



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 02:50 PM UTC

PDB ID : 7DCO / pdb_00007dco
EMDB ID : EMD-30637
Title : Cryo-EM structure of the activated spliceosome (Bact complex) at an atomic resolution of 2.5 angstrom
Authors : Bai, R.; Wan, R.; Yan, C.; Qi, J.; Zhang, P.; Lei, J.; Shi, Y.
Deposited on : 2020-10-26
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

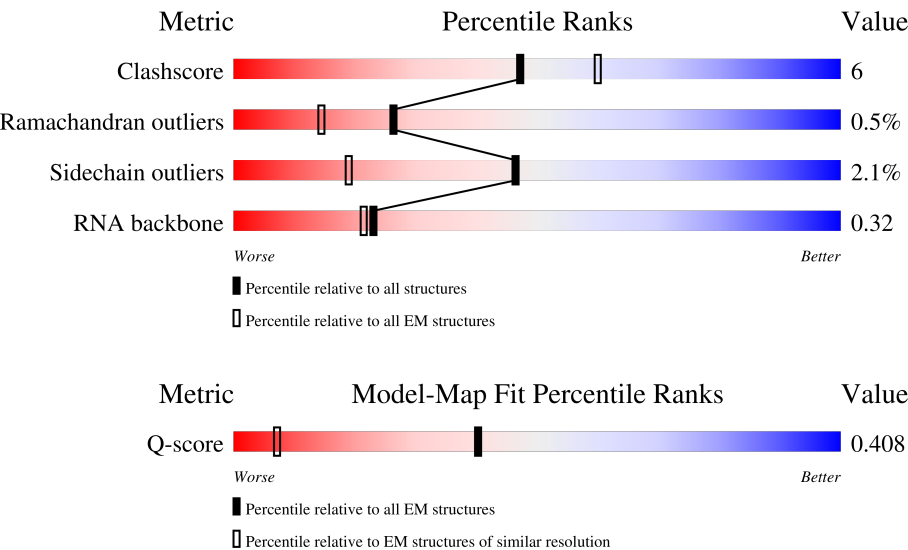
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7115 (2.00 - 3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	A	2413	79%12%9%
2	B	214	43% 40%31%11%16%
3	C	1008	14% 77%13%9%

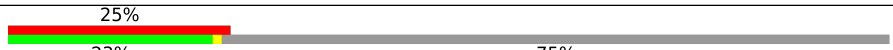
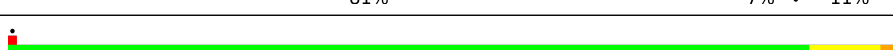
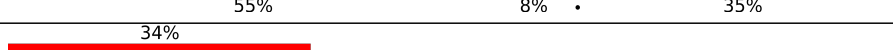
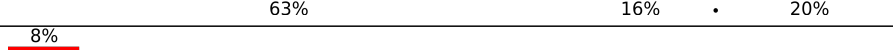
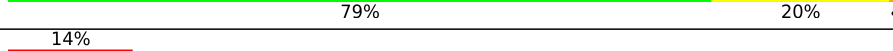
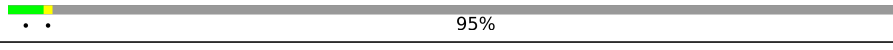
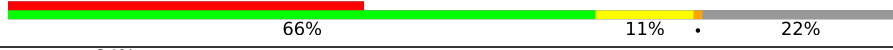
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Mol	Chain	Length	Quality of chain
4	D	2163	
5	d	101	
6	a	196	
6	h	196	
7	b	146	
7	m	146	
8	c	110	
8	n	110	
9	e	94	
9	i	94	
10	f	86	
10	j	86	
11	g	77	
11	k	77	
12	F	112	
13	G	162	
14	H	1175	
15	o	238	
16	p	111	
17	l	81	
18	u	530	
19	w	280	
20	v	266	
21	1	971	
22	2	238	

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Mol	Chain	Length	Quality of chain
23	3	1361	
24	4	213	
25	5	107	
26	6	84	
27	L	590	
28	q	503	
28	r	503	
28	s	503	
28	t	503	
29	K	175	
30	N	157	
31	T	337	
32	P	379	
33	Q	364	
34	R	261	
35	S	175	
36	Y	204	
37	X	128	
38	Z	121	
39	W	455	
40	U	135	
41	V	577	
42	M	259	
43	z	301	
44	y	185	

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Mol	Chain	Length	Quality of chain
45	J	687	60% 71% 10% 19%
46	I	859	68% 59% 8% 32%
47	x	876	62% 66% 8% 25%

2 Entry composition [i](#)

There are 53 unique types of molecules in this entry. The entry contains 129875 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called PRP8 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2205	Total	C	N	O	S	0	0
			18135	11656	3091	3324	64		

- Molecule 2 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	179	Total	C	N	O	P	0	0
			3795	1699	660	1258	178		

- Molecule 3 is a protein called SNU114 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	918	Total	C	N	O	S	0	0
			7328	4725	1218	1355	30		

- Molecule 4 is a protein called BRR2 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	1828	Total	C	N	O	S	0	0
			14666	9388	2437	2784	57		

- Molecule 5 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	d	79	Total	C	N	O	0	0
			316	158	79	79		

- Molecule 6 is a protein called BJ4_G0014900.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	a	73	Total	C	N	O	0	0
			292	146	73	73		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	h	78	Total	C	N	O	S	0	0
			610	389	110	108	3		

- Molecule 7 is a protein called SMD1 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	b	77	Total	C	N	O		0	0
			308	154	77	77			
7	m	82	Total	C	N	O	S	0	0
			644	409	110	123	2		

- Molecule 8 is a protein called BJ4_G0037700.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	c	90	Total	C	N	O		0	0
			360	180	90	90			
8	n	65	Total	C	N	O	S	0	0
			528	340	102	84	2		

- Molecule 9 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	e	72	Total	C	N	O		0	0
			288	144	72	72			
9	i	75	Total	C	N	O	S	0	0
			575	379	92	101	3		

- Molecule 10 is a protein called Sm protein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	f	70	Total	C	N	O		0	0
			280	140	70	70			
10	j	70	Total	C	N	O	S	0	0
			554	355	98	100	1		

- Molecule 11 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	g	70	Total	C	N	O		0	0
			280	140	70	70			
11	k	69	Total	C	N	O	S	0	0
			529	337	93	97	2		

- Molecule 12 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	103	Total	C	N	O	P	0	0
			2192	982	391	716	103		

- Molecule 13 is a RNA chain called pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	105	Total	C	N	O	P	0	0
			2099	942	330	723	104		

- Molecule 14 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H	169	Total	C	N	O	P	0	0
			3566	1594	595	1208	169		

- Molecule 15 is a protein called HLJ1_G0053790.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	o	135	Total	C	N	O	0	0
			841	538	142	161		

- Molecule 16 is a protein called BJ4_G0027490.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	p	75	Total	C	N	O	0	0
			476	310	83	83		

- Molecule 17 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	l	81	Total	C	N	O	S	0	0
			611	390	106	113	2		

- Molecule 18 is a protein called PRP9 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	u	461	Total	C	N	O	S	0	0
			3899	2477	675	732	15		

- Molecule 19 is a protein called Pre-mRNA-splicing factor PRP21.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	w	127	Total	C	N	O	S	0	0
			1084	689	193	196	6		

- Molecule 20 is a protein called PRP11 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	v	207	Total	C	N	O	S	0	0
			1621	1014	281	319	7		

- Molecule 21 is a protein called HSH155 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	1	930	Total	C	N	O	S	0	0
			7376	4723	1262	1348	43		

- Molecule 22 is a protein called HLJ1_G0043010.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	2	220	Total	C	N	O	S	0	0
			1793	1158	311	314	10		

