILE:HD12	1.97	0.45
50:v:168:PHE:HA	50:v:171:ILE:HD12	1.97	0.45
4:4:160:PHE:HA	4:4:167:MET:HA	1.99	0.45
5:5:110:C:H5'	41:b:50:ARG:HH22	1.82	0.45
7:A:1614:ILE:HG21	7:A:1618:LYS:HD2	1.98	0.45
9:C:548:VAL:O	9:C:552:VAL:HG23	2.17	0.45
9:C:1439:TRP:CG	9:C:1440:LYS:H	2.34	0.45
11:E:519:ASP:HA	11:E:522:LYS:HE2	1.99	0.45
12:F:418:LEU:O	12:F:422:THR:HG23	2.16	0.45
12:F:432:LEU:HD22	12:F:476:VAL:HG23	1.98	0.45
12:F:462:LEU:HD11	12:F:466:ARG:HE	1.81	0.45
36:W:426:ARG:HA	36:W:426:ARG:HD3	1.80	0.45
42:c:44:ILE:HD12	42:c:52:LEU:HB2	1.98	0.45
44:e:86:LEU:HD21	46:g:62:ILE:HG22	1.98	0.45
7:A:1777:ILE:HG12	7:A:1860:GLN:HB2	1.97	0.45
8:B:724:TRP:HZ3	8:B:732:ILE:HD11	1.81	0.45
9:C:1627:MET:HE3	9:C:1627:MET:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:11:TRP:CZ2	11:E:41:LYS:HG2	2.52	0.45
12:F:518:PRO:O	12:F:522:ILE:HG13	2.17	0.45
7:A:465:LYS:HA	7:A:465:LYS:HD3	1.68	0.45
7:A:1382:SER:HB2	7:A:1416:ILE:H	1.82	0.45
8:B:367:ARG:O	8:B:371:GLU:CB	2.65	0.45
9:C:1259:PHE:HB2	9:C:1261:PRO:HD2	1.99	0.45
9:C:2013:ARG:HG2	9:C:2052:ILE:HG13	1.98	0.45
33:T:490:LYS:HD2	33:T:490:LYS:HA	1.78	0.45
33:T:866:ASN:OD1	33:T:868:LYS:HG2	2.17	0.45
33:T:989:LEU:HD21	33:T:1152:HIS:CE1	2.38	0.45
4:4:203:ILE:HB	4:4:218:PHE:HB2	1.98	0.44
7:A:1676:ILE:HG23	7:A:1713:SER:HB2	1.99	0.44
8:B:94:ILE:HD12	17:K:275:LEU:HB2	1.98	0.44
9:C:2063:GLY:H	9:C:2111:ASP:CG	2.24	0.44
12:F:502:SER:O	12:F:506:VAL:HG23	2.17	0.44
18:L:73:GLU:HB3	18:L:93:LYS:HD3	1.98	0.44
26:M:44:ALA:HB1	26:M:84:LEU:HG	2.00	0.44
33:T:746:ILE:HD12	33:T:748:TYR:HE1	1.82	0.44
33:T:909:ARG:HE	33:T:909:ARG:HB2	1.59	0.44
33:T:993:LEU:O	33:T:997:VAL:HG23	2.17	0.44
9:C:869:LEU:HD21	9:C:879:TYR:CD1	2.52	0.44
11:E:314:GLY:O	11:E:318:GLU:HG2	2.17	0.44
34:U:58:LEU:HD12	34:U:58:LEU:C	2.42	0.44
35:V:257:SER:HA	35:V:260:VAL:HG12	1.99	0.44
3:2:28:U:H2'	3:2:29:A:C8	2.53	0.44
5:5:36:C:H2'	5:5:37:G:H8	1.82	0.44
6:6:80:G:C8	12:F:427:LYS:HB3	2.52	0.44
9:C:930:LEU:HD23	9:C:949:LEU:HD23	1.98	0.44
9:C:1071:LYS:C	9:C:1072:LEU:HD22	2.41	0.44
9:C:1356:LYS:HD2	9:C:1490:LEU:HB3	1.99	0.44
33:T:789:ALA:HA	33:T:792:ILE:HG22	1.99	0.44
36:W:450:LEU:HB2	36:W:467:TYR:HB2	1.99	0.44
3:2:77:U:H5'	3:2:78:U:H5'	1.99	0.44
8:B:449:ILE:HD12	8:B:465:MET:HE3	2.00	0.44
9:C:537:LYS:HG2	9:C:584:GLN:HA	2.00	0.44
33:T:743:PRO:HB3	53:y:57:LYS:HE2	2.00	0.44
35:V:624:THR:O	35:V:628:ILE:HG12	2.17	0.44
36:W:383:LEU:HD11	36:W:434:LEU:HB2	1.99	0.44
46:g:28:GLN:HE22	46:g:48:MET:HG3	1.83	0.44
4:4:156:ALA:HB1	4:4:158:LYS:HE2	1.99	0.44
8:B:141:GLY:HA3	8:B:258:ASN:HD22	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:2023:VAL:HB	9:C:2026:LYS:HB2	1.99	0.44
10:D:56:GLN:HE21	10:D:60:MET:HG2	1.82	0.44
26:M:47:PRO:HA	26:M:50:TYR:CE2	2.53	0.44
33:T:474:GLN:HA	33:T:477:MET:SD	2.57	0.44
33:T:767:ILE:HD12	33:T:898:LYS:HD2	1.99	0.44
33:T:868:LYS:HE3	33:T:868:LYS:HB3	1.82	0.44
1:O:-6:U:O2	1:O:-6:U:C2'	2.66	0.44
8:B:696:LEU:O	8:B:700:ILE:HG12	2.18	0.44
9:C:479:LYS:HB2	9:C:479:LYS:HE3	1.82	0.44
9:C:1683:ASP:O	9:C:1687:MET:HG3	2.18	0.44
13:G:482:GLU:HA	13:G:485:LYS:HB2	1.99	0.44
34:U:138:ALA:CB	50:v:228:MET:HE1	2.46	0.44
34:U:139:PHE:CG	50:v:228:MET:HE2	2.52	0.44
35:V:533:TYR:CE2	35:V:568:ILE:HG12	2.52	0.44
36:W:274:LYS:HB2	36:W:276:TRP:HE1	1.83	0.44
9:C:1559:VAL:HG13	9:C:1660:LEU:HG	1.99	0.44
26:M:125:LEU:HD23	26:M:125:LEU:HA	1.77	0.44
44:e:77:ILE:HG23	45:f:71:TYR:HB2	1.99	0.44
4:4:137:GLU:HB2	4:4:151:VAL:HG23	1.99	0.44
9:C:735:ALA:HB2	9:C:810:VAL:HG11	1.99	0.44
13:G:433:ARG:NH1	13:G:463:GLY:HA2	2.33	0.44
33:T:785:GLU:CD	33:T:785:GLU:H	2.25	0.44
35:V:221:ILE:HD11	35:V:359:LEU:HD13	1.99	0.44
42:c:110:LEU:HD23	42:c:110:LEU:HA	1.86	0.44
44:e:76:ARG:HH12	45:f:5:LEU:HD23	1.82	0.44
50:v:255:PHE:HD2	50:v:400:ILE:HG22	1.83	0.44
4:4:245:GLY:HA2	4:4:283:PRO:HD3	1.99	0.44
7:A:984:MET:HE3	7:A:984:MET:HB2	1.86	0.44
8:B:314:TYR:HA	8:B:417:ARG:HG3	1.99	0.44
9:C:712:ILE:O	9:C:716:ALA:HB2	2.17	0.44
9:C:1493:SER:HB3	9:C:1721:PRO:HB3	2.00	0.44
17:K:363:LYS:HB3	17:K:363:LYS:HE3	1.87	0.44
33:T:630:VAL:HG21	33:T:660:TYR:OH	2.17	0.44
33:T:668:ARG:HD3	33:T:984:PRO:HB3	2.00	0.44
44:e:77:ILE:HD13	45:f:73:ARG:HB2	1.99	0.44
46:g:6:PRO:HA	46:g:36:PRO:HA	2.00	0.44
7:A:615:ARG:HE	7:A:615:ARG:HB3	1.66	0.43
7:A:1850:ARG:HE	7:A:1850:ARG:HB2	1.57	0.43
8:B:105:MET:HE2	8:B:105:MET:HB3	1.65	0.43
11:E:187:LYS:HE2	11:E:187:LYS:HB3	1.78	0.43
33:T:426:LEU:HD12	33:T:427:PRO:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:T:563:GLU:HA	33:T:568:TYR:CG	2.53	0.43
50:v:85:GLY:HA2	50:v:370:ARG:HH21	1.83	0.43
50:v:200:GLN:O	50:v:204:VAL:HG13	2.17	0.43
54:z:133:TYR:CZ	54:z:196:VAL:HG11	2.53	0.43
7:A:609:LYS:O	7:A:613:TYR:HB2	2.19	0.43
7:A:1757:GLU:HB3	7:A:1759:THR:HG23	2.00	0.43
8:B:698:GLU:HA	8:B:701:GLU:HG2	2.00	0.43
9:C:1871:LEU:HD23	9:C:1874:LYS:HE2	2.00	0.43
11:E:206:ARG:NH2	13:G:229:LYS:HB2	2.33	0.43
12:F:414:ALA:O	12:F:418:LEU:HG	2.18	0.43
12:F:737:GLN:HA	12:F:740:PHE:HB3	2.00	0.43
18:L:25:ALA:HB3	18:L:28:ARG:HD3	2.01	0.43
44:e:78:MET:HB2	45:f:72:ILE:HD12	1.99	0.43
46:g:21:LEU:N	46:g:21:LEU:HD22	2.33	0.43
50:v:92:PHE:CD1	50:v:185:VAL:HG11	2.53	0.43
4:4:205:ILE:HD11	4:4:218:PHE:HE1	1.83	0.43
7:A:591:MET:HG2	7:A:598:LEU:HD11	2.00	0.43
7:A:1644:LEU:HD22	7:A:1677:GLU:HB3	1.99	0.43
7:A:2315:LEU:HD12	7:A:2315:LEU:HA	1.86	0.43
8:B:342:ARG:HG3	8:B:347:ILE:HD13	1.99	0.43
8:B:814:ARG:HG3	8:B:952:PHE:HB3	2.00	0.43
16:J:230:MET:HE3	16:J:230:MET:HB3	1.86	0.43
33:T:659:LYS:HG2	33:T:661:MET:HB2	2.00	0.43
33:T:768:HIS:CD2	33:T:807:LEU:HD22	2.53	0.43
33:T:1045:LEU:HA	33:T:1048:VAL:HG22	2.01	0.43
50:v:79:ILE:HG22	50:v:216:LEU:HB3	2.00	0.43
6:6:52:A:H2'	6:6:53:G:H8	1.82	0.43
8:B:531:TRP:HB3	8:B:538:HIS:HB3	2.01	0.43
8:B:671:SER:HA	34:U:122:HIS:CE1	2.54	0.43
9:C:1555:PRO:HA	9:C:1588:ARG:HH22	1.83	0.43
12:F:563:LYS:HA	12:F:563:LYS:HD3	1.71	0.43
26:M:27:THR:HB	26:M:28:GLN:H	1.68	0.43
33:T:777:LEU:HD12	33:T:851:ILE:HD12	2.00	0.43
37:X:659:ASN:HD21	37:X:669:PRO:HB2	1.83	0.43
7:A:1090:ARG:HG3	7:A:1095:ILE:HG22	2.00	0.43
8:B:481:MET:HE3	8:B:481:MET:HB3	1.77	0.43
10:D:251:LEU:HD13	10:D:261:VAL:HG22	2.01	0.43
16:J:119:LEU:HD21	16:J:230:MET:HE3	2.01	0.43
16:J:243:GLN:HA	16:J:246:LYS:HG3	2.00	0.43
26:M:50:TYR:O	26:M:54:ARG:HG2	2.17	0.43
33:T:694:THR:HA	33:T:697:LEU:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:v:202:TYR:HD1	50:v:202:TYR:HA	1.72	0.43
4:4:149:CYS:HB2	4:4:157:MET:HE1	2.00	0.43
6:6:72:A:H61	13:G:381:LYS:NZ	2.16	0.43
7:A:535:ARG:HH22	38:Y:110:TRP:HA	1.83	0.43
7:A:2028:GLU:O	7:A:2031:LYS:HB2	2.18	0.43
9:C:140:LEU:HD13	9:C:182:TYR:HE1	1.83	0.43
12:F:420:LYS:O	12:F:424:VAL:HG23	2.19	0.43
12:F:465:ARG:HH21	12:F:474:GLU:HG2	1.83	0.43
12:F:494:GLU:HG2	12:F:498:GLY:HA3	1.99	0.43
13:G:262:ARG:NH2	13:G:291:GLN:HG2	2.33	0.43
13:G:490:ASN:HB3	13:G:493:ALA:HB3	2.00	0.43
35:V:648:LYS:HE2	35:V:648:LYS:HB3	1.77	0.43
42:c:44:ILE:HD13	42:c:65:MET:HE1	2.01	0.43
3:2:9:A:H2'	3:2:10:A:C8	2.53	0.43
7:A:2108:LYS:HE2	7:A:2112:LYS:HE3	2.01	0.43
28:O:18:THR:HA	28:O:159:ILE:HA	2.01	0.43
34:U:23:LEU:HD23	34:U:23:LEU:HA	1.85	0.43
44:e:78:MET:HG3	45:f:11:LEU:HD21	2.00	0.43
2:1:186:A:H61	36:W:233:THR:HA	1.84	0.43
2:1:215:U:O2	2:1:215:U:H2'	2.19	0.43
3:2:13:U:H2'	3:2:14:A:C4	2.54	0.43
7:A:1683:LYS:HD3	7:A:1683:LYS:HA	1.71	0.43
7:A:1776:ILE:HB	7:A:1858:PRO:HA	2.01	0.43
8:B:531:TRP:CZ3	8:B:553:GLU:HB2	2.54	0.43
9:C:596:ILE:HD12	9:C:596:ILE:HA	1.91	0.43
9:C:1136:PRO:O	9:C:1140:VAL:HG23	2.19	0.43
9:C:1763:ARG:HA	9:C:1763:ARG:HD2	1.85	0.43
10:D:157:CYS:HB2	10:D:169:THR:HG22	2.00	0.43
12:F:697:PRO:HA	12:F:704:TRP:CD1	2.54	0.43
12:F:737:GLN:HG3	54:z:127:TRP:CZ2	2.54	0.43
33:T:1101:VAL:O	33:T:1105:LYS:HG3	2.18	0.43
41:b:3:LEU:HD12	41:b:3:LEU:HA	1.89	0.43
50:v:189:ALA:O	50:v:193:LEU:HB2	2.19	0.43
54:z:206:GLN:HA	54:z:209:ARG:HB2	2.00	0.43
6:6:53:G:H2'	6:6:54:G:C8	2.54	0.43
6:6:80:G:H2'	6:6:81:G:C8	2.51	0.43
7:A:1976:TRP:HA	7:A:1979:VAL:HG12	2.01	0.43
8:B:64:LYS:HD2	27:N:209:ARG:HH12	1.83	0.43
8:B:826:ARG:HD3	8:B:826:ARG:HA	1.78	0.43
9:C:1088:ALA:O	9:C:1092:MET:HB2	2.19	0.43
9:C:1098:ILE:HG23	9:C:1102:ARG:CZ	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:1344:ASP:H	9:C:1486:ARG:HE	1.66	0.43
9:C:1346:VAL:HG12	9:C:1510:SER:HB2	2.00	0.43
9:C:1818:ILE:HD13	9:C:1929:VAL:HG22	2.00	0.43
9:C:1985:ILE:HA	9:C:1988:MET:HE1	2.00	0.43
10:D:89:LEU:HD22	10:D:106:LYS:HG2	2.01	0.43