- Molecule 23 is a protein called RSE1 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	3	1207	Total	C	N	O	S	0	0
			9599	6134	1613	1801	51		

- Molecule 24 is a protein called HSH49 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	4	174	Total	C	N	O	S	0	0
			1433	932	240	259	2		

- Molecule 25 is a protein called BJ4_G0056610.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	5	103	Total	C	N	O	S	0	0
			814	503	154	143	14		

- Molecule 26 is a protein called RDS3 complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	6	84	Total	C	N	O	S	0	0
			693	429	130	132	2		

- Molecule 27 is a protein called Pre-mRNA-splicing factor CEF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	L	435	Total	C	N	O	S	0	0
			2901	1799	538	557	7		

- Molecule 28 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	s	124	Total	C	N	O	S	0	0
			819	518	132	167	2		
28	t	128	Total	C	N	O	S	0	0
			843	533	136	172	2		
28	q	129	Total	C	N	O	S	0	0
			850	537	137	174	2		
28	r	125	Total	C	N	O	S	0	0
			823	521	133	167	2		

- Molecule 29 is a protein called SNT309 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	K	155	Total	C	N	O	S	0	0
			920	581	159	179	1		

- Molecule 30 is a protein called BUD31 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	N	157	Total	C	N	O	S	0	0
			1291	808	240	232	11		

- Molecule 31 is a protein called HLJ1_G0054350.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	T	337	Total	C	N	O	S	0	0
			2646	1669	466	501	10		

- Molecule 32 is a protein called Pre-mRNA-processing protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	P	246	Total	C	N	O	S	0	0
			1978	1233	359	380	6		

- Molecule 33 is a protein called Pre-mRNA-splicing factor SLT11.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Q	292	Total	C	N	O	S	0	0
			2301	1461	399	426	15		

- Molecule 34 is a protein called Pre-mRNA-splicing factor CWC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	R	261	Total	C	N	O	S	0	0
			2089	1320	369	388	12		

- Molecule 35 is a protein called Pre-mRNA-splicing factor CWC15.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	S	71	Total	C	N	O	S	0	0
			578	361	117	99	1		

- Molecule 36 is a protein called Pre-mRNA leakage protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Y	174	Total	C	N	O	S	0	0
			1386	868	233	275	10		

- Molecule 37 is a protein called SX2_G0027210.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	X	128	Total	C	N	O	S	0	0
			1051	662	181	208			

- Molecule 38 is a protein called Pre-mRNA-splicing factor CWC26.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Z	121	Total	C	N	O	S	0	0
			920	575	161	182	2		

- Molecule 39 is a protein called CDC40 isoform 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	W	23	Total	C	N	O	0	0
			195	122	41	32		

- Molecule 40 is a protein called Pre-mRNA-splicing factor CWC21.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	U	27	Total	C	N	O	0	0
			190	112	38	40		

- Molecule 41 is a protein called CWC22 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	V	450	Total	C	N	O	S	0	0
			3660	2346	605	691	18		

- Molecule 42 is a protein called Pre-mRNA-splicing factor CWC24.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	M	176	Total	C	N	O	S	0	0
			1360	852	235	260	13		

- Molecule 43 is a protein called CWC27 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	z	150	Total	C	N	O	S	0	0
			1224	789	206	223	6		

- Molecule 44 is a protein called Pre-mRNA-splicing factor SPP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	y	73	Total	C	N	O	S	0	0
			572	371	93	107	1		

- Molecule 45 is a protein called CLF1 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	J	554	Total	C	N	O	S	0	0
			3595	2231	680	676	8		

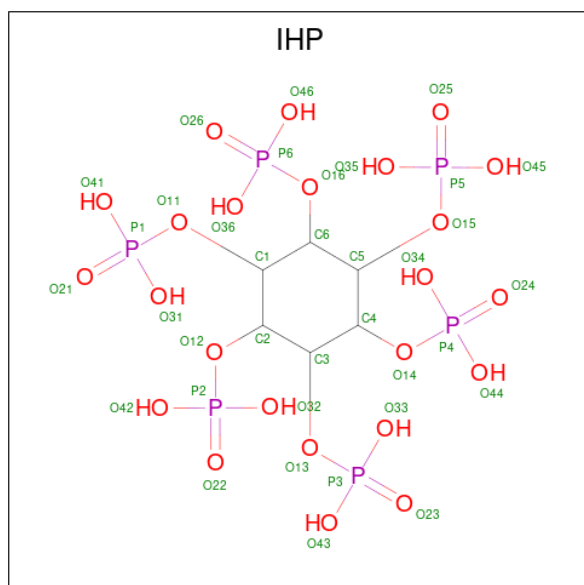
- Molecule 46 is a protein called SYF1 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	I	580	Total	C	N	O	S	0	0
			3101	1897	590	613	1		

- Molecule 47 is a protein called Pre-mRNA-splicing factor ATP-dependent RNA helicase-like protein PRP2.

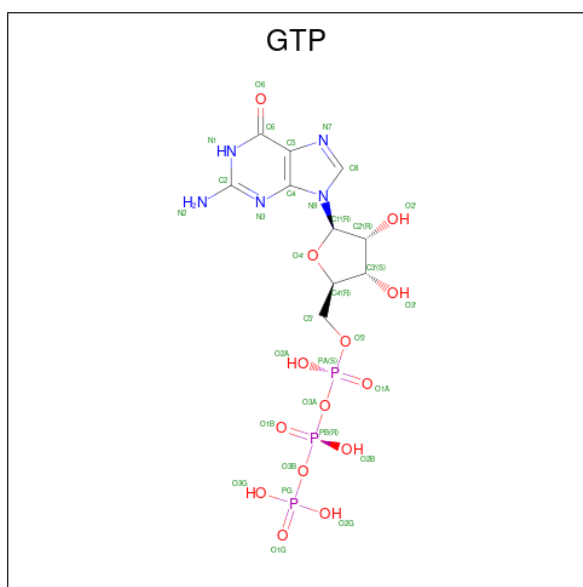
Mol	Chain	Residues	Atoms					AltConf	Trace
47	x	653	Total	C	N	O	S	0	0
			5193	3313	891	956	33		

- Molecule 48 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 49 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
49	C	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 50 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
50	C	1	Total	Mg	0
			1	1	
50	F	4	Total	Mg	0
			4	4	
50	3	1	Total	Mg	0
			1	1	

- Molecule 51 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
51	C	1	Total	Ca	0
			1	1	

- Molecule 52 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
52	u	2	Total	Zn	0
			2	2	

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Mol	Chain	Residues	Atoms		AltConf
52	v	1	Total 1	Zn 1	0
52	5	3	Total 3	Zn 3	0
52	N	3	Total 3	Zn 3	0
52	Q	2	Total 2	Zn 2	0
52	R	1	Total 1	Zn 1	0
52	M	3	Total 3	Zn 3	0

- Molecule 53 is water.

Mol	Chain	Residues	Atoms		AltConf
53	A	582	Total 582	O 582	0
53	B	127	Total 127	O 127	0
53	C	8	Total 8	O 8	0
53	D	2	Total 2	O 2	0
53	F	109	Total 109	O 109	0
53	G	56	Total 56	O 56	0
53	H	70	Total 70	O 70	0
53	v	29	Total 29	O 29	0
53	1	185	Total 185	O 185	0
53	2	51	Total 51	O 51	0
53	3	218	Total 218	O 218	0
53	5	53	Total 53	O 53	0
53	6	42	Total 42	O 42	0

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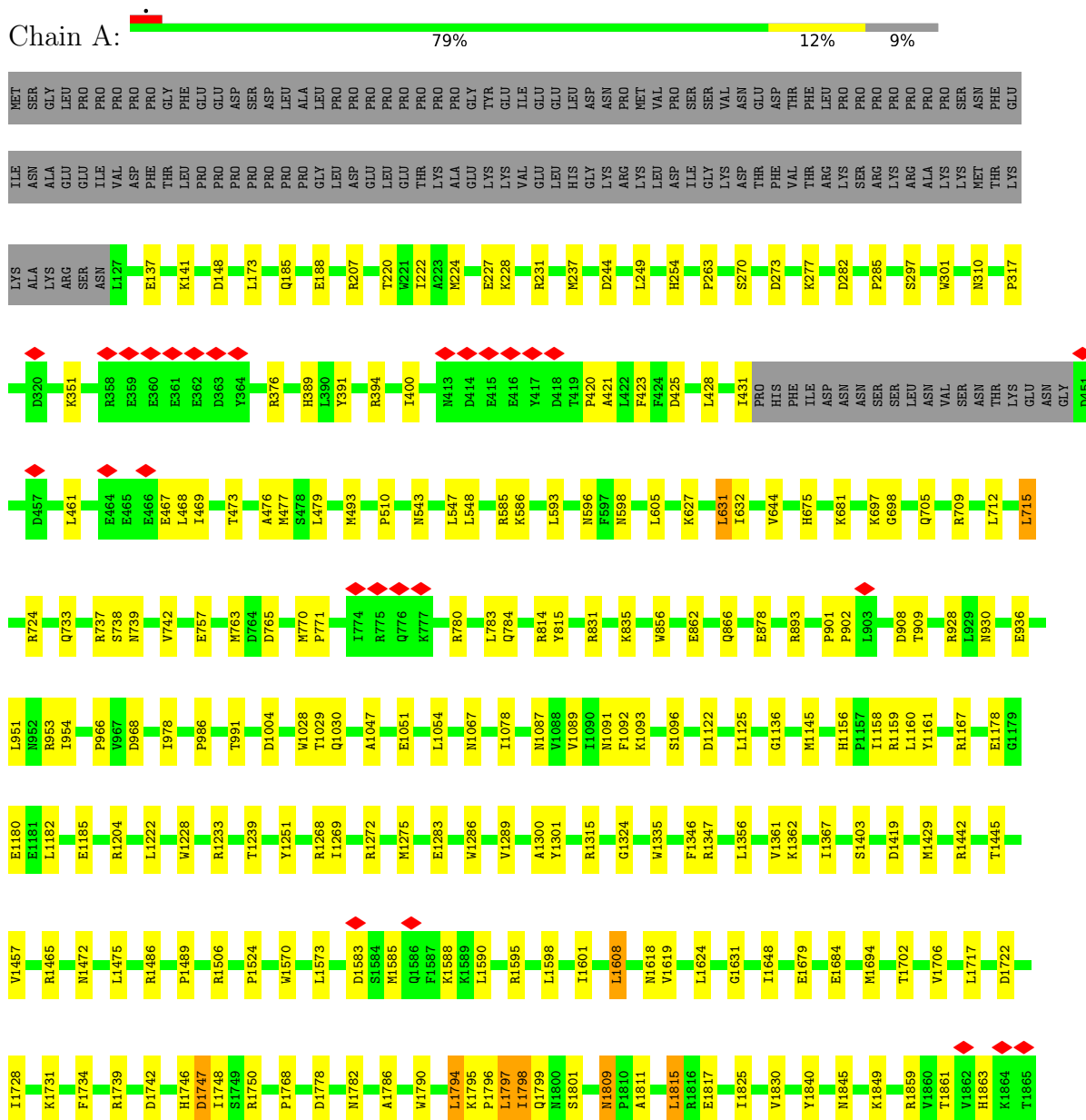
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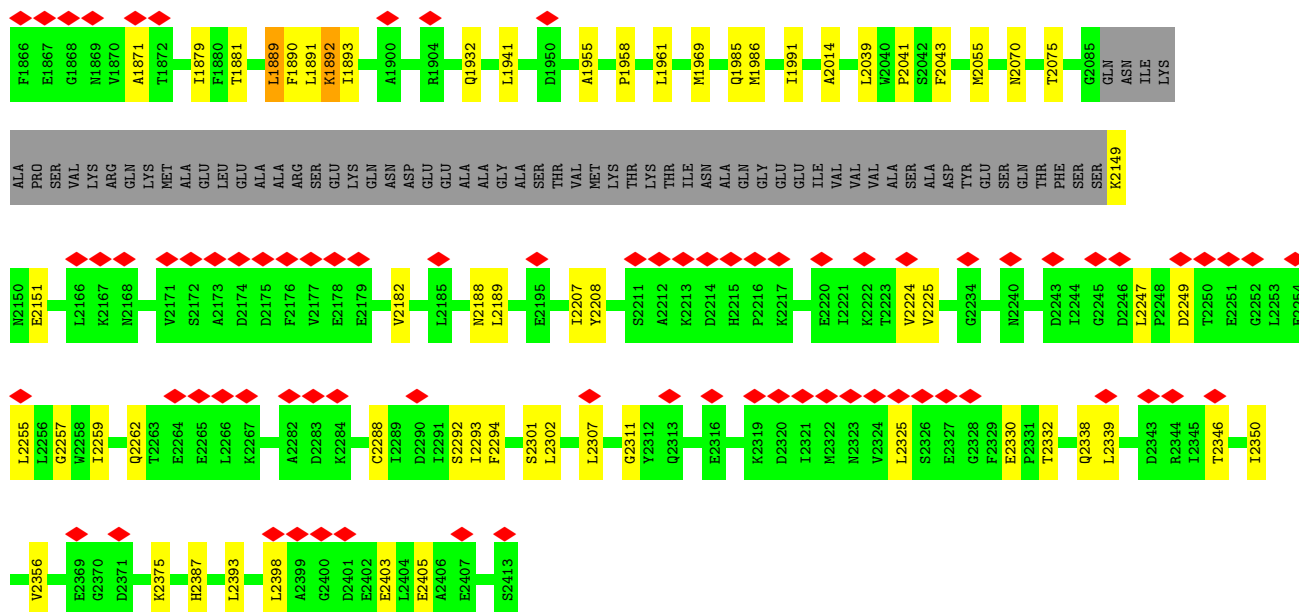
Mol	Chain	Residues	Atoms		AltConf
53	L	18	Total 18	O 18	0
53	N	12	Total 12	O 12	0
53	T	39	Total 39	O 39	0
53	P	26	Total 26	O 26	0
53	R	8	Total 8	O 8	0
53	S	9	Total 9	O 9	0
53	X	13	Total 13	O 13	0
53	Z	9	Total 9	O 9	0
53	U	6	Total 6	O 6	0
53	V	21	Total 21	O 21	0
53	M	21	Total 21	O 21	0

3 Residue-property plots

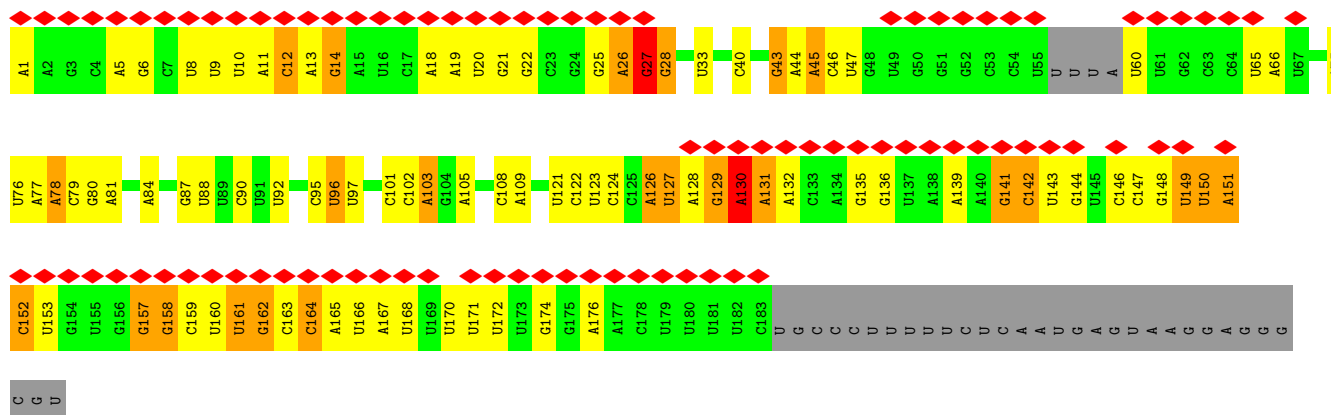
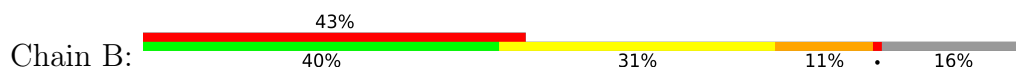
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: PRP8 isoform 1