32:S:84:HIS:CD2	32:S:85:GLN:HE21	2.36	0.43
34:U:135:LEU:O	50:v:202:TYR:OH	2.33	0.43
5:5:17:U:H2'	5:5:18:C:C6	2.53	0.43
7:A:1768:TYR:CE2	32:S:324:MET:HE1	2.54	0.43
8:B:692:LEU:CD2	8:B:693:GLU:H	2.31	0.43
10:D:218:LYS:HB3	10:D:227:LEU:HD13	2.01	0.43
4:4:119:ILE:HD12	4:4:119:ILE:HA	1.92	0.42
4:4:348:ARG:HA	4:4:348:ARG:HD2	1.91	0.42
7:A:1017:ILE:HD11	7:A:1031:ILE:HD11	2.01	0.42
8:B:349:PHE:HB3	8:B:371:GLU:OE2	2.19	0.42
11:E:77:LEU:HD22	16:J:285:ALA:HA	2.01	0.42
12:F:734:TYR:O	12:F:735:ASN:HB2	2.18	0.42
17:K:207:VAL:HB	17:K:480:ALA:HB1	2.01	0.42
27:N:76:ARG:HE	27:N:76:ARG:HB3	1.62	0.42
32:S:358:LYS:HD2	32:S:358:LYS:HA	1.81	0.42
52:x:96:TYR:HD2	52:x:130:ALA:HA	1.84	0.42
1:0:-15:C:H42	50:v:148:GLU:N	2.17	0.42
6:6:32:C:O2'	6:6:33:C:H6	2.03	0.42
7:A:362:ARG:HH22	8:B:864:PRO:HG2	1.83	0.42
7:A:976:MET:HG2	7:A:1187:PHE:HB3	2.00	0.42
9:C:603:ARG:HA	9:C:603:ARG:HD3	1.86	0.42
9:C:1214:VAL:HG22	9:C:1275:TRP:HH2	1.84	0.42
9:C:1525:LEU:HD12	9:C:1702:CYS:HB3	2.01	0.42
10:D:176:VAL:HB	10:D:190:PHE:HD2	1.84	0.42
14:H:123:LYS:O	14:H:127:LEU:HG	2.18	0.42
16:J:311:LYS:HE3	16:J:311:LYS:HA	2.01	0.42
33:T:933:LYS:HZ2	33:T:972:LEU:HD12	1.84	0.42
34:U:133:GLU:HA	34:U:136:ARG:HG2	1.99	0.42
51:w:29:ARG:HD2	51:w:33:LYS:HB3	2.02	0.42
52:x:67:GLN:HG3	52:x:152:ARG:HA	2.00	0.42
4:4:92:VAL:HA	4:4:446:ASN:HA	2.00	0.42
8:B:676:ALA:HB3	8:B:815:VAL:HB	2.02	0.42
9:C:541:ILE:HA	9:C:588:CYS:O	2.19	0.42
9:C:1062:LEU:HD23	9:C:1062:LEU:HA	1.79	0.42
9:C:1559:VAL:HA	9:C:1660:LEU:O	2.19	0.42
33:T:1005:MET:O	33:T:1009:VAL:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:T:1147:GLU:HG3	33:T:1148:TRP:CD1	2.54	0.42
35:V:194:ARG:HH11	35:V:382:LEU:HB3	1.83	0.42
35:V:316:PHE:CZ	35:V:343:ARG:HD3	2.55	0.42
51:w:7:PHE:HD2	51:w:63:LYS:HE3	1.84	0.42
6:G:69:A:H62	13:G:315:LYS:HE2	1.84	0.42
7:A:36:LYS:HD3	7:A:36:LYS:HA	1.92	0.42
7:A:1454:TRP:CD1	7:A:1454:TRP:H	2.37	0.42
8:B:721:LYS:HD2	8:B:721:LYS:HA	1.80	0.42
9:C:482:ASN:O	9:C:486:SER:HB2	2.19	0.42
9:C:551:MET:HE2	9:C:551:MET:HB2	1.84	0.42
13:G:181:ASN:HB2	37:X:691:THR:HG23	2.01	0.42
33:T:1189:LEU:CD1	33:T:1190:SER:H	2.29	0.42
51:w:63:LYS:HE3	51:w:94:ILE:HG23	2.00	0.42
7:A:840:ILE:HG13	33:T:1198:LEU:HD13	2.01	0.42
7:A:1144:LYS:HB3	7:A:1144:LYS:HE2	1.86	0.42
9:C:2021:TYR:HB3	9:C:2039:VAL:HG13	2.01	0.42
12:F:593:LYS:HG3	12:F:631:MET:HE1	2.01	0.42
12:F:698:ARG:HG2	12:F:738:VAL:HG11	2.01	0.42
18:L:71:ALA:HB3	18:L:95:MET:HE2	2.01	0.42
33:T:1085:ILE:HA	33:T:1088:ARG:HE	1.84	0.42
33:T:1150:VAL:HG12	33:T:1166:THR:O	2.20	0.42
34:U:130:LYS:O	34:U:133:GLU:HG2	2.20	0.42
35:V:242:ARG:O	35:V:246:ARG:HG2	2.19	0.42
8:B:210:ASN:HB3	8:B:636:TYR:HB2	2.01	0.42
8:B:924:GLN:HB3	8:B:928:HIS:HB2	2.01	0.42
9:C:731:THR:HB	9:C:810:VAL:HG22	2.01	0.42
9:C:733:LYS:HD2	9:C:733:LYS:HA	1.74	0.42
9:C:1681:ILE:HD12	9:C:1684:VAL:HB	2.02	0.42
9:C:1736:PHE:HD2	9:C:1792:THR:HG21	1.85	0.42
17:K:392:PRO:HG3	17:K:415:ILE:HA	2.00	0.42
32:S:59:ILE:HG12	32:S:82:LEU:HD12	2.00	0.42
33:T:797:MET:SD	33:T:807:LEU:HB3	2.60	0.42
33:T:1002:SER:O	33:T:1006:LEU:HB2	2.20	0.42
34:U:59:ASP:O	34:U:63:LYS:HG3	2.20	0.42
37:X:643:PRO:HD2	37:X:719:ILE:HD11	2.00	0.42
37:X:696:LEU:HD12	37:X:696:LEU:HA	1.88	0.42
37:X:703:LYS:HA	37:X:703:LYS:HD3	1.87	0.42
7:A:644:ILE:HD12	7:A:644:ILE:HA	1.88	0.42
9:C:552:VAL:HG13	9:C:566:VAL:HG22	2.00	0.42
9:C:962:LEU:HD23	9:C:962:LEU:HA	1.92	0.42
10:D:312:TRP:CD1	10:D:319:ILE:HG12	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:G:413:GLU:HA	13:G:416:TYR:CE1	2.55	0.42
13:G:430:GLU:HA	13:G:433:ARG:HG3	2.02	0.42
33:T:1031:LYS:HD3	33:T:1034:LYS:HD2	2.01	0.42
33:T:1051:SER:O	33:T:1055:ASN:HB2	2.20	0.42
34:U:132:ASN:O	34:U:136:ARG:HG2	2.19	0.42
4:4:345:ALA:O	4:4:349:GLU:HG3	2.20	0.42
7:A:1330:MET:HE1	7:A:1369:TYR:HB2	2.02	0.42
8:B:404:THR:OG1	8:B:407:GLU:HG3	2.19	0.42
8:B:477:HIS:CE1	8:B:577:PHE:HB2	2.54	0.42
8:B:822:MET:HE3	8:B:949:ILE:HG21	2.02	0.42
9:C:1387:GLU:HA	9:C:1390:TYR:HB3	2.02	0.42
10:D:259:VAL:HB	10:D:277:PHE:HB2	2.02	0.42
17:K:353:THR:HG22	17:K:369:THR:HG22	2.02	0.42
33:T:986:GLU:HB3	33:T:989:LEU:HG	2.01	0.42
51:w:36:TYR:HB3	51:w:50:LYS:HG2	2.01	0.42
52:x:78:THR:HG22	52:x:145:SER:HB3	2.02	0.42
7:A:579:GLN:HG3	7:A:629:PHE:H	1.84	0.42
9:C:496:ASP:HB3	9:C:519:ARG:HH21	1.85	0.42
32:S:106:VAL:HG22	32:S:151:PRO:HB2	2.01	0.42
33:T:1169:ASP:HB2	33:T:1172:TRP:NE1	2.35	0.42
42:c:53:LEU:HB2	42:c:71:LYS:HZ2	1.85	0.42
50:v:242:LYS:HA	50:v:242:LYS:HD3	1.83	0.42
50:v:340:GLY:H	50:v:367:ARG:NH2	2.17	0.42
4:4:323:SER:O	4:4:327:GLU:HG2	2.20	0.42
7:A:1072:LEU:HD22	7:A:1087:LEU:HD22	2.01	0.42
8:B:133:THR:HG21	8:B:219:LEU:HD23	2.00	0.42
26:M:30:GLN:HE21	26:M:30:GLN:HA	1.85	0.42
27:N:229:LYS:HD2	27:N:229:LYS:HA	1.69	0.42
33:T:768:HIS:CE1	33:T:807:LEU:HD13	2.55	0.42
33:T:810:LEU:HD23	33:T:810:LEU:HA	1.82	0.42
33:T:1086:MET:SD	33:T:1091:LEU:HB2	2.60	0.42
35:V:397:LYS:HA	35:V:397:LYS:HD2	1.63	0.42
42:c:71:LYS:HG3	42:c:93:ASP:OD1	2.19	0.42
7:A:2012:LEU:HD23	7:A:2012:LEU:HA	1.84	0.41
8:B:421:LYS:HB2	8:B:421:LYS:HE3	1.80	0.41
17:K:320:LYS:HE2	17:K:320:LYS:HB2	1.83	0.41
30:Q:851:ILE:HA	30:Q:1060:LEU:O	2.20	0.41
33:T:1168:ILE:HD12	33:T:1169:ASP:H	1.85	0.41
36:W:273:PHE:CE2	36:W:307:ILE:HG21	2.55	0.41
45:f:5:LEU:HG	45:f:10:PHE:HB2	2.02	0.41
45:f:42:MET:HB3	45:f:64:ILE:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:v:124:LYS:HA	50:v:124:LYS:HD3	1.93	0.41
7:A:1950:ALA:O	7:A:1954:LEU:HG	2.20	0.41
8:B:461:LEU:HA	8:B:461:LEU:HD12	1.75	0.41
9:C:1046:ILE:HD13	9:C:1046:ILE:HA	1.94	0.41
9:C:2118:GLN:HB3	9:C:2120:TYR:CE1	2.56	0.41
12:F:606:TRP:HA	14:H:118:ARG:HH12	1.84	0.41
17:K:371:HIS:CE1	17:K:396:LYS:HG3	2.55	0.41
26:M:92:GLU:HG3	26:M:96:HIS:CE1	2.54	0.41
33:T:1150:VAL:HG13	33:T:1166:THR:HB	2.02	0.41
36:W:250:ASN:HD21	36:W:269:MET:HG2	1.85	0.41
36:W:466:ARG:HB3	54:z:214:LEU:HD12	2.02	0.41
41:b:70:LEU:HB2	42:c:98:LYS:HB2	2.02	0.41
42:c:71:LYS:HB2	42:c:95:TYR:CE1	2.55	0.41
54:z:197:LYS:HD2	54:z:197:LYS:HA	1.82	0.41
4:4:224:SER:HB3	4:4:243:LYS:HB2	2.02	0.41
6:6:124:U:H5'	6:6:125:U:H5'	2.02	0.41
7:A:1562:MET:HE3	7:A:1562:MET:HB3	1.82	0.41
7:A:2152:GLY:HA3	7:A:2157:VAL:HA	2.03	0.41
8:B:367:ARG:O	8:B:371:GLU:HB2	2.20	0.41
9:C:406:ARG:HH22	9:C:974:LYS:HB3	1.85	0.41
9:C:495:THR:HG21	9:C:671:LYS:HE2	2.02	0.41
9:C:681:ARG:HH21	9:C:854:GLY:HA2	1.84	0.41
9:C:1405:VAL:HG22	9:C:1424:ILE:HD11	2.01	0.41
9:C:1936:LEU:HA	9:C:1936:LEU:HD23	1.85	0.41
13:G:247:LYS:HE3	13:G:247:LYS:HB2	1.85	0.41
17:K:227:THR:HG22	17:K:243:THR:HG22	2.02	0.41
29:P:11:GLY:O	29:P:77:ILE:HA	2.20	0.41
33:T:1004:GLU:O	33:T:1008:ILE:HG23	2.19	0.41
35:V:297:LEU:HD12	35:V:297:LEU:HA	1.79	0.41
7:A:203:VAL:O	7:A:207:PHE:HB2	2.20	0.41
7:A:608:LEU:HD13	7:A:632:ALA:HB1	2.03	0.41
8:B:129:ILE:HG13	8:B:441:PRO:HG2	2.03	0.41
8:B:374:LEU:HD23	8:B:374:LEU:HA	1.82	0.41
9:C:1034:LYS:HB3	9:C:1034:LYS:HE2	1.89	0.41
10:D:166:LEU:HD13	10:D:178:LEU:HD21	2.02	0.41
13:G:427:LYS:HA	13:G:427:LYS:HD2	1.79	0.41
35:V:304:LEU:HB3	35:V:312:ILE:HD13	2.02	0.41
36:W:277:ASN:HB2	36:W:285:LEU:HD11	2.03	0.41
46:g:19:LEU:HB3	46:g:27:VAL:O	2.21	0.41
51:w:61:GLU:HG3	52:x:76:PHE:CZ	2.55	0.41
2:1:196:U:H2'	2:1:197:C:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:162:LYS:HD3	32:S:169:ARG:HH21	1.86	0.41
7:A:1157:ILE:HD13	7:A:1157:ILE:HA	1.86	0.41
7:A:2083:LEU:O	7:A:2087:THR:HG23	2.20	0.41
8:B:227:LEU:HD21	8:B:239:THR:HG23	2.02	0.41
8:B:481:MET:HE1	8:B:556:ASP:HB2	2.03	0.41
9:C:117:LEU:HB3	9:C:1032:GLU:HB3	2.03	0.41
9:C:1194:THR:HG22	9:C:1723:PRO:HG3	2.02	0.41
9:C:2103:ASN:HA	9:C:2123:SER:HA	2.02	0.41
12:F:462:LEU:HG	12:F:466:ARG:HH21	1.86	0.41
26:M:157:ARG:O	26:M:161:GLN:HG2	2.21	0.41
46:g:17:LEU:HA	46:g:71:GLU:O	2.20	0.41
2:1:206:C:N4	3:2:15:U:H3	2.18	0.41
6:6:9:U:H2'	6:6:10:G:H8	1.85	0.41
6:6:93:C:H2'	6:6:94:C:C6	2.55	0.41
7:A:543:ALA:HB2	7:A:651:TRP:HB3	2.01	0.41
9:C:151:LYS:HD2	9:C:151:LYS:HA	1.89	0.41
9:C:1973:ARG:HB2	9:C:1997:LEU:HD11	2.02	0.41
32:S:126:MET:HE3	32:S:126:MET:HB3	1.91	0.41
33:T:447:PRO:HA	33:T:450:ARG:HG3	2.02	0.41
35:V:570:LEU:HD23	35:V:570:LEU:HA	1.85	0.41
45:f:21:VAL:HG13	45:f:72:ILE:HG13	2.03	0.41
51:w:10:ARG:O	51:w:90:LEU:HA	2.20	0.41
1:0:-7:C:O5'	1:0:-7:C:H6	2.04	0.41
5:5:96:A:C4'	42:c:47:ARG:HH21	2.34	0.41
7:A:1607:GLU:HB2	7:A:1634:SER:HA	2.03	0.41
8:B:168:THR:HG23	8:B:184:THR:HB	2.03	0.41
9:C:557:LYS:HB2	9:C:557:LYS:HE3	1.92	0.41
9:C:572:ASP:HB3	9:C:575:LEU:HB3	2.03	0.41
9:C:786:HIS:CD2	9:C:789:MET:HE3	2.55	0.41
9:C:827:ILE:HG22	9:C:868:ILE:HD13	2.02	0.41
9:C:1075:PHE:O	9:C:1076:ALA:C	2.63	0.41
9:C:1129:LEU:HD12	9:C:1140:VAL:HG22	2.03	0.41
12:F:629:TYR:CG	12:F:663:HIS:HB3	2.55	0.41
18:L:132:ARG:NH2	26:M:162:ILE:HA	2.36	0.41
32:S:293:ARG:HA	32:S:312:ASP:OD1	2.20	0.41
34:U:58:LEU:HD12	34:U:59:ASP:N	2.36	0.41
35:V:391:PHE:O	35:V:395:GLU:HG2	2.21	0.41
35:V:392:MET:HE3	35:V:392:MET:HB3	1.89	0.41
54:z:151:LYS:HE2	54:z:155:GLU:HB3	2.02	0.41
7:A:380:LEU:HD23	7:A:380:LEU:HA	1.96	0.41
10:D:92:LEU:HD12	10:D:103:ALA:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:J:1:MET:HB2	16:J:2:ALA:H	1.56	0.41
40:a:40:LEU:HD11	40:a:77:LEU:HD22	2.01	0.41
44:e:85:THR:HG22	46:g:66:SER:HB2	2.02	0.41
3:2:17:A:H2'	3:2:18:G:H8	1.86	0.41
5:5:31:U:H2'	5:5:32:C:C6	2.56	0.41
5:5:95:G:C6	45:f:24:LYS:HB3	2.55	0.41
7:A:43:LYS:HB3	7:A:43:LYS:HE2	1.82	0.41
7:A:599:MET:O	7:A:603:ARG:HG3	2.21	0.41
7:A:1074:PHE:CD2	7:A:1080:GLU:HG2	2.55	0.41
9:C:426:LYS:H	9:C:426:LYS:HG2	1.50	0.41
9:C:630:ALA:HB2	9:C:893:MET:HE1	2.02	0.41
9:C:850:LEU:HD23	9:C:850:LEU:HA	1.95	0.41
9:C:1036:GLU:OE2	9:C:1072:LEU:HD12	2.21	0.41
9:C:1294:LYS:HA	9:C:1294:LYS:HD3	1.84	0.41
12:F:536:GLU:H	12:F:536:GLU:HG2	1.71	0.41
16:J:107:SER:HB3	16:J:108:LYS:H	1.76	0.41
18:L:81:TYR:HD2	18:L:89:VAL:HG21	1.85	0.41
26:M:73:LEU:HD23	26:M:73:LEU:HA	1.95	0.41
32:S:156:GLN:HA	32:S:157:PRO:HD3	1.94	0.41
32:S:190:LEU:HD12	32:S:190:LEU:HA	1.93	0.41
32:S:192:LYS:HG3	38:Y:81:ALA:HB1	2.01	0.41
33:T:481:ALA:O	33:T:484:LYS:HG2	2.21	0.41
33:T:933:LYS:HD3	33:T:933:LYS:HA	1.93	0.41
33:T:995:MET:HE3	33:T:999:LEU:HG	2.02	0.41
33:T:1041:ASP:HA	33:T:1044:THR:HB	2.02	0.41
35:V:159:TRP:CD1	35:V:385:PHE:HB2	2.54	0.41
35:V:596:LEU:HD12	35:V:596:LEU:HA	1.85	0.41
41:b:25:VAL:HG13	41:b:43:VAL:HG13	2.03	0.41
42:c:43:LEU:HD11	42:c:51:LYS:HB3	2.03	0.41
50:v:115:THR:HG23	50:v:118:LEU:H	1.86	0.41
50:v:189:ALA:H	50:v:218:SER:HB2	1.85	0.41
5:5:36:C:H2'	5:5:37:G:C8	2.56	0.41
7:A:2218:PHE:HD1	7:A:2218:PHE:HA	1.81	0.41
8:B:140:HIS:CD2	8:B:230:ASP:HB2	2.55	0.41
8:B:666:VAL:HG22	8:B:787:VAL:HG23	2.03	0.41
9:C:641:MET:HE2	9:C:641:MET:HB2	1.98	0.41
11:E:48:ALA:O	11:E:52:GLU:HG2	2.21	0.41
12:F:637:LYS:HG2	12:F:638:ARG:HH21	1.85	0.41
12:F:740:PHE:O	12:F:744:GLN:HG2	2.21	0.41
12:F:782:GLU:HB3	54:z:180:ARG:HH21	1.85	0.41
33:T:1036:HIS:CE1	33:T:1140:ALA:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:V:171:ASN:HB3	50:v:276:THR:O	2.21	0.41
42:c:43:LEU:HD13	42:c:53:LEU:HG	2.03	0.41
42:c:56:VAL:HG13	42:c:65:MET:HB2	2.02	0.41
50:v:100:LEU:HD23	50:v:100:LEU:HA	1.86	0.41
52:x:113:LEU:HD13	52:x:114:LYS:O	2.21	0.41
7:A:1288:LEU:HD13	7:A:1330:MET:HG2	2.03	0.40
7:A:1827:TRP:HB3	7:A:1833:LEU:HD11	2.02	0.40
8:B:603:MET:HB2	8:B:651:ILE:HD11	2.03	0.40
10:D:253:ASN:HB2	10:D:291:CYS:SG	2.60	0.40
13:G:409:GLU:H	13:G:409:GLU:HG2	1.58	0.40
33:T:663:ASP:HB2	33:T:693:HIS:HB3	2.02	0.40
33:T:755:ASP:HB3	33:T:758:ASP:HB2	2.03	0.40
50:v:79:ILE:HG13	50:v:238:ARG:HA	2.02	0.40
50:v:112:LEU:HD11	50:v:204:VAL:HG21	2.04	0.40
50:v:224:GLU:O	50:v:227:GLU:HG2	2.21	0.40
50:v:355:PRO:HG3	50:v:364:ARG:NE	2.36	0.40
5:5:14:U:H2'	5:5:15:C:H6	1.86	0.40
7:A:273:ILE:H	7:A:273:ILE:HG12	1.54	0.40
7:A:2014:MET:HA	37:X:758:ARG:HH11	1.85	0.40
9:C:1916:LEU:HD23	9:C:1916:LEU:HA	1.89	0.40
10:D:336:HIS:HB3	10:D:339:GLU:O	2.22	0.40
12:F:656:ILE:HD13	12:F:656:ILE:HA	1.91	0.40
16:J:115:LYS:HB2	16:J:115:LYS:HE3	1.87	0.40
16:J:291:LEU:HD23	16:J:291:LEU:HA	1.89	0.40
32:S:43:ARG:CZ	32:S:51:GLU:HB2	2.51	0.40
32:S:331:ALA:HB2	32:S:350:LEU:HD11	2.04	0.40
2:1:196:U:H2'	2:1:197:C:H6	1.87	0.40
7:A:648:LEU:HD23	7:A:648:LEU:HA	1.79	0.40
9:C:969:LEU:HD13	9:C:998:VAL:HG11	2.03	0.40
9:C:1378:TYR:HA	9:C:1452:VAL:O	2.21	0.40
12:F:734:TYR:C	12:F:736:THR:H	2.29	0.40
13:G:431:ARG:HH11	16:J:10:PRO:HG3	1.86	0.40
26:M:37:LEU:HD23	26:M:76:PHE:HB2	2.02	0.40
33:T:977:GLY:O	33:T:980:MET:HB2	2.21	0.40
35:V:186:LEU:HD11	35:V:405:ILE:HG21	2.04	0.40
35:V:235:LYS:HD3	35:V:370:LEU:HD21	2.04	0.40
50:v:126:LEU:HD23	50:v:126:LEU:HA	1.95	0.40
52:x:68:ARG:HG2	52:x:73:TRP:CH2	2.56	0.40
2:1:195:U:H2'	2:1:196:U:H6	1.87	0.40
4:4:197:GLU:HG2	4:4:200:THR:H	1.85	0.40
7:A:1555:LEU:HD21	7:A:1570:LYS:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1937:ILE:HD13	7:A:1937:ILE:HA	1.81	0.40
10:D:308:PHE:HE1	10:D:324:PRO:HB3	1.85	0.40
26:M:35:GLN:H	26:M:35:GLN:HG2	1.55	0.40
26:M:63:LEU:HD21	26:M:94:ILE:HD11	2.03	0.40
33:T:1032:LYS:HG2	33:T:1036:HIS:CD2	2.57	0.40
34:U:55:PRO:HA	34:U:58:LEU:CG	2.51	0.40
36:W:302:PRO:HG2	36:W:346:HIS:ND1	2.37	0.40
44:e:30:ARG:HB3	44:e:90:VAL:HA	2.04	0.40
44:e:36:TYR:HD2	44:e:85:THR:HG23	1.86	0.40
50:v:297:MET:HA	50:v:297:MET:HE3	2.03	0.40
4:4:184:TYR:HB3	4:4:192:SER:H	1.86	0.40
7:A:1038:SER:O	7:A:1042:GLN:HG2	2.20	0.40
8:B:696:LEU:HD21	8:B:718:PHE:CE1	2.55	0.40
8:B:772:TRP:CG	8:B:813:ARG:HD3	2.56	0.40
9:C:905:ILE:HD13	9:C:970:VAL:HG21	2.03	0.40
9:C:1407:LEU:HD23	9:C:1426:ILE:HB	2.02	0.40
9:C:1964:PRO:HD2	9:C:2007:VAL:HG12	2.02	0.40
12:F:67:SER:O	12:F:71:TRP:CB	2.70	0.40
12:F:747:LYS:HZ1	12:F:774:GLN:HB2	1.85	0.40
16:J:202:MET:HE1	18:L:61:GLU:HB3	2.04	0.40
16:J:222:PRO:HA	16:J:223:PRO:HD2	1.96	0.40
18:L:41:ILE:HD12	18:L:41:ILE:HA	1.91	0.40
42:c:109:VAL:HB	45:f:63:LEU:HB2	2.03	0.40
51:w:7:PHE:CE1	51:w:9:LEU:HB2	2.56	0.40
51:w:112:VAL:HG13	51:w:121:LEU:HB3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	4	403/646 (62%)	396 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	A	2277/2335 (98%)	2203 (97%)	74 (3%)	0	100	100
8	B	898/972 (92%)	832 (93%)	62 (7%)	4 (0%)	30	65
9	C	1917/2136 (90%)	1824 (95%)	87 (4%)	6 (0%)	36	70
10	D	306/357 (86%)	298 (97%)	8 (3%)	0	100	100
11	E	596/802 (74%)	583 (98%)	13 (2%)	0	100	100
12	F	733/855 (86%)	695 (95%)	36 (5%)	2 (0%)	36	70
13	G	637/848 (75%)	611 (96%)	26 (4%)	0	100	100
14	H	42/166 (25%)	38 (90%)	4 (10%)	0	100	100
15	I	46/285 (16%)	45 (98%)	1 (2%)	0	100	100
16	J	227/536 (42%)	206 (91%)	18 (8%)	3 (1%)	9	38
17	K	400/514 (78%)	382 (96%)	18 (4%)	0	100	100
18	L	137/367 (37%)	133 (97%)	4 (3%)	0	100	100
19	L2	93/95 (98%)	88 (95%)	5 (5%)	0	100	100
20	L3	83/102 (81%)	82 (99%)	1 (1%)	0	100	100
21	L4	78/139 (56%)	75 (96%)	3 (4%)	0	100	100
22	L5	80/91 (88%)	74 (92%)	6 (8%)	0	100	100
23	L6	73/80 (91%)	70 (96%)	3 (4%)	0	100	100
24	L7	87/103 (84%)	85 (98%)	2 (2%)	0	100	100
25	L8	94/96 (98%)	92 (98%)	2 (2%)	0	100	100
26	M	171/198 (86%)	163 (95%)	7 (4%)	1 (1%)	21	56
27	N	94/229 (41%)	85 (90%)	9 (10%)	0	100	100
28	O	157/166 (95%)	149 (95%)	8 (5%)	0	100	100
29	P	77/301 (26%)	76 (99%)	1 (1%)	0	100	100
30	Q	1319/1485 (89%)	1289 (98%)	30 (2%)	0	100	100
31	R	159/161 (99%)	157 (99%)	2 (1%)	0	100	100
32	S	268/586 (46%)	253 (94%)	15 (6%)	0	100	100
33	T	776/1220 (64%)	714 (92%)	61 (8%)	1 (0%)	48	80
34	U	126/2752 (5%)	123 (98%)	2 (2%)	1 (1%)	16	50
35	V	460/908 (51%)	452 (98%)	6 (1%)	2 (0%)	30	65
36	W	344/544 (63%)	314 (91%)	30 (9%)	0	100	100
37	X	140/758 (18%)	133 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	Y	57/112 (51%)	56 (98%)	1 (2%)	0	100	100
39	Z	29/415 (7%)	21 (72%)	8 (28%)	0	100	100
40	a	69/240 (29%)	69 (100%)	0	0	100	100
40	h	69/240 (29%)	69 (100%)	0	0	100	100
41	b	80/119 (67%)	78 (98%)	2 (2%)	0	100	100
41	i	79/119 (66%)	76 (96%)	3 (4%)	0	100	100
42	c	94/118 (80%)	92 (98%)	2 (2%)	0	100	100
42	j	94/118 (80%)	90 (96%)	4 (4%)	0	100	100
43	d	83/126 (66%)	81 (98%)	2 (2%)	0	100	100
43	k	79/126 (63%)	74 (94%)	5 (6%)	0	100	100
44	e	75/92 (82%)	72 (96%)	3 (4%)	0	100	100
44	l	75/92 (82%)	75 (100%)	0	0	100	100
45	f	71/86 (83%)	69 (97%)	2 (3%)	0	100	100
45	m	71/86 (83%)	71 (100%)	0	0	100	100
46	g	72/76 (95%)	66 (92%)	5 (7%)	1 (1%)	9	36
46	n	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
47	p	48/476 (10%)	47 (98%)	1 (2%)	0	100	100
48	q	135/504 (27%)	133 (98%)	2 (2%)	0	100	100
48	r	133/504 (26%)	130 (98%)	3 (2%)	0	100	100
48	s	136/504 (27%)	134 (98%)	2 (2%)	0	100	100
48	t	134/504 (27%)	131 (98%)	3 (2%)	0	100	100
49	u	223/225 (99%)	213 (96%)	10 (4%)	0	100	100
50	v	388/411 (94%)	373 (96%)	15 (4%)	0	100	100
51	w	142/146 (97%)	139 (98%)	3 (2%)	0	100	100
52	x	89/174 (51%)	84 (94%)	5 (6%)	0	100	100
53	y	143/413 (35%)	141 (99%)	2 (1%)	0	100	100
54	z	112/233 (48%)	105 (94%)	7 (6%)	0	100	100
All	All	16150/27168 (59%)	15479 (96%)	650 (4%)	21 (0%)	49	80