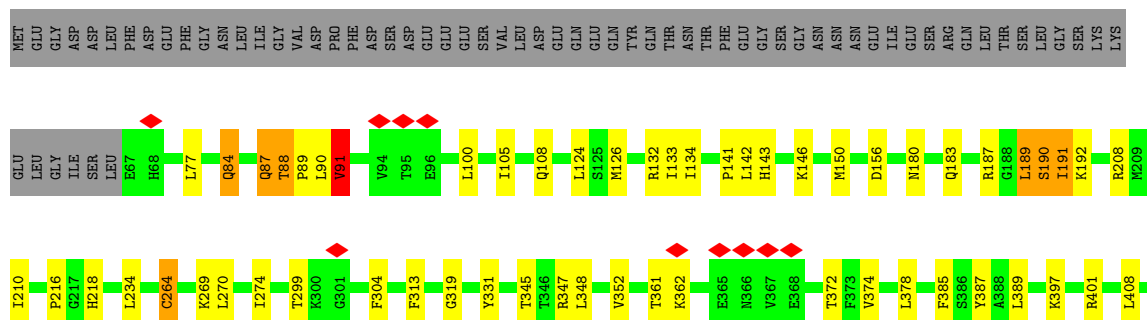
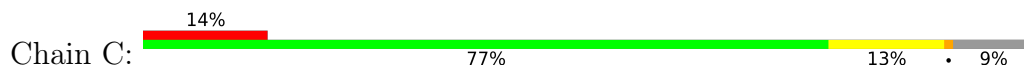


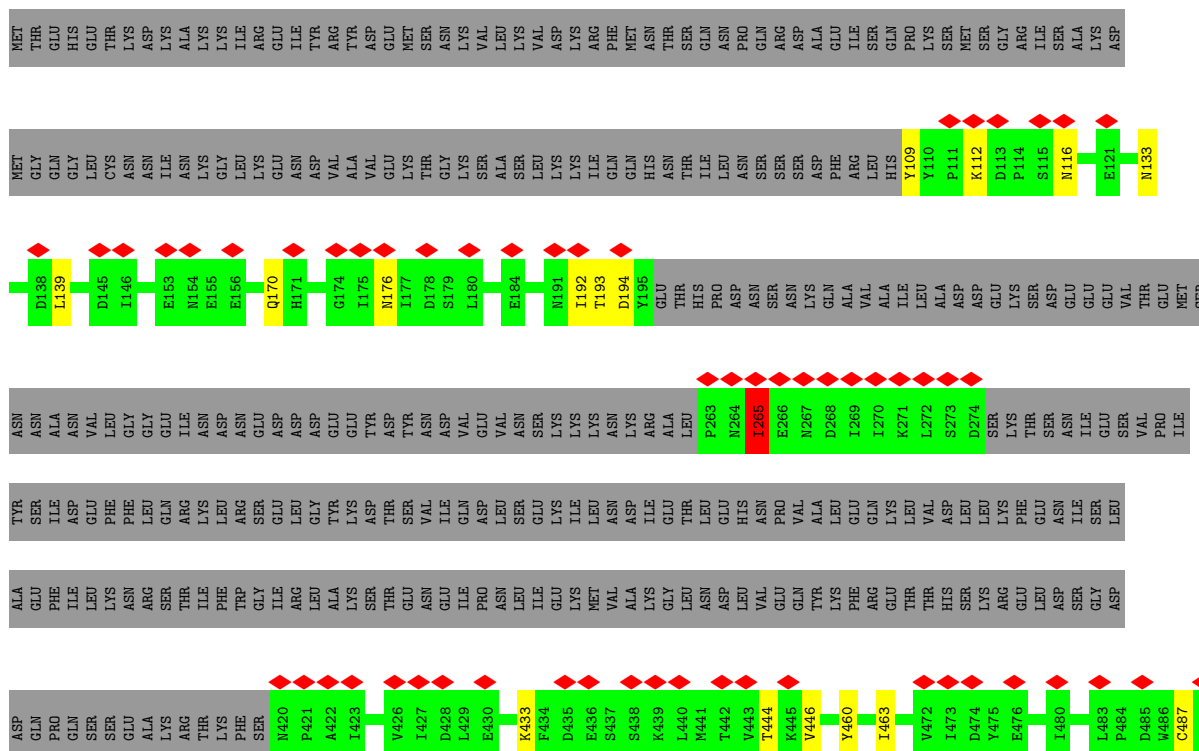


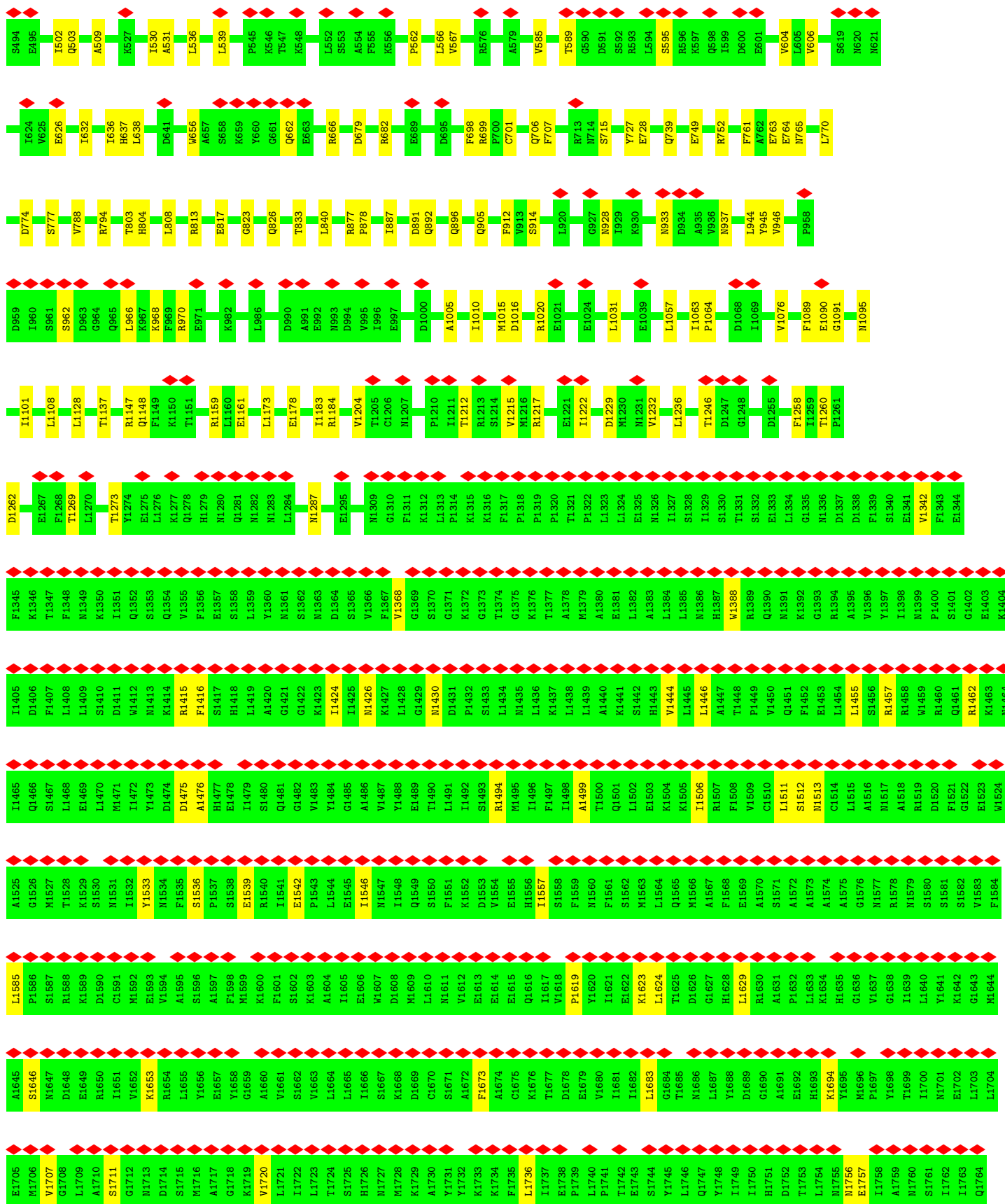
• Molecule 2: U5 snRNA

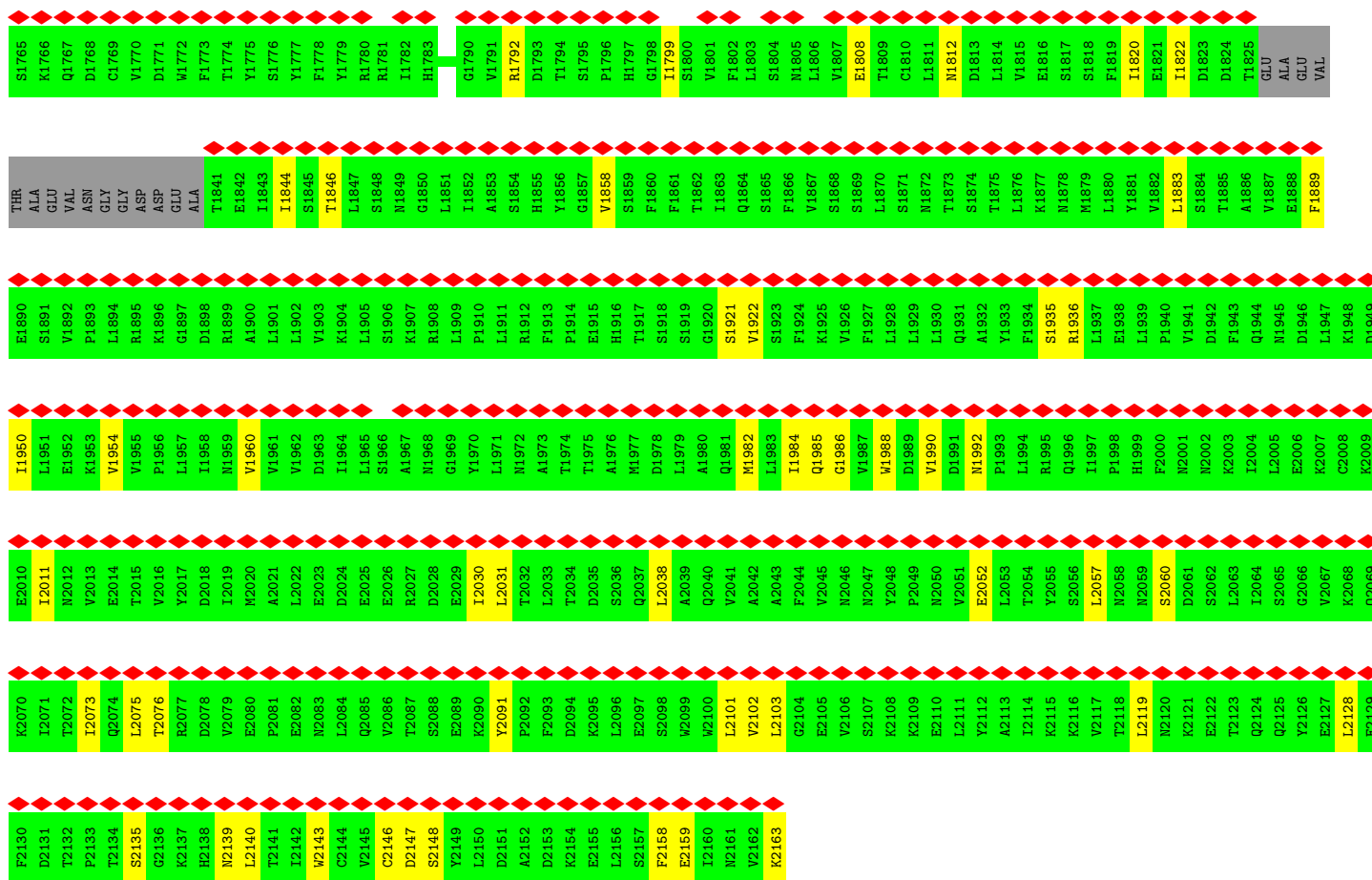


• Molecule 3: SNU114 isoform 1

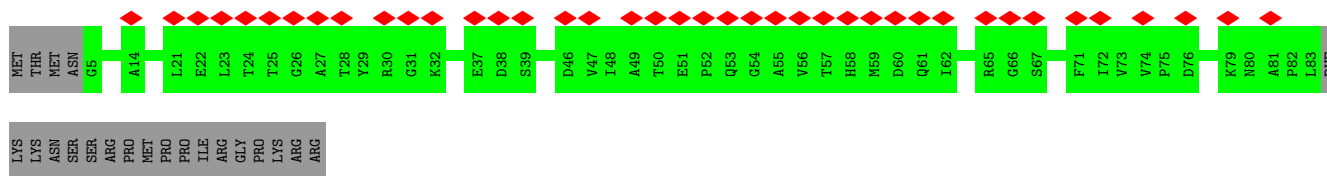
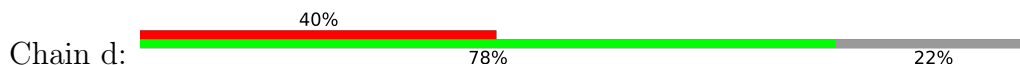