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	C	480	THR

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Mol	Chain	Res	Type
9	C	1996	LEU
12	F	354	PRO
35	V	559	SER
8	B	371	GLU
8	B	756	LYS
9	C	1412	THR
9	C	1439	TRP
16	J	98	TYR
16	J	261	THR
34	U	136	ARG
8	B	535	ALA
9	C	531	ILE
16	J	104	GLN
26	M	27	THR
33	T	1189	LEU
46	g	21	LEU
9	C	697	ALA
35	V	353	ILE
8	B	710	ASN
12	F	554	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	4	363/572 (64%)	362 (100%)	1 (0%)	86	91
7	A	2063/2108 (98%)	2032 (98%)	31 (2%)	57	80
8	B	800/866 (92%)	776 (97%)	24 (3%)	36	69
9	C	1617/1908 (85%)	1605 (99%)	12 (1%)	76	86
10	D	264/300 (88%)	263 (100%)	1 (0%)	84	90
11	E	245/709 (35%)	238 (97%)	7 (3%)	37	70
12	F	327/749 (44%)	324 (99%)	3 (1%)	70	85
13	G	299/751 (40%)	296 (99%)	3 (1%)	68	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	H	26/143 (18%)	26 (100%)	0	100	100
16	J	171/457 (37%)	170 (99%)	1 (1%)	78	88
17	K	297/441 (67%)	292 (98%)	5 (2%)	53	78
18	L	119/326 (36%)	119 (100%)	0	100	100
26	M	135/171 (79%)	132 (98%)	3 (2%)	45	74
27	N	91/203 (45%)	88 (97%)	3 (3%)	33	67
32	S	240/520 (46%)	232 (97%)	8 (3%)	33	67
33	T	692/1085 (64%)	682 (99%)	10 (1%)	59	80
34	U	63/2432 (3%)	63 (100%)	0	100	100
35	V	420/838 (50%)	415 (99%)	5 (1%)	63	82
36	W	301/460 (65%)	296 (98%)	5 (2%)	53	78
37	X	126/655 (19%)	123 (98%)	3 (2%)	43	73
38	Y	53/99 (54%)	48 (91%)	5 (9%)	8	32
39	Z	25/366 (7%)	24 (96%)	1 (4%)	28	62
40	a	67/177 (38%)	66 (98%)	1 (2%)	57	80
41	b	77/101 (76%)	76 (99%)	1 (1%)	61	81
42	c	93/110 (84%)	91 (98%)	2 (2%)	45	74
43	d	74/101 (73%)	74 (100%)	0	100	100
44	e	72/84 (86%)	68 (94%)	4 (6%)	19	52
45	f	61/74 (82%)	60 (98%)	1 (2%)	55	79
46	g	64/66 (97%)	62 (97%)	2 (3%)	35	68
47	p	1/395 (0%)	1 (100%)	0	100	100
50	v	345/361 (96%)	340 (99%)	5 (1%)	59	80
51	w	132/134 (98%)	126 (96%)	6 (4%)	24	59
52	x	76/143 (53%)	75 (99%)	1 (1%)	61	81
53	y	5/368 (1%)	5 (100%)	0	100	100
54	z	98/209 (47%)	96 (98%)	2 (2%)	48	76
All	All	9902/18482 (54%)	9746 (98%)	156 (2%)	54	79

All (156) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	4	389	VAL

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Mol	Chain	Res	Type
7	A	54	VAL
7	A	57	GLN
7	A	61	MET
7	A	97	HIS
7	A	229	GLN
7	A	273	ILE
7	A	371	LEU
7	A	535	ARG
7	A	569	VAL
7	A	621	VAL
7	A	682	ASP
7	A	690	MET
7	A	703	GLN
7	A	978	GLU
7	A	980	ARG
7	A	1030	ILE
7	A	1165	VAL
7	A	1284	LEU
7	A	1438	VAL
7	A	1505	LYS
7	A	1541	THR
7	A	1609	VAL
7	A	1613	THR
7	A	1767	ASN
7	A	1768	TYR
7	A	1791	HIS
7	A	1961	ILE
7	A	2028	GLU
7	A	2036	GLN
7	A	2223	CYS
7	A	2261	MET
8	B	95	LYS
8	B	162	ASP
8	B	165	LEU
8	B	213	ASP
8	B	215	VAL
8	B	293	SER
8	B	298	LEU
8	B	300	LEU
8	B	319	THR
8	B	375	GLU
8	B	389	ASP

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Mol	Chain	Res	Type
8	B	422	LYS
8	B	475	MET
8	B	486	ASP
8	B	571	ASN
8	B	610	VAL
8	B	683	ASN
8	B	692	LEU
8	B	733	TRP
8	B	735	PHE
8	B	835	GLU
8	B	945	GLU
8	B	949	ILE
8	B	953	PHE
9	C	425	ASN
9	C	517	MET
9	C	609	VAL
9	C	673	LEU
9	C	847	LEU
9	C	883	LEU
9	C	964	LEU
9	C	1072	LEU
9	C	1271	VAL
9	C	1320	LEU
9	C	1967	THR
9	C	1982	VAL
10	D	157	CYS
11	E	4	ILE
11	E	10	VAL
11	E	104	LEU
11	E	201	LYS
11	E	302	ILE
11	E	363	LEU
11	E	517	ASP
12	F	441	GLU
12	F	553	VAL
12	F	769	MET
13	G	225	LEU
13	G	270	ASP
13	G	482	GLU
16	J	278	VAL
17	K	220	VAL
17	K	252	VAL

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Mol	Chain	Res	Type
17	K	360	VAL
17	K	450	VAL
17	K	478	LEU
26	M	27	THR
26	M	30	GLN
26	M	72	THR
27	N	193	VAL
27	N	199	LYS
27	N	208	LYS
32	S	52	VAL
32	S	70	VAL
32	S	97	SER
32	S	111	ILE
32	S	127	THR
32	S	133	CYS
32	S	324	MET
32	S	362	GLU
33	T	442	VAL
33	T	602	LEU
33	T	646	ILE
33	T	705	VAL
33	T	851	ILE
33	T	898	LYS
33	T	1035	PHE
33	T	1036	HIS
33	T	1103	VAL
33	T	1189	LEU
35	V	181	ILE
35	V	218	LEU
35	V	392	MET
35	V	452	LEU
35	V	576	THR
36	W	225	LEU
36	W	272	THR
36	W	290	LEU
36	W	488	LEU
36	W	490	THR
37	X	685	LEU
37	X	691	THR
37	X	734	HIS
38	Y	55	LEU
38	Y	59	THR

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Mol	Chain	Res	Type
38	Y	97	ASP
38	Y	100	THR
38	Y	105	ILE
39	Z	353	VAL
40	a	66	VAL
41	b	45	MET
42	c	11	MET
42	c	115	ILE
44	e	39	VAL
44	e	48	ILE
44	e	85	THR
44	e	86	LEU
45	f	59	LEU
46	g	42	ILE
46	g	60	VAL
50	v	73	ILE
50	v	186	LEU
50	v	202	TYR
50	v	286	THR
50	v	331	LEU
51	w	8	TYR
51	w	46	VAL
51	w	55	HIS
51	w	67	ASP
51	w	133	CYS
51	w	138	LEU
52	x	90	HIS
54	z	134	PHE
54	z	144	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (85) such sidechains are listed below:

Mol	Chain	Res	Type
4	4	334	GLN
7	A	38	GLN
7	A	243	ASN
7	A	400	ASN
7	A	461	HIS
7	A	793	ASN
7	A	957	GLN
7	A	1014	ASN
7	A	1122	ASN

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Mol	Chain	Res	Type
7	A	1363	GLN
7	A	1367	ASN
7	A	1450	GLN
7	A	1767	ASN
7	A	1944	HIS
7	A	1946	ASN
7	A	1995	ASN
7	A	2276	GLN
8	B	505	GLN
8	B	807	GLN
9	C	573	HIS
9	C	678	ASN
9	C	726	HIS
9	C	786	HIS
9	C	820	ASN
9	C	902	ASN
9	C	980	GLN
9	C	1086	GLN
9	C	1113	ASN
9	C	1250	HIS
9	C	1480	GLN
9	C	1568	GLN
9	C	1749	GLN
9	C	1814	ASN
9	C	1933	ASN
9	C	1965	HIS
9	C	2003	GLN
10	D	287	ASN
11	E	81	GLN
11	E	231	ASN
13	G	275	ASN
13	G	291	GLN
13	G	479	GLN
16	J	133	GLN
16	J	231	HIS
16	J	242	GLN
16	J	279	HIS
17	K	329	HIS
18	L	15	HIS
18	L	17	GLN
26	M	30	GLN
26	M	55	GLN

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Mol	Chain	Res	Type
32	S	85	GLN
32	S	174	ASN
33	T	576	GLN
33	T	581	ASN
33	T	1036	HIS
33	T	1037	GLN
33	T	1054	ASN
33	T	1104	GLN
33	T	1152	HIS
34	U	60	HIS
34	U	132	ASN
35	V	174	ASN
35	V	183	GLN
35	V	262	HIS
35	V	270	HIS
35	V	390	ASN
35	V	609	GLN
36	W	277	ASN
37	X	732	HIS
38	Y	93	ASN
40	a	22	GLN
40	a	76	ASN
41	b	64	ASN
42	c	39	ASN
42	c	49	ASN
43	d	57	GLN
43	d	79	ASN
46	g	65	ASN
50	v	71	GLN
50	v	81	GLN
50	v	108	GLN
51	w	88	GLN
51	w	113	ASN
54	z	126	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	24/57 (42%)	10 (41%)	2 (8%)
2	1	52/277 (18%)	26 (50%)	3 (5%)
3	2	40/150 (26%)	9 (22%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	5	107/117 (91%)	25 (23%)	1 (0%)
6	6	110/125 (88%)	31 (28%)	2 (1%)
All	All	333/726 (45%)	101 (30%)	8 (2%)

All (101) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	-24	A
1	0	-17	A
1	0	-15	C
1	0	-14	C
1	0	-13	G
1	0	-11	C
1	0	-7	C
1	0	-6	U
1	0	-4	C
1	0	-1	G
2	1	11	U
2	1	12	A
2	1	13	A
2	1	15	C
2	1	17	U
2	1	18	G
2	1	19	U
2	1	20	A
2	1	21	G
2	1	22	A
2	1	186	A
2	1	187	U
2	1	188	G
2	1	189	A
2	1	190	U
2	1	191	G
2	1	194	U
2	1	195	U
2	1	196	U
2	1	202	A
2	1	206	C
2	1	207	A
2	1	213	G
2	1	218	C
2	1	219	G

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Mol	Chain	Res	Type
2	1	220	C
3	2	2	U
3	2	6	U
3	2	7	U
3	2	8	A
3	2	13	U
3	2	14	A
3	2	15	U
3	2	30	A
3	2	77	U
5	5	8	G
5	5	9	G
5	5	20	G
5	5	21	A
5	5	22	U
5	5	24	G
5	5	35	U
5	5	45	C
5	5	53	U
5	5	71	C
5	5	72	U
5	5	73	C
5	5	77	G
5	5	78	U
5	5	87	A
5	5	88	A
5	5	90	U
5	5	94	U
5	5	95	G
5	5	98	G
5	5	105	U
5	5	106	U
5	5	107	U
5	5	108	G
5	5	115	C
6	6	19	G
6	6	21	A
6	6	27	G
6	6	33	C
6	6	38	G
6	6	46	U
6	6	47	G

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Mol	Chain	Res	Type
6	6	63	C
6	6	66	G
6	6	67	A
6	6	68	C
6	6	70	A
6	6	71	C
6	6	72	A
6	6	74	G
6	6	76	A
6	6	78	A
6	6	86	G
6	6	99	A
6	6	100	C
6	6	101	U
6	6	109	A
6	6	110	U
6	6	111	C
6	6	116	C
6	6	117	A
6	6	118	U
6	6	120	G
6	6	121	U
6	6	122	U
6	6	124	U

All (8) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	-7	C
1	0	-2	A
2	1	17	U
2	1	186	A
2	1	195	U
5	5	105	U
6	6	65	U
6	6	121	U

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are 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
16	SEP	J	224	16	8,9,10	1.51	1 (12%)	8,12,14	1.68	2 (25%)
16	SEP	J	232	16	8,9,10	1.54	1 (12%)	8,12,14	1.72	2 (25%)

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
16	SEP	J	224	16	-	0/5/8/10	-
16	SEP	J	232	16	-	3/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	J	232	SEP	P-O1P	3.30	1.61	1.50
16	J	224	SEP	P-O1P	3.29	1.61	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	J	232	SEP	P-OG-CB	-3.37	109.00	118.30
16	J	224	SEP	P-OG-CB	-3.19	109.50	118.30
16	J	232	SEP	OG-CB-CA	3.01	111.07	108.14
16	J	224	SEP	OG-CB-CA	2.97	111.03	108.14

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	J	232	SEP	CB-OG-P-O2P
16	J	232	SEP	CB-OG-P-O3P
16	J	232	SEP	CB-OG-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 12 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
59	ADP	C	2202	55	27,29,29	1.35	4 (14%)	42,45,45	1.96	11 (26%)
57	IHP	A	3000	-	36,36,36	1.82	6 (16%)	54,60,60	1.36	5 (9%)
61	ATP	v	702	55	29,33,33	0.31	0	44,52,52	0.52	1 (2%)
58	GTP	B	1501	55	30,34,34	0.97	1 (3%)	46,54,54	1.75	10 (21%)
59	ADP	C	2201	-	27,29,29	1.36	4 (14%)	42,45,45	1.95	10 (23%)

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
59	ADP	C	2202	55	-	3/16/32/32	0/3/3/3
57	IHP	A	3000	-	-	3/30/54/54	0/1/1/1
61	ATP	v	702	55	-	1/22/38/38	0/3/3/3
58	GTP	B	1501	55	-	4/22/38/38	0/3/3/3
59	ADP	C	2201	-	-	3/16/32/32	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	A	3000	IHP	P2-O12	4.94	1.68	1.59
59	C	2201	ADP	C5-C4	4.57	1.47	1.39
59	C	2202	ADP	C5-C4	4.52	1.47	1.39
57	A	3000	IHP	P5-O15	4.17	1.67	1.59
57	A	3000	IHP	P6-O16	3.99	1.66	1.59
57	A	3000	IHP	P4-O14	3.94	1.66	1.59
57	A	3000	IHP	P3-O13	3.60	1.66	1.59
57	A	3000	IHP	P1-O11	3.59	1.66	1.59
59	C	2201	ADP	C5-C6	2.71	1.48	1.41
59	C	2202	ADP	C5-C6	2.67	1.48	1.41
59	C	2201	ADP	C8-N7	2.45	1.36	1.31
59	C	2202	ADP	C8-N7	2.42	1.36	1.31
58	B	1501	GTP	C5-N7	-2.18	1.34	1.39
59	C	2201	ADP	C5-N7	-2.15	1.35	1.39
59	C	2202	ADP	C5-N7	-2.14	1.35	1.39

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	C	2201	ADP	C5-C4-N3	-6.16	118.72	126.75
59	C	2202	ADP	C5-C4-N3	-6.11	118.77	126.75
57	A	3000	IHP	O13-C3-C2	4.82	120.05	108.69
59	C	2202	ADP	N3-C4-N9	4.78	134.96	127.08
59	C	2201	ADP	N3-C4-N9	4.76	134.93	127.08
58	B	1501	GTP	C5-C4-N3	-4.70	120.84	128.46
58	B	1501	GTP	C2-N3-C4	4.40	120.14	112.30
58	B	1501	GTP	PA-O3A-PB	-3.88	119.52	132.83
59	C	2201	ADP	C2-N3-C4	3.86	120.87	111.75
59	C	2202	ADP	C2-N3-C4	3.83	120.80	111.75
57	A	3000	IHP	O12-C2-C3	3.66	117.33	108.69
57	A	3000	IHP	C3-C2-C1	-3.43	102.90	110.41
59	C	2202	ADP	PA-O3A-PB	-3.32	121.44	132.83
59	C	2201	ADP	PA-O3A-PB	-3.32	121.45	132.83
59	C	2201	ADP	C4-C5-N7	-3.29	106.61	110.62
58	B	1501	GTP	PB-O3B-PG	-3.28	121.57	132.83
59	C	2202	ADP	C4-C5-N7	-3.28	106.62	110.62
59	C	2202	ADP	N3-C2-N1	-3.18	123.63	128.60
59	C	2201	ADP	N3-C2-N1	-3.17	123.64	128.60
58	B	1501	GTP	N9-C4-N3	3.03	132.01	125.94
59	C	2202	ADP	C5-N7-C8	2.79	107.47	103.51
58	B	1501	GTP	N9-C8-N7	-2.76	108.18	113.39
59	C	2201	ADP	C5-N7-C8	2.75	107.42	103.51
58	B	1501	GTP	C2-N1-C6	-2.69	120.20	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	B	1501	GTP	C5-C6-N1	2.62	119.84	113.19
59	C	2202	ADP	C4-N9-C8	2.61	108.56	105.73
59	C	2201	ADP	C4-N9-C8	2.47	108.41	105.73
58	B	1501	GTP	C8-N7-C5	2.43	108.64	104.24
57	A	3000	IHP	C5-C4-C3	-2.43	105.09	110.41
59	C	2202	ADP	C3'-C2'-C1'	2.38	105.94	101.43
59	C	2201	ADP	C3'-C2'-C1'	2.36	105.91	101.43
58	B	1501	GTP	O6-C6-C5	-2.33	120.41	126.60
59	C	2201	ADP	C6-C5-N7	2.21	136.13	132.02
57	A	3000	IHP	O11-C1-C2	2.21	113.89	108.69
59	C	2202	ADP	C6-C5-N7	2.18	136.08	132.02
59	C	2202	ADP	N9-C8-N7	-2.07	111.08	113.91
61	v	702	ATP	PB-O3B-PG	2.05	139.85	132.83

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	A	3000	IHP	C2-C3-O13-P3
57	A	3000	IHP	C3-O13-P3-O33
57	A	3000	IHP	C6-O16-P6-O46
58	B	1501	GTP	C5'-O5'-PA-O1A
59	C	2201	ADP	C5'-O5'-PA-O1A
59	C	2201	ADP	C5'-O5'-PA-O3A
59	C	2202	ADP	C5'-O5'-PA-O3A
58	B	1501	GTP	O4'-C4'-C5'-O5'
58	B	1501	GTP	C3'-C4'-C5'-O5'
59	C	2202	ADP	C3'-C4'-C5'-O5'
58	B	1501	GTP	C5'-O5'-PA-O3A
59	C	2202	ADP	C5'-O5'-PA-O1A
61	v	702	ATP	PB-O3A-PA-O2A
59	C	2201	ADP	O4'-C4'-C5'-O5'

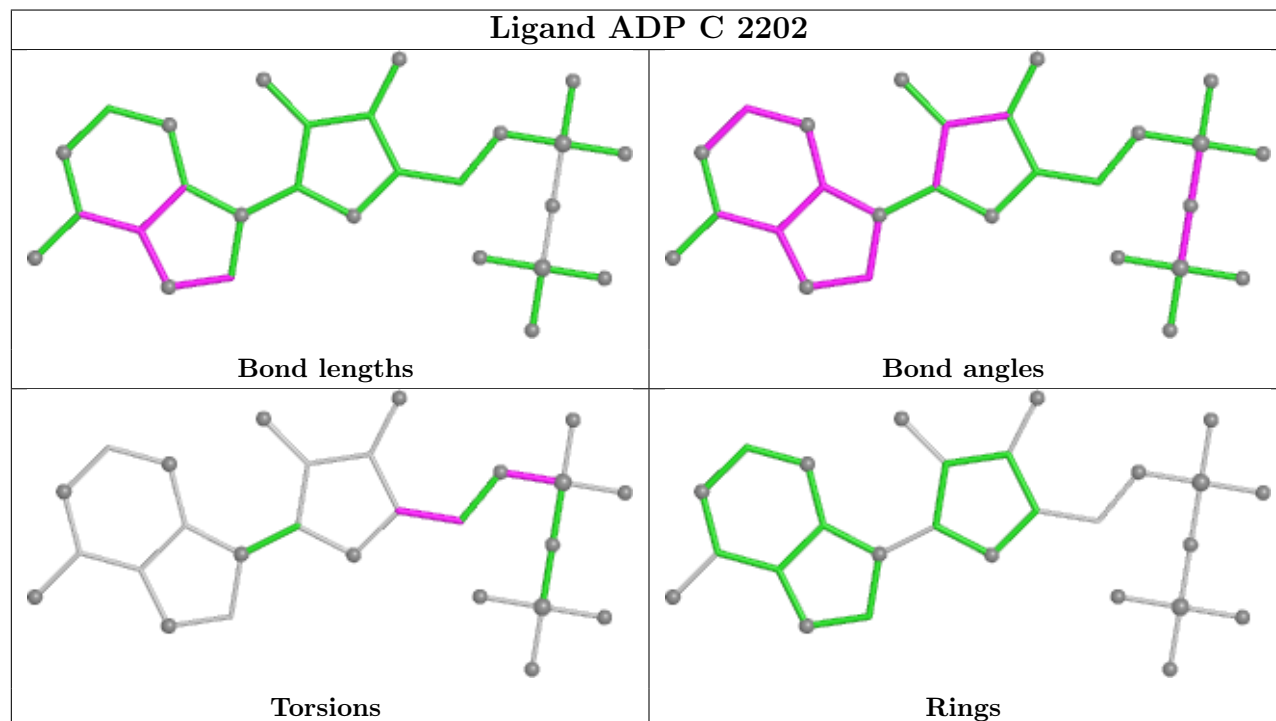
There are no ring outliers.

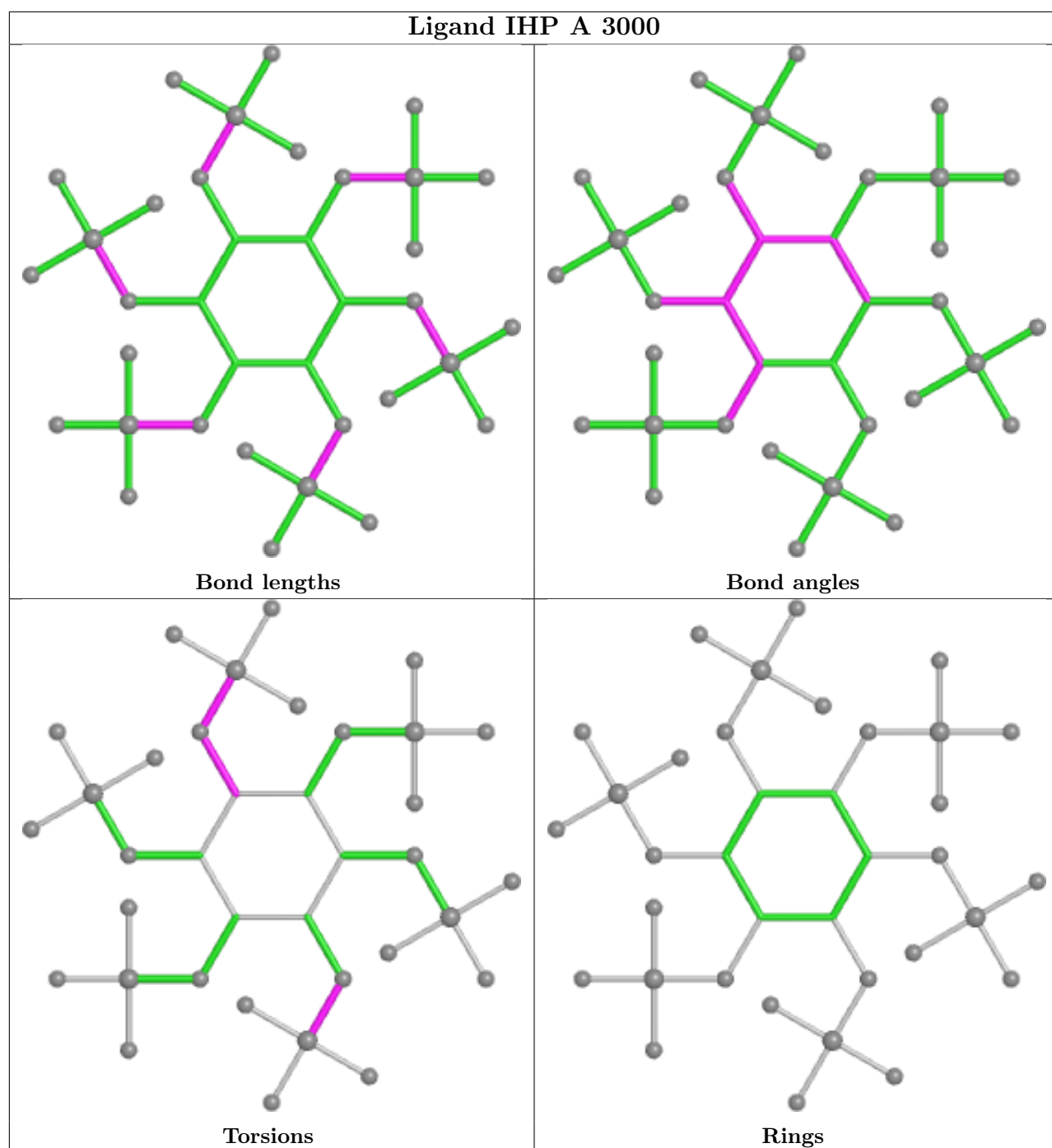
1 monomer is involved in 1 short contact:

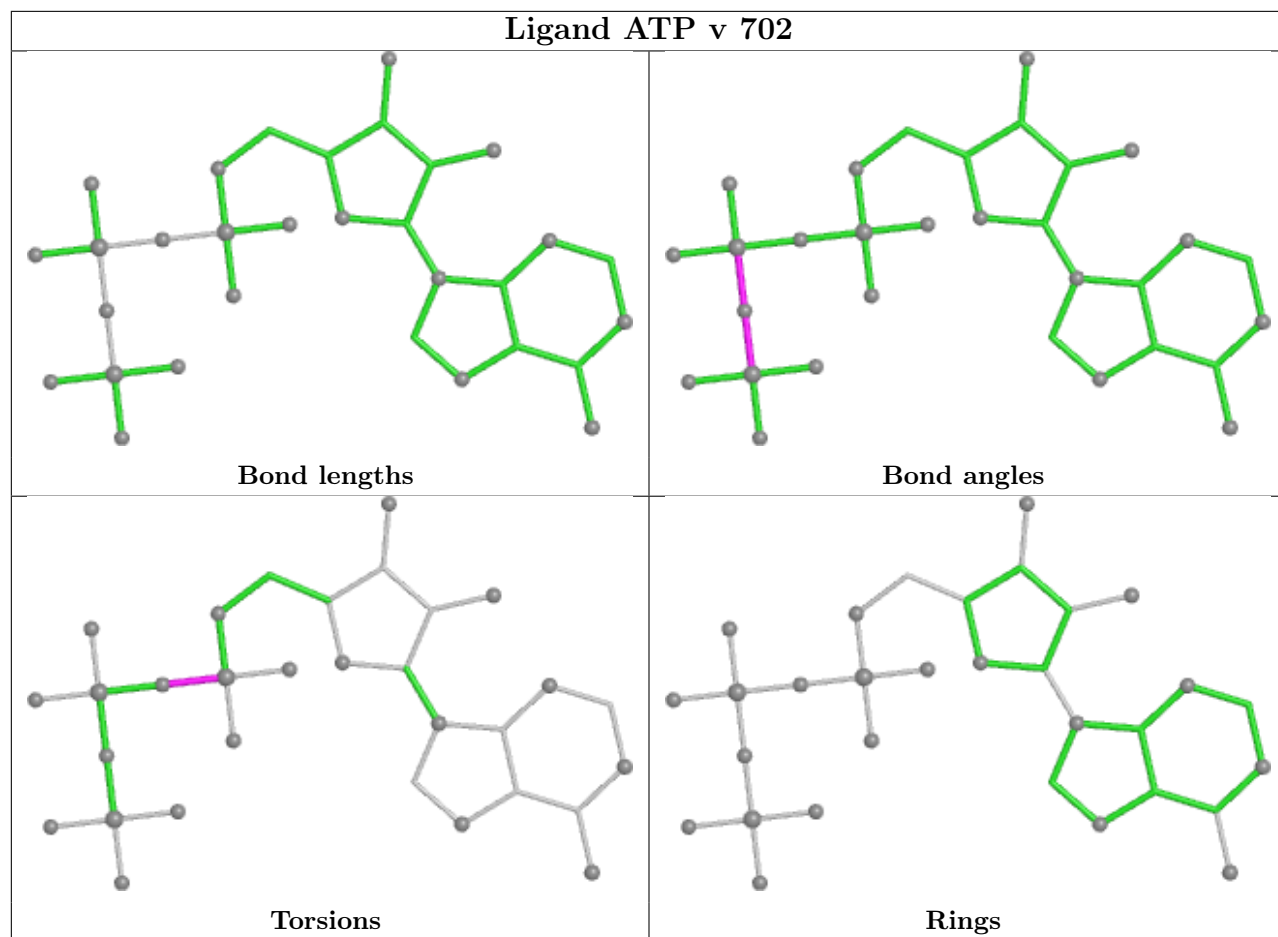
Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	B	1501	GTP	1	0