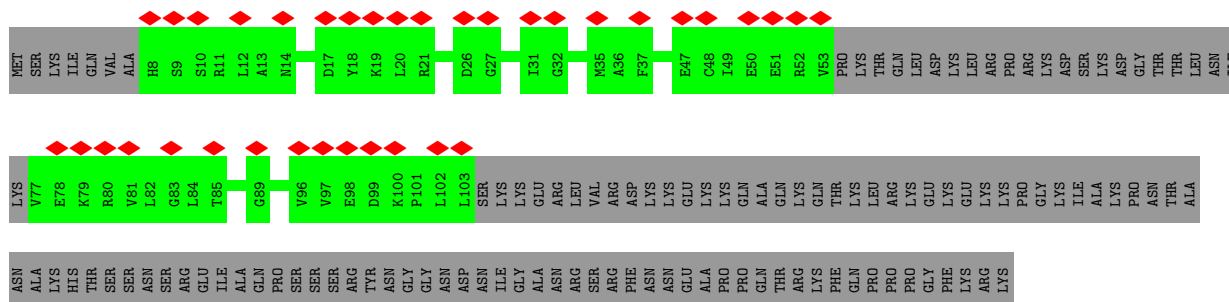


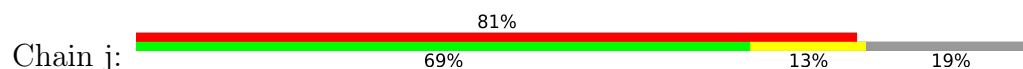


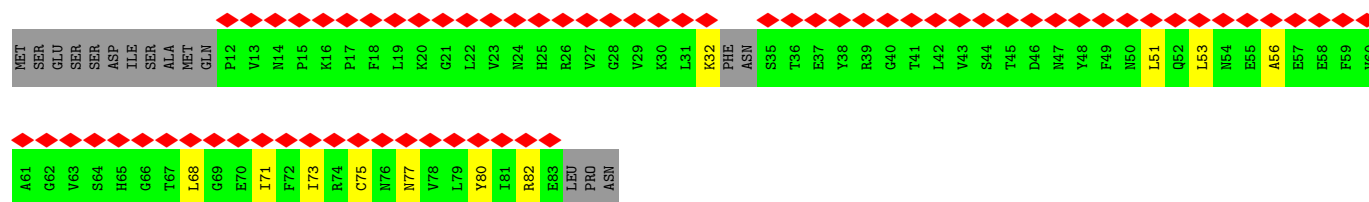
• Molecule 5: Small nuclear ribonucleoprotein Sm D3



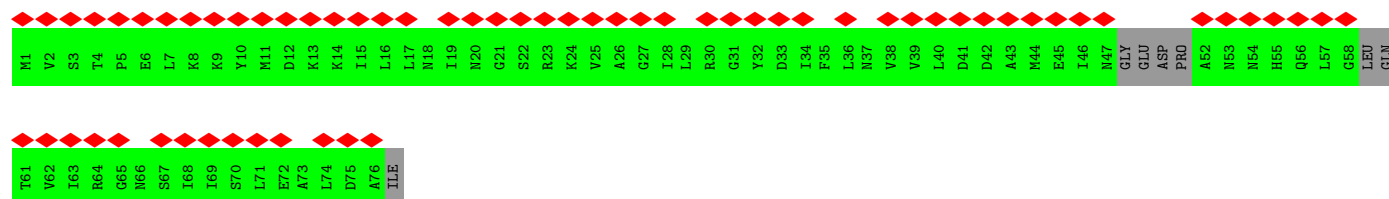
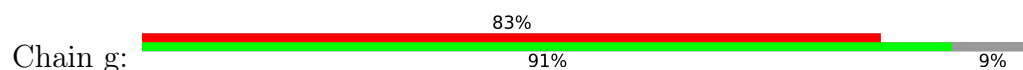
• Molecule 6: BJ4_G0014900.mRNA.1.CDS.1



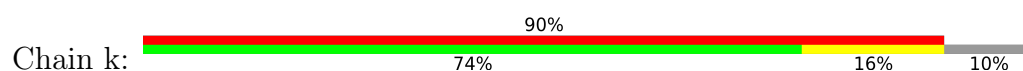




• Molecule 11: Small nuclear ribonucleoprotein G



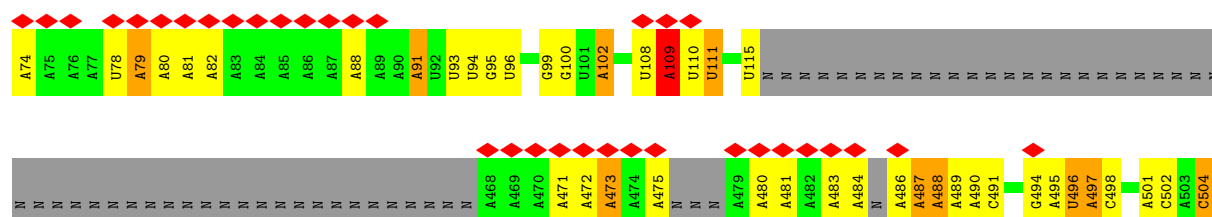
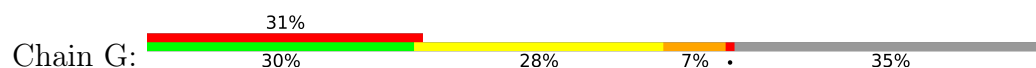
• Molecule 11: Small nuclear ribonucleoprotein G

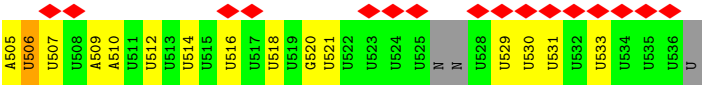


• Molecule 12: U6 snRNA

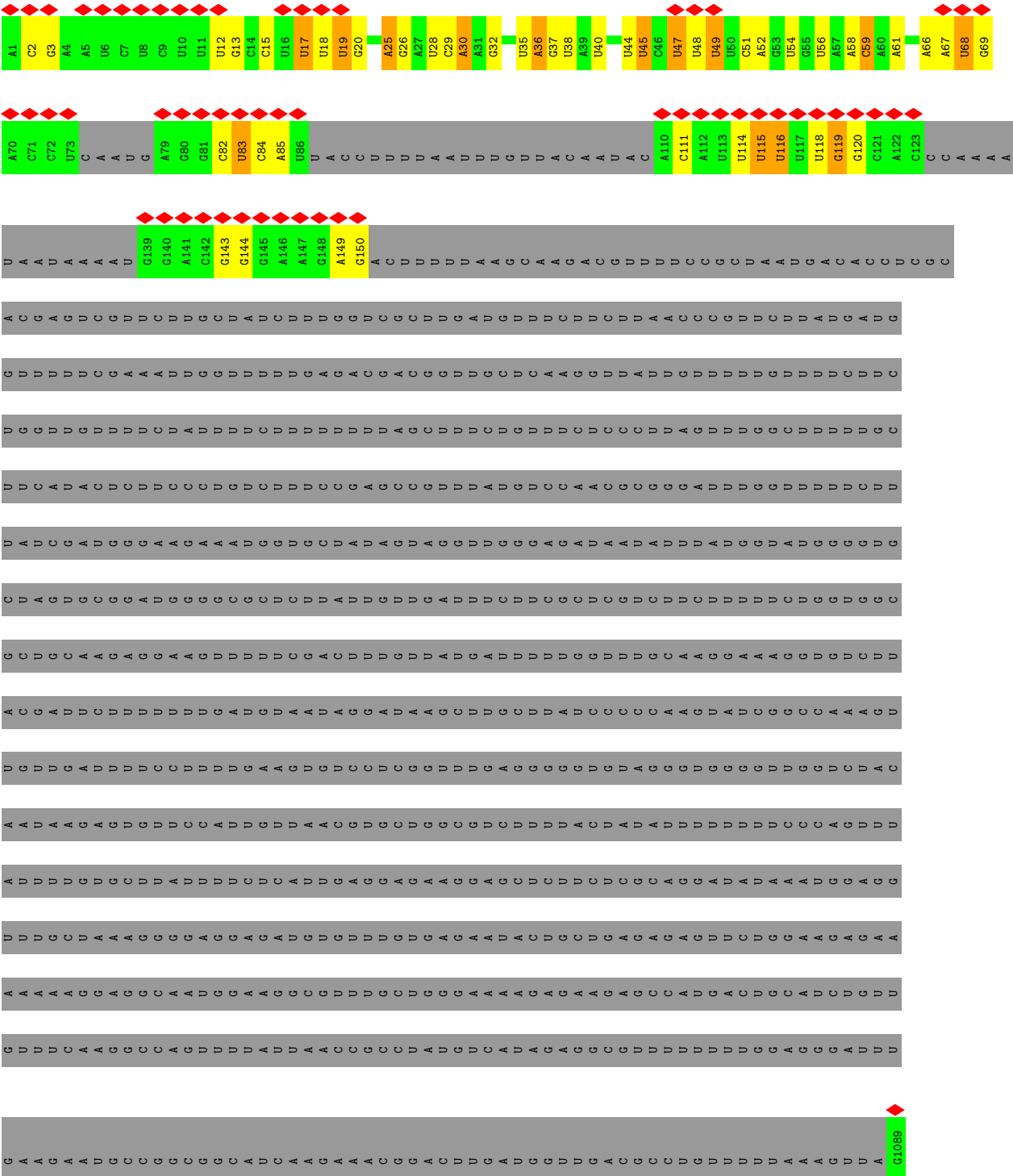


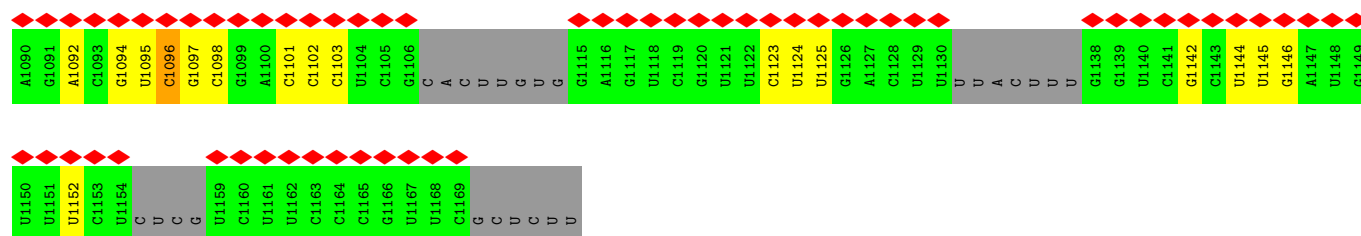
• Molecule 13: pre-mRNA



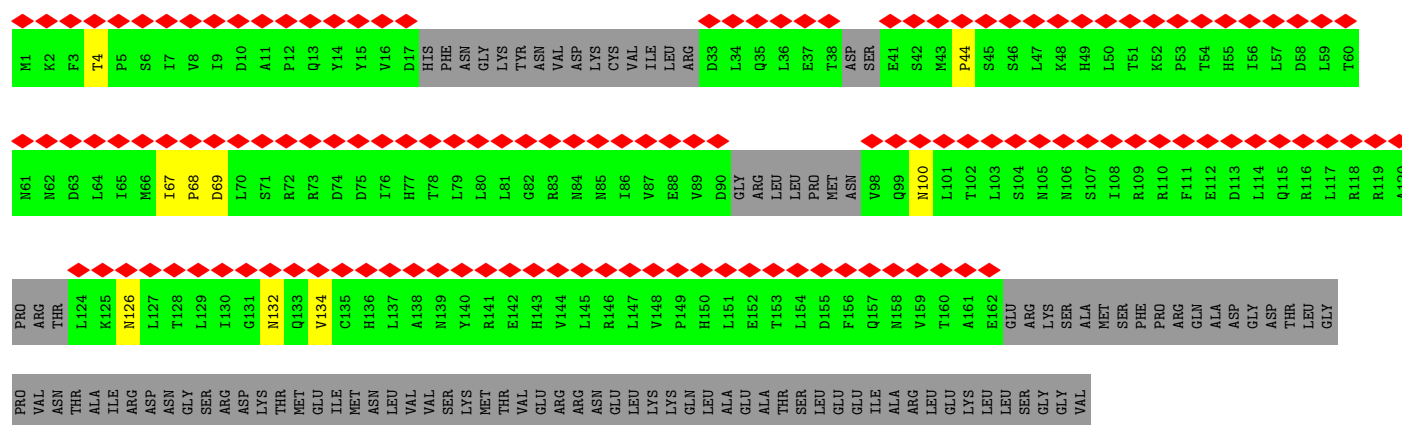


• Molecule 14: U2 snRNA

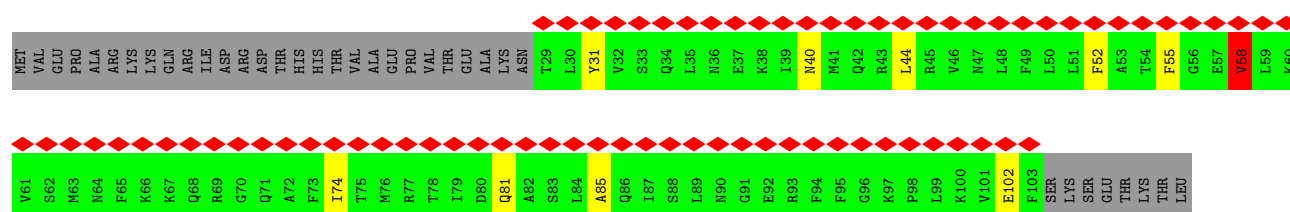




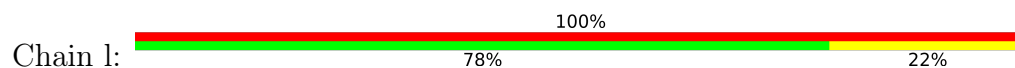
• Molecule 15: HLJ1_G0053790.mRNA.1.CDS.1