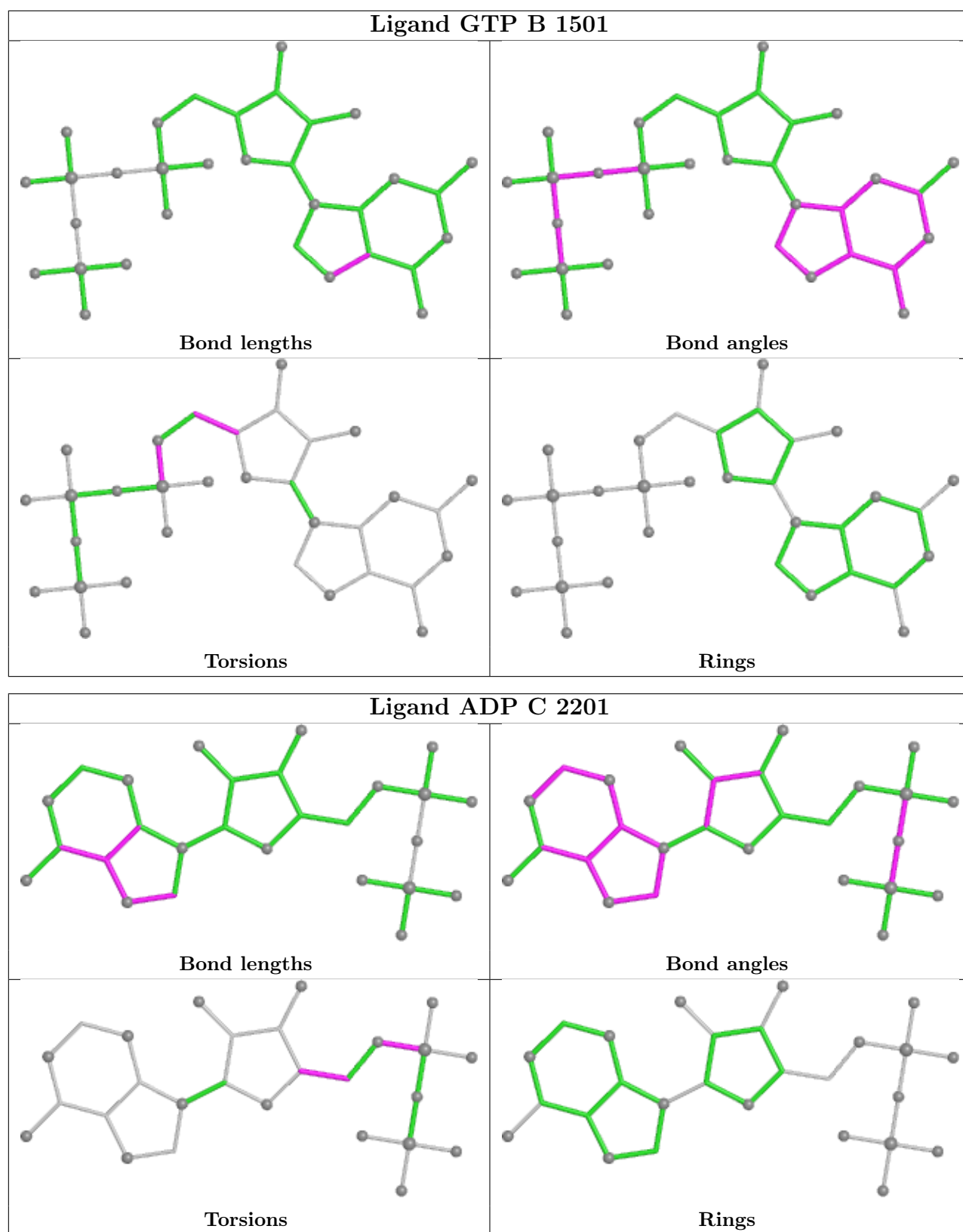
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

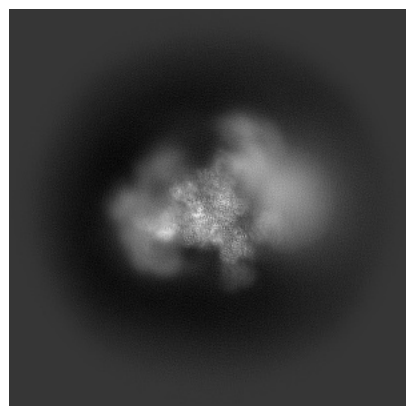
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-67263. These allow visual inspection of the internal detail of the map and identification of artifacts.

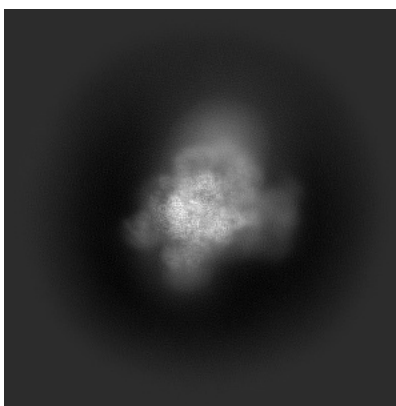
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

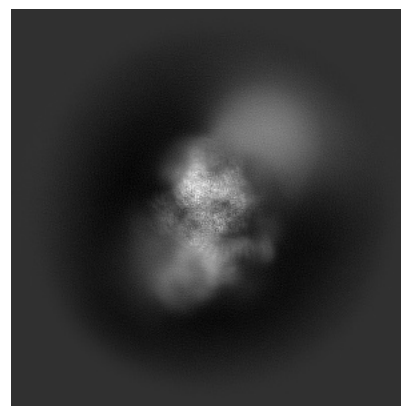
6.1.1 Primary map



X

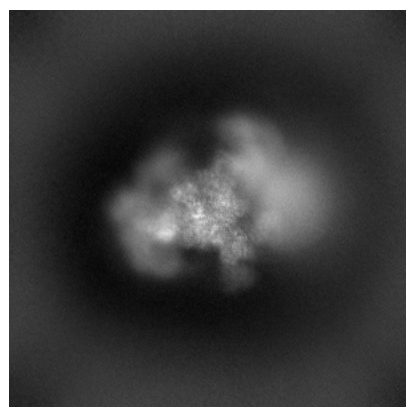


Y

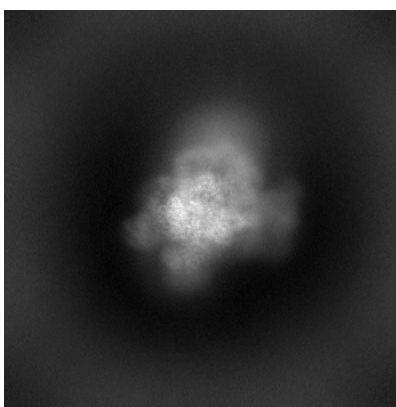


Z

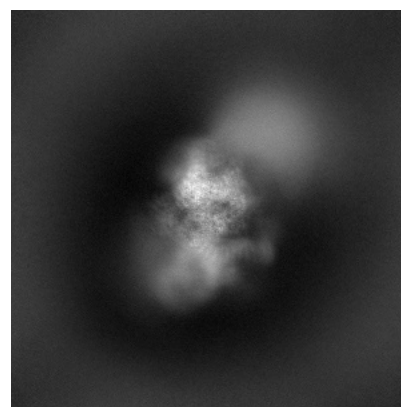
6.1.2 Raw map



X



Y

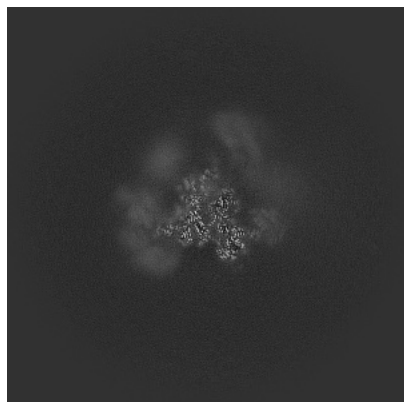


Z

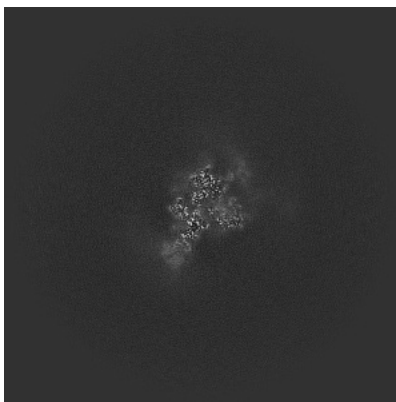
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

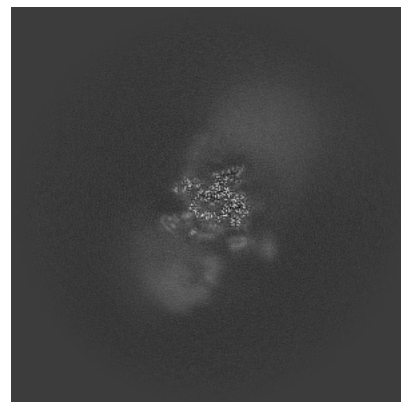
6.2.1 Primary map



X Index: 320

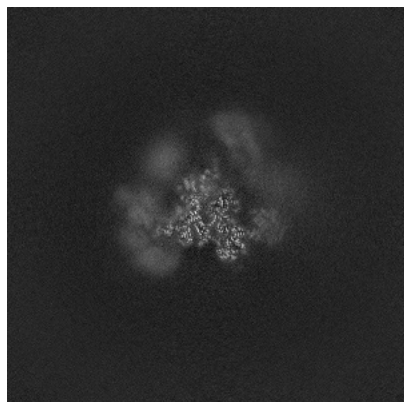


Y Index: 320

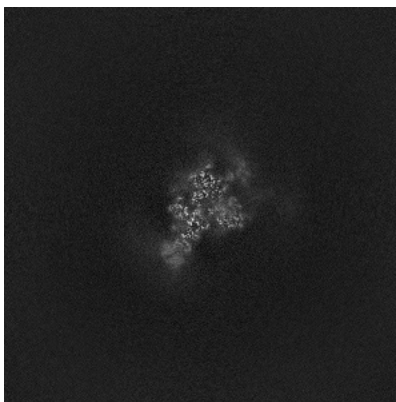


Z Index: 320

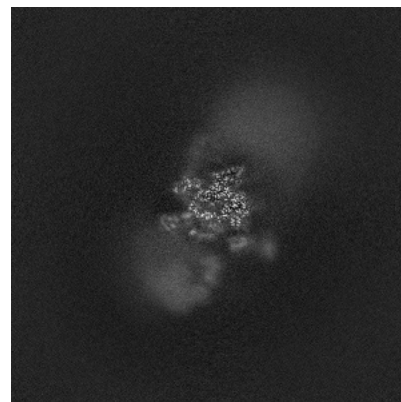
6.2.2 Raw map



X Index: 320



Y Index: 320

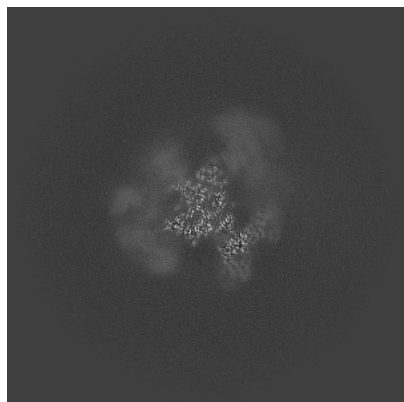


Z Index: 320

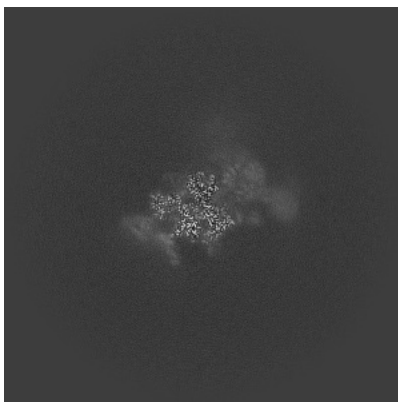
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

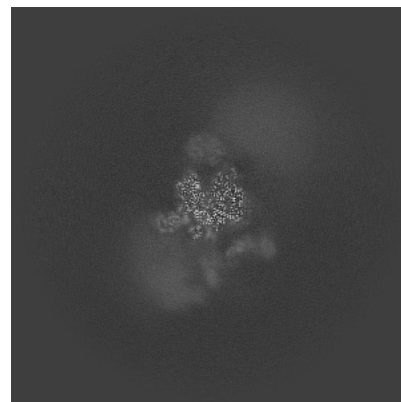
6.3.1 Primary map



X Index: 306

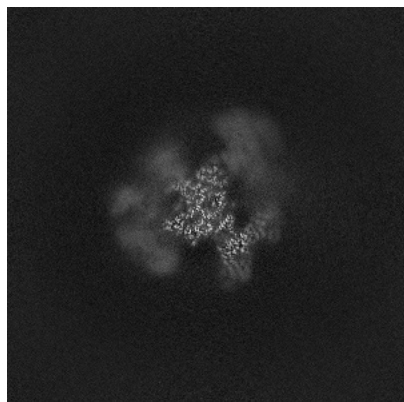


Y Index: 343

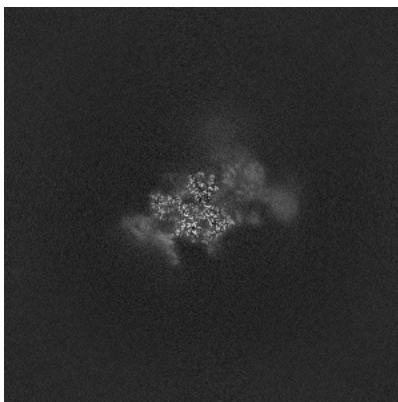


Z Index: 310

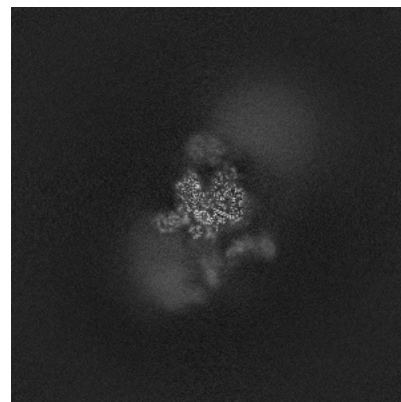
6.3.2 Raw map



X Index: 306



Y Index: 343

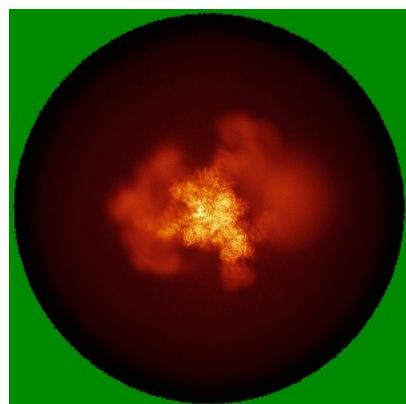


Z Index: 310

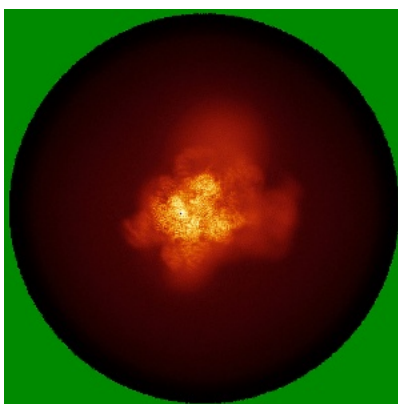
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

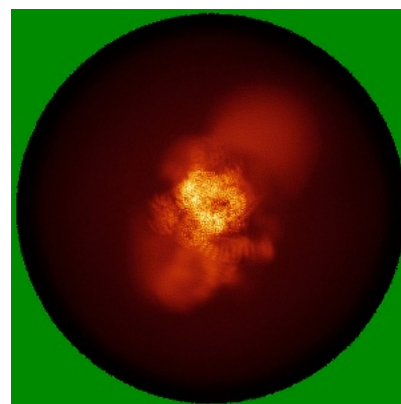
6.4.1 Primary map



X

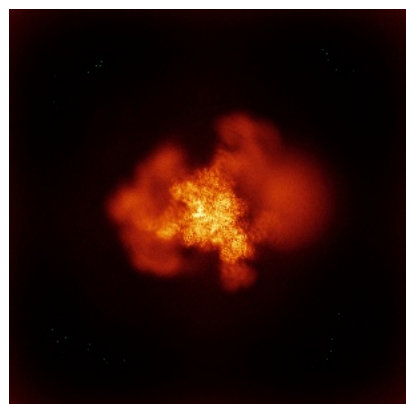


Y

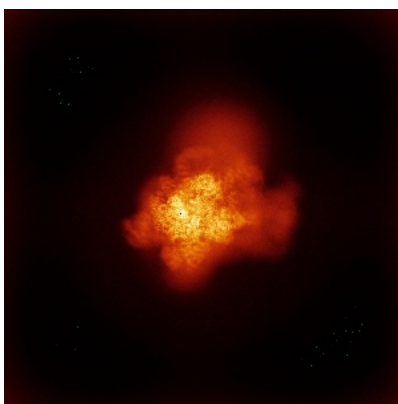


Z

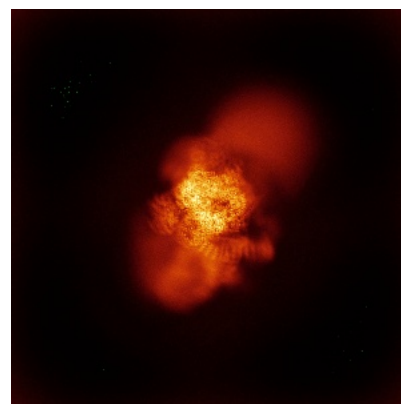
6.4.2 Raw map



X



Y

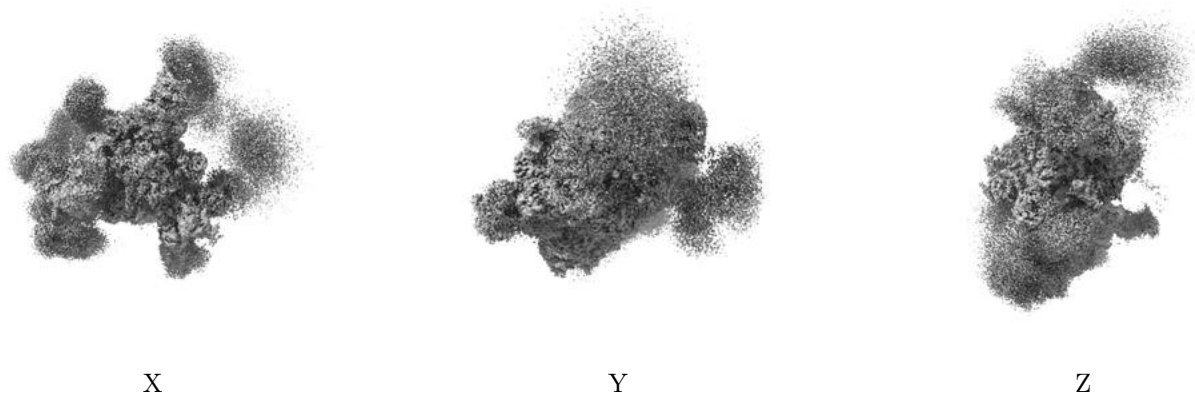


Z

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

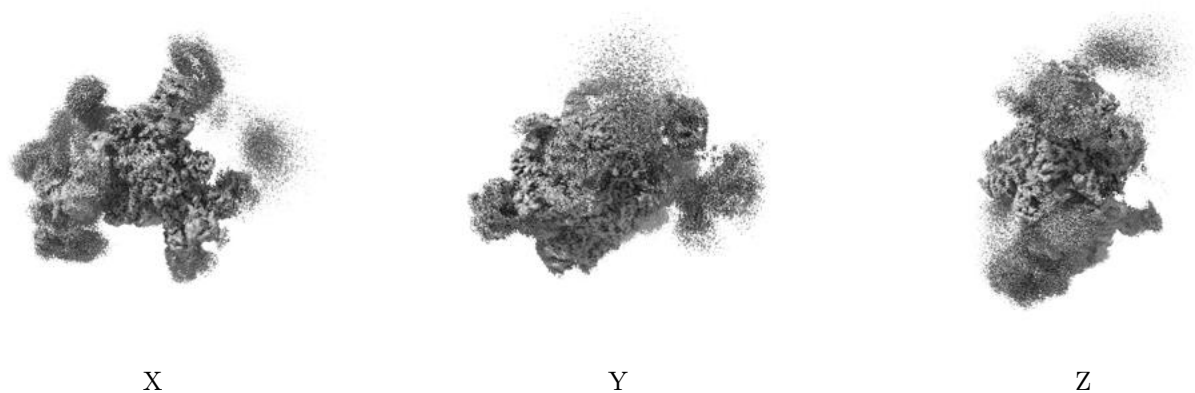
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.36. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

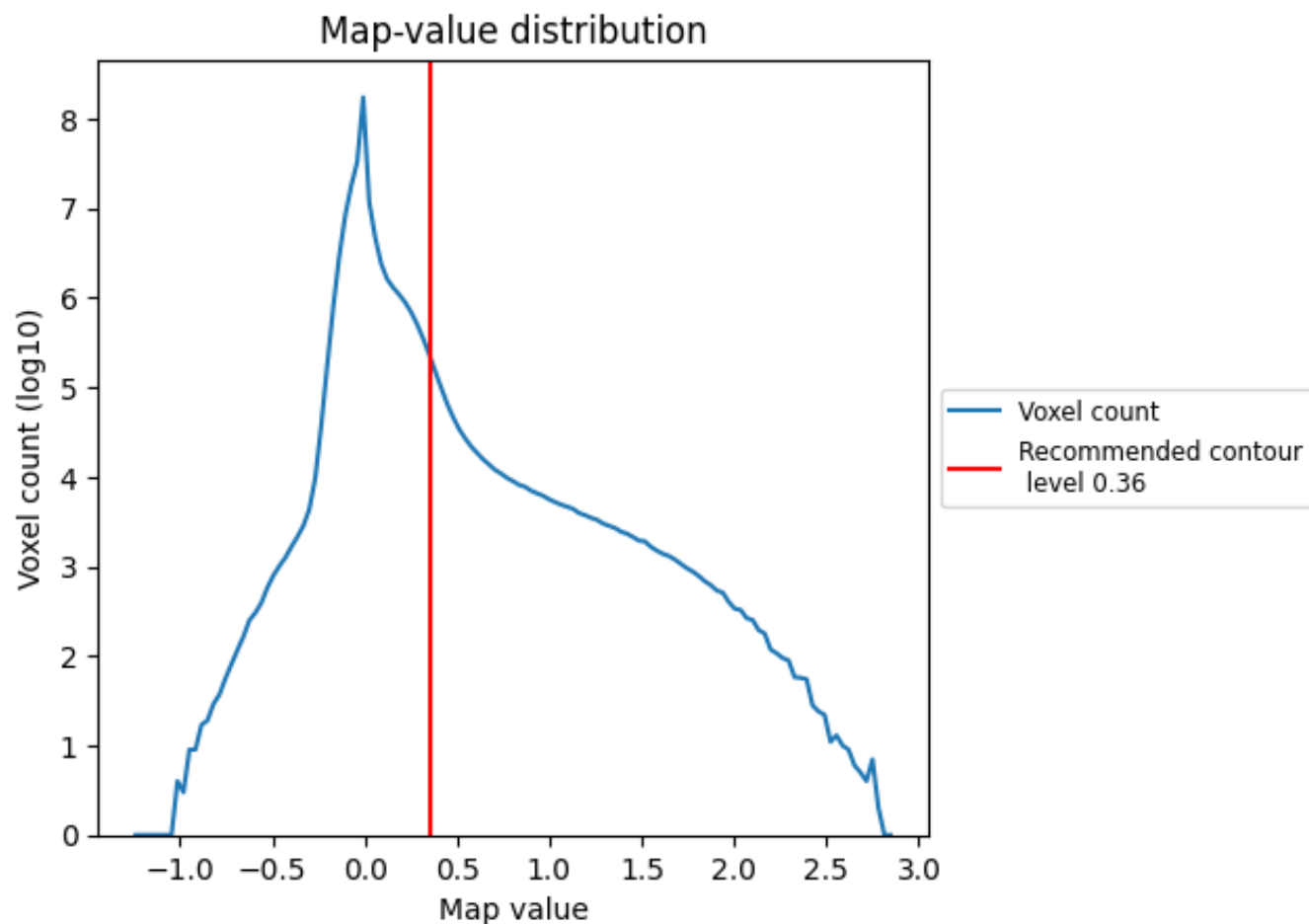
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

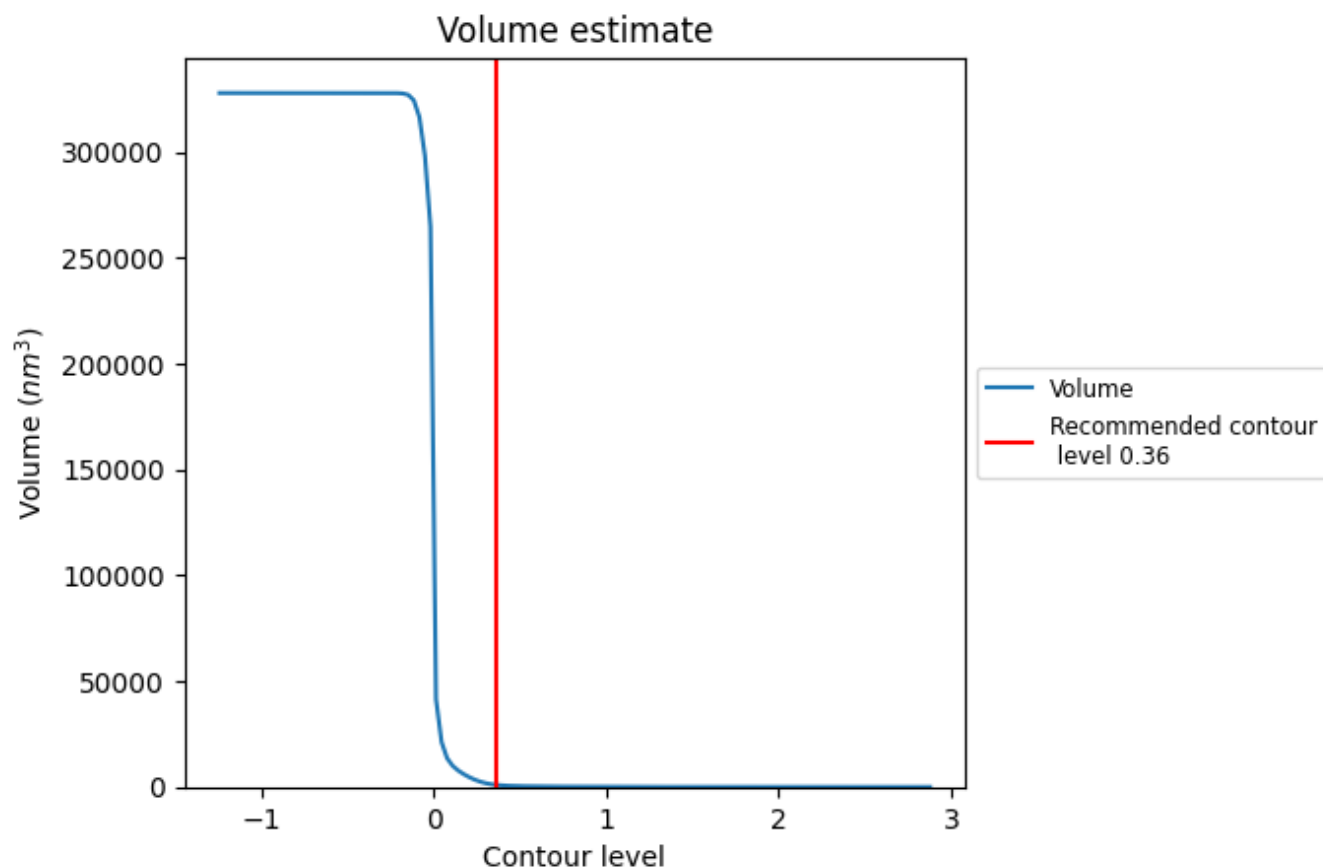
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

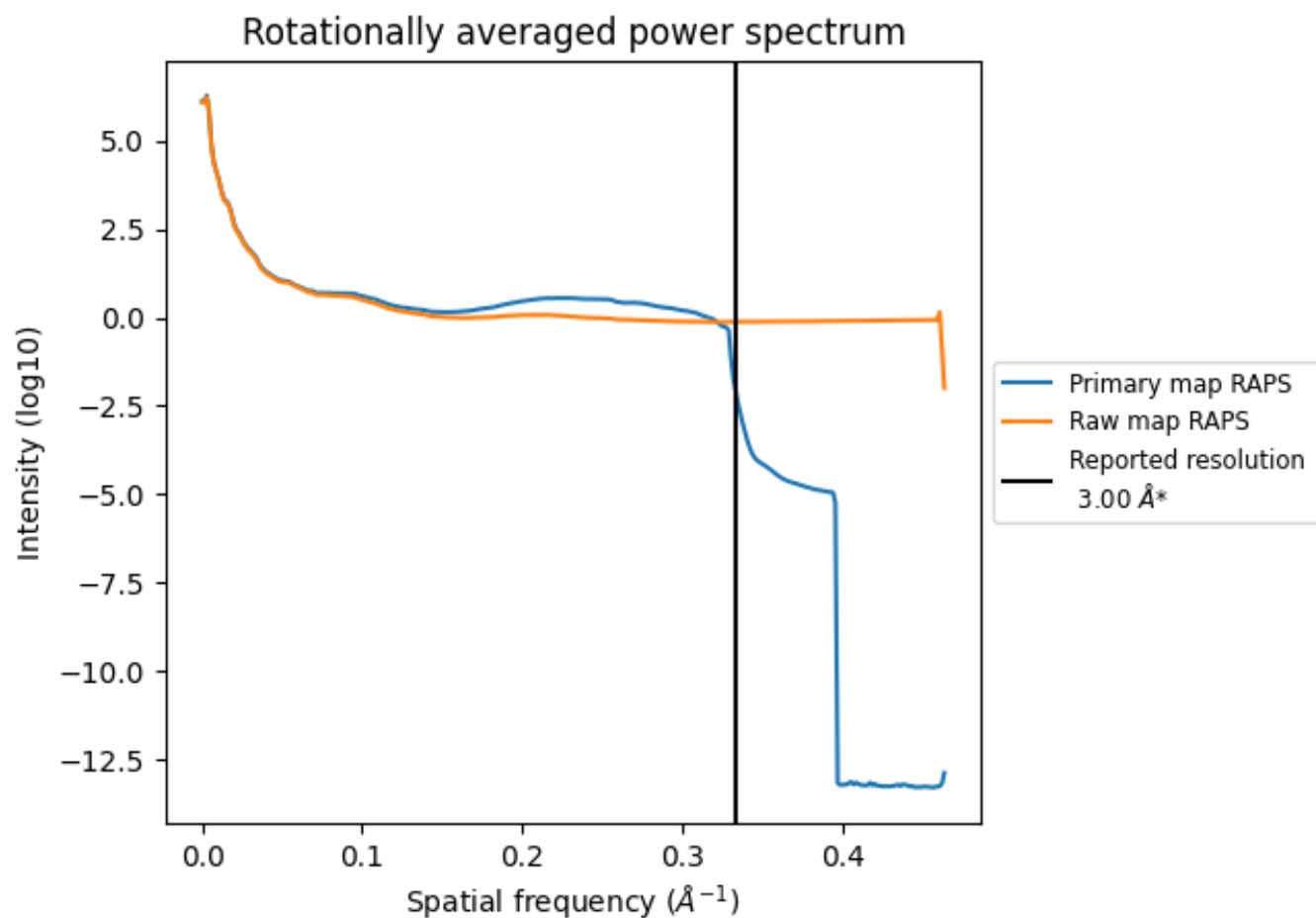
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 998 nm^3 ; this corresponds to an approximate mass of 902 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

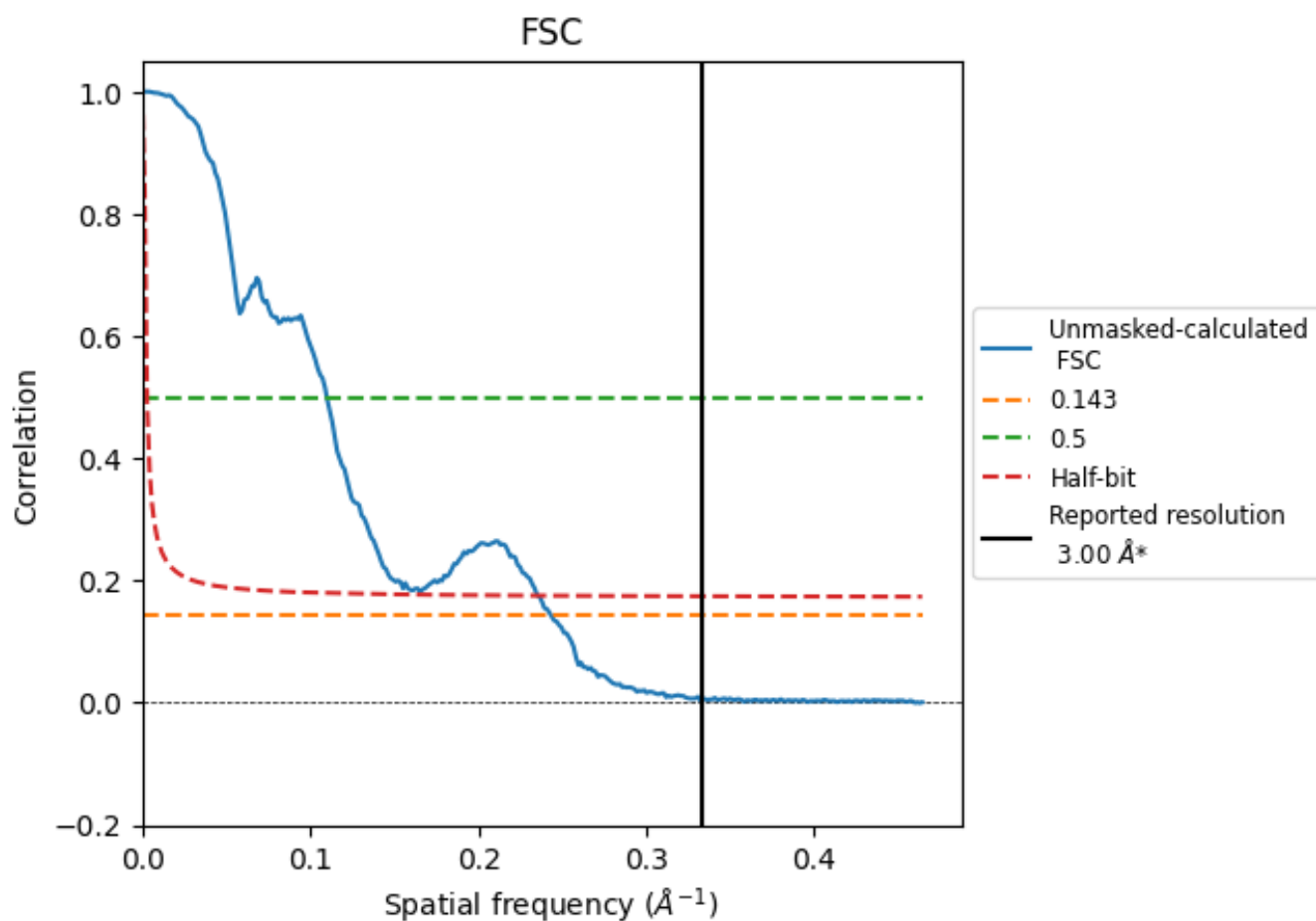


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

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 0.333 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

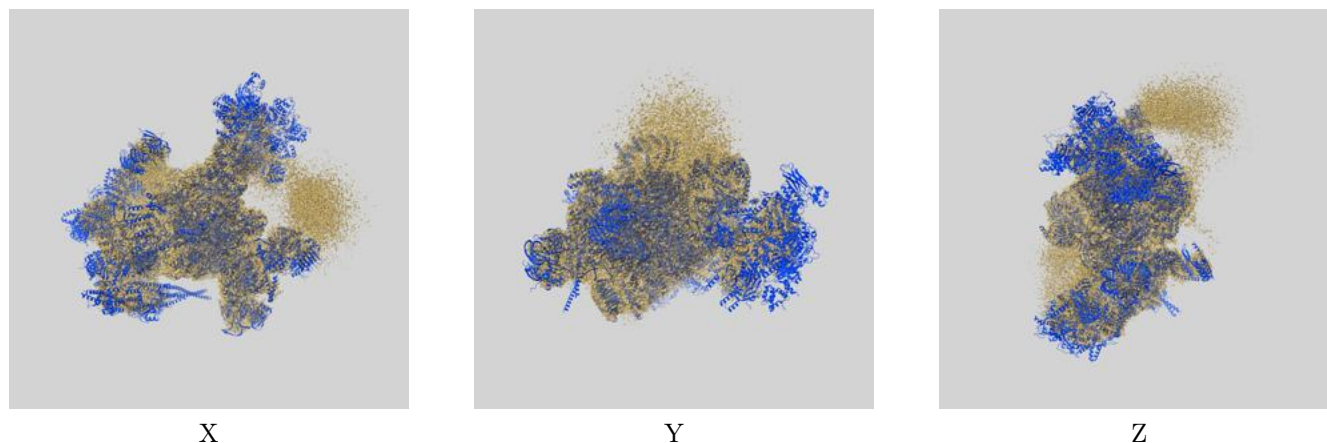
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.11	9.10	4.25

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.11 differs from the reported value 3.0 by more than 10 %

9 Map-model fit [i](#)

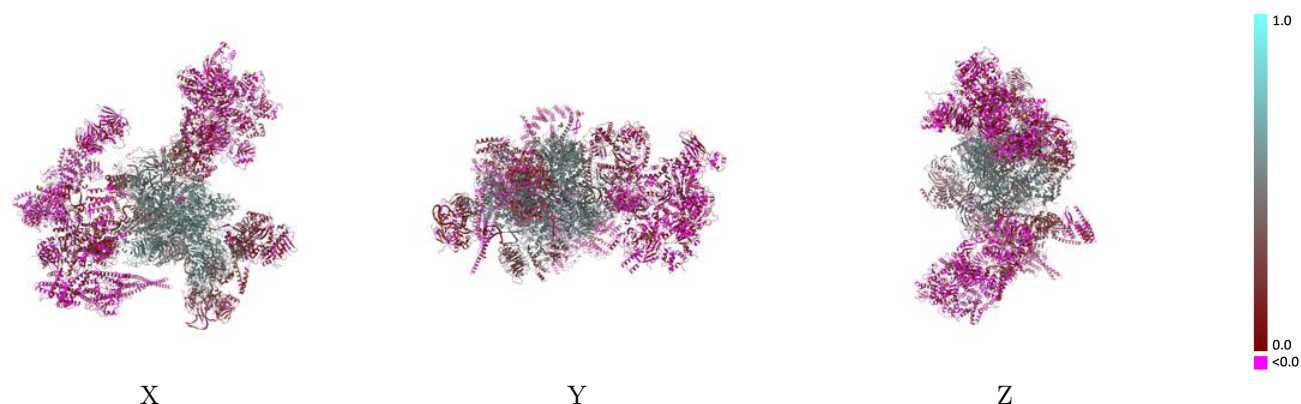
This section contains information regarding the fit between EMDB map EMD-67263 and PDB model 9XU3. Per-residue inclusion information can be found in section [3](#) on page [18](#).

9.1 Map-model overlay [i](#)



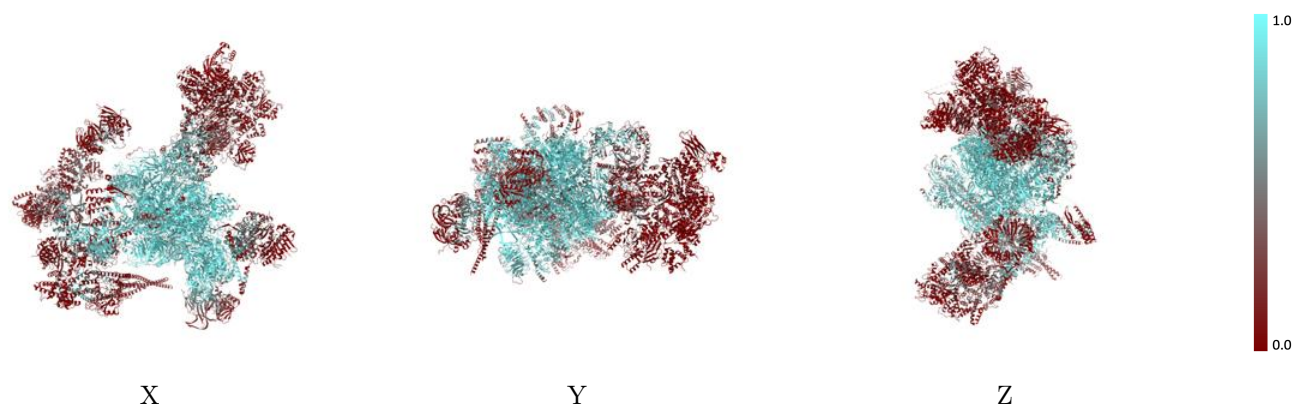
The images above show the 3D surface view of the map at the recommended contour level 0.36 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



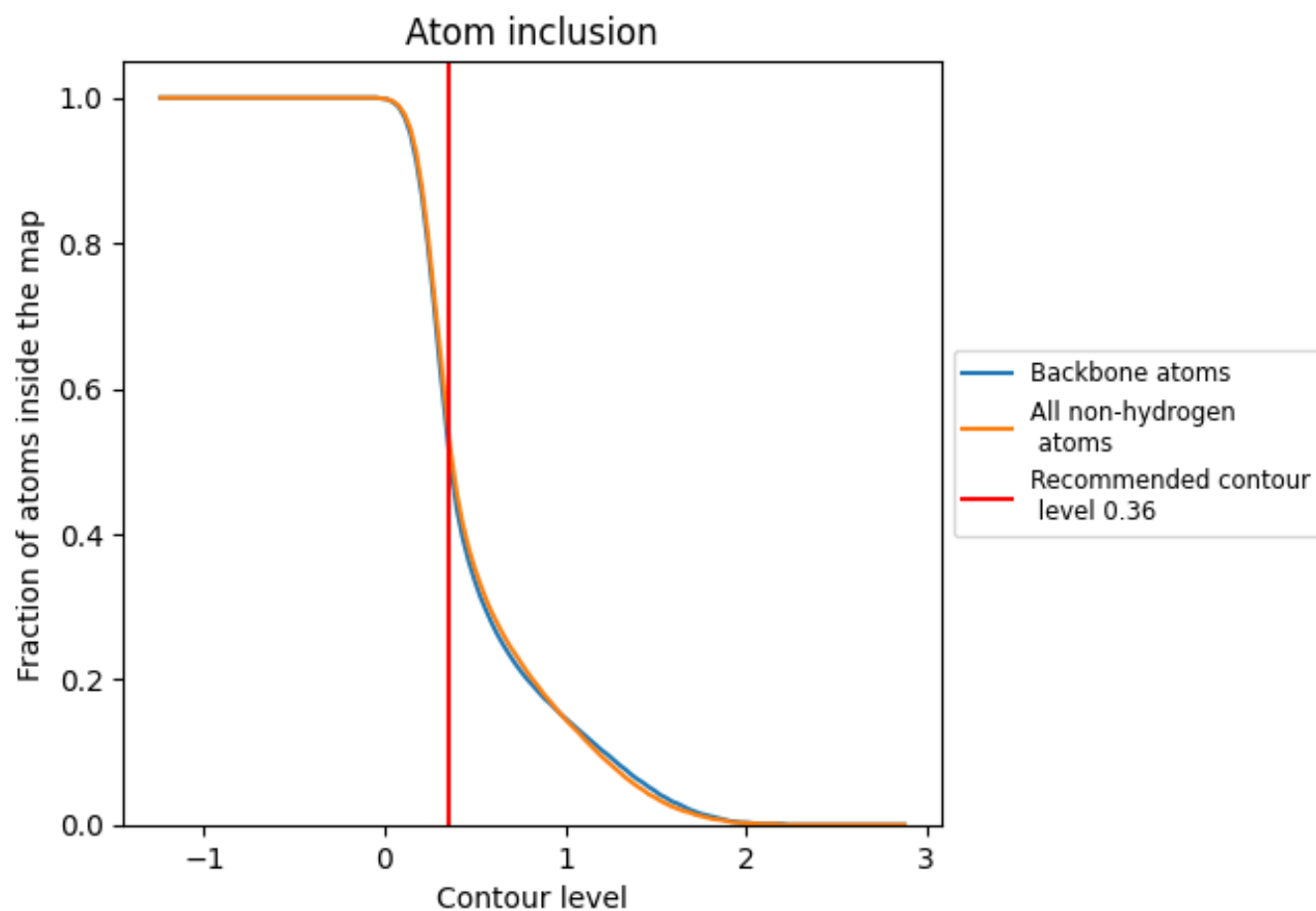
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.36).

9.4 Atom inclusion [i](#)



At the recommended contour level, 50% of all backbone atoms, 53% 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 (0.36) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5260	 0.2750
0	 0.5740	 0.3350
1	 0.9420	 0.4260
2	 0.8820	 0.3670
4	 0.0530	 0.0490
5	 0.7850	 0.3600
6	 0.7110	 0.3010
A	 0.8710	 0.5000
B	 0.9320	 0.5170
C	 0.0410	 0.0570
D	 0.7790	 0.3230
E	 0.5370	 0.2940
F	 0.5980	 0.1350
G	 0.7200	 0.3080
H	 0.5180	 0.1260
I	 0.0840	 0.0670
J	 0.7540	 0.3990
K	 0.8920	 0.5220
L	 0.9250	 0.4360
L2	 0.1630	 0.0580
L3	 0.1280	 0.0560
L4	 0.1160	 0.0210
L5	 0.0200	 0.0770
L6	 0.0410	 0.0850
L7	 0.0500	 0.0740
L8	 0.1800	 0.0620
M	 0.7410	 0.2690
N	 0.8620	 0.4780
O	 0.2640	 0.0410
P	 0.1410	 0.0620
Q	 0.1300	 0.0340
R	 0.0290	 0.0420
S	 0.8200	 0.4840
T	 0.5050	 0.2040
U	 0.4310	 0.2860



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Chain	Atom inclusion	Q-score
V	 0.6840	 0.3960
W	 0.9480	 0.4940
X	 0.8020	 0.3980
Y	 0.9070	 0.5200
Z	 0.7290	 0.4830
a	 0.6020	 0.2600
b	 0.4910	 0.1460
c	 0.2450	 0.1470
d	 0.6380	 0.3550
e	 0.1300	 0.1430
f	 0.1290	 0.1570
g	 0.3110	 0.2380
h	 0.1860	 0.0410
i	 0.1770	 0.0510
j	 0.1170	 0.0660
k	 0.1800	 0.0470
l	 0.1940	 0.0680
m	 0.1350	 0.0550
n	 0.1590	 0.0230
p	 0.2870	 0.3670
q	 0.1940	 0.0700
r	 0.1290	 0.0420
s	 0.1710	 0.0080
t	 0.0990	 0.0660
u	 0.1030	 0.0500
v	 0.4370	 0.2410
w	 0.0560	 0.1360
x	 0.0360	 0.1500
y	 0.1750	 0.1800
z	 0.8130	 0.3820