• Molecule 16: BJ4_G0027490.mRNA.1.CDS.1



• Molecule 17: Small nuclear ribonucleoprotein Sm D3

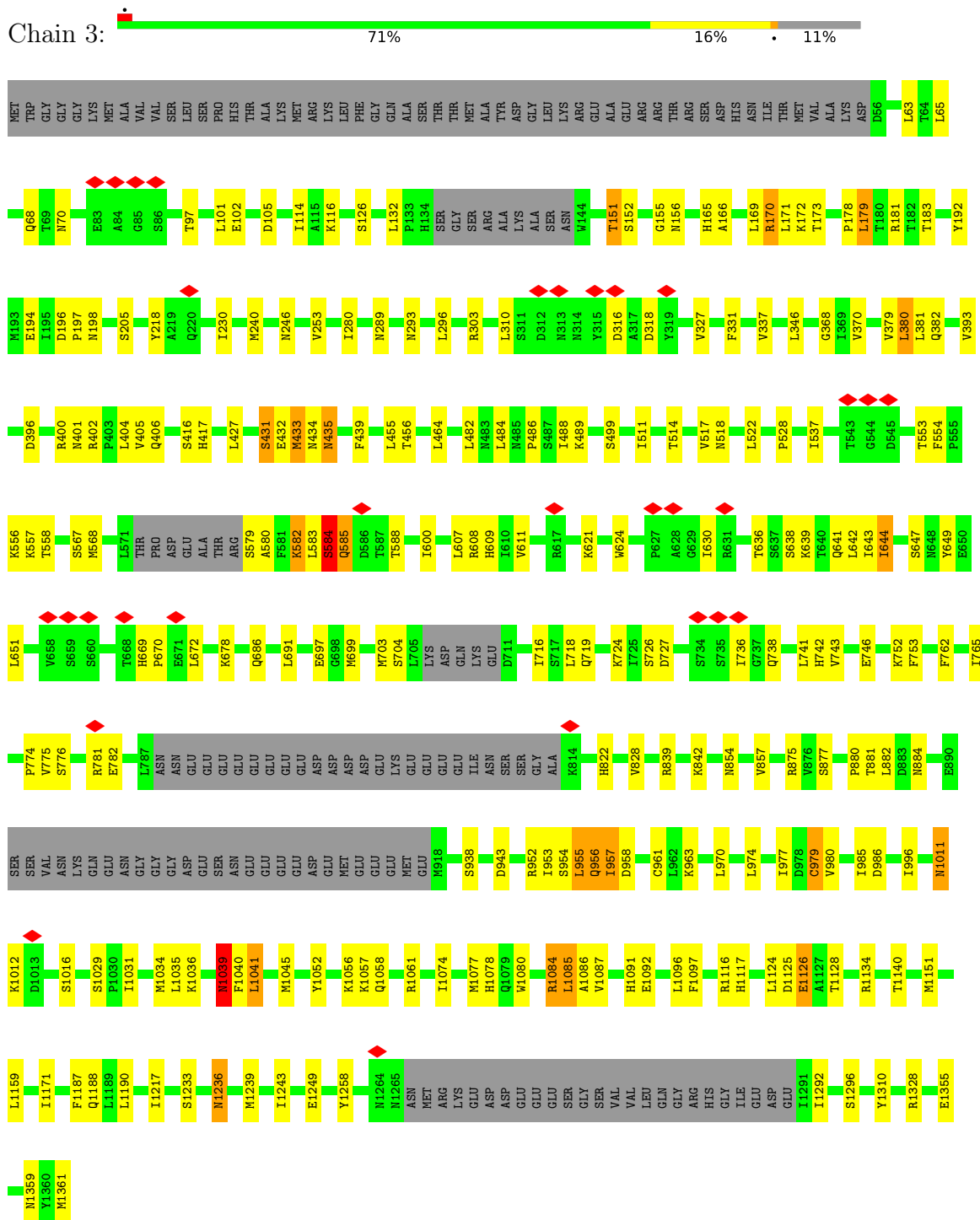


• Molecule 18: PRP9 isoform 1



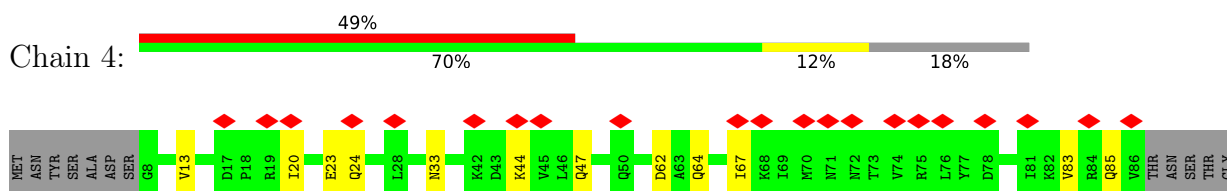
• Molecule 23: RSE1 isoform 1

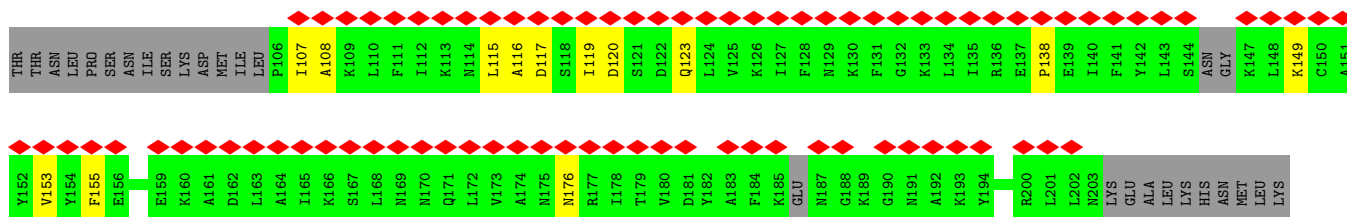
Chain 3:



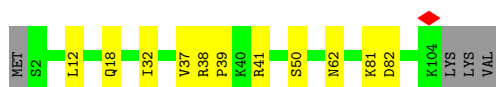
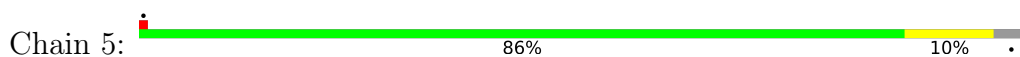
• Molecule 24: HSH49 isoform 1

Chain 4:





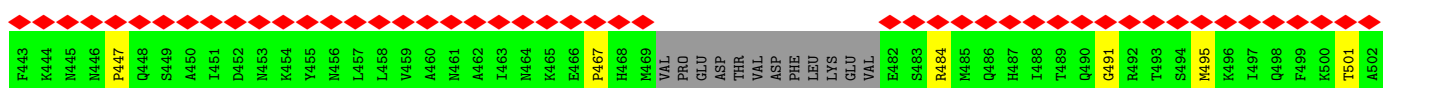
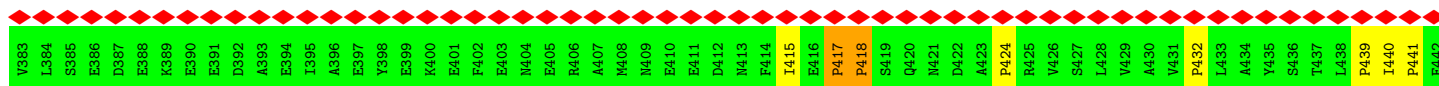
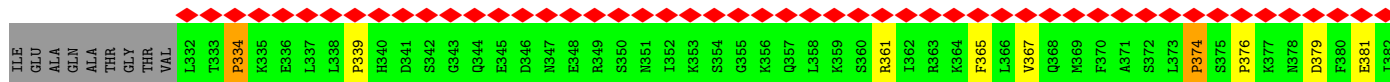
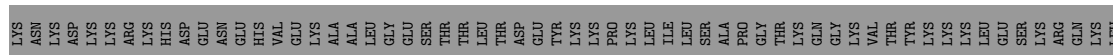
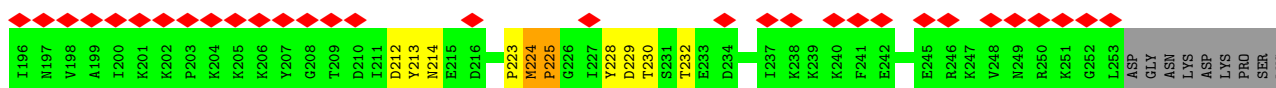
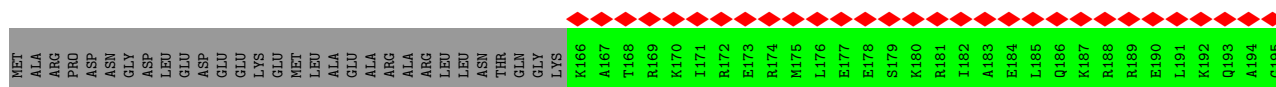
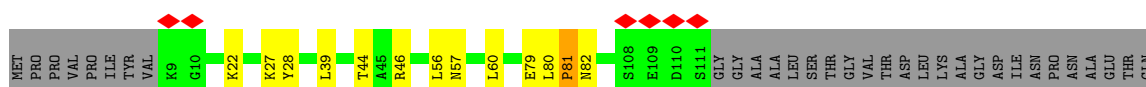
- Molecule 25: BJ4_G0056610.mRNA.1.CDS.1

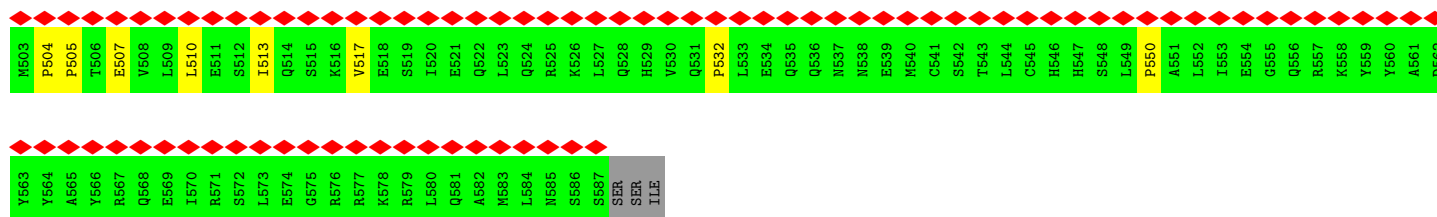


- Molecule 26: RDS3 complex subunit 10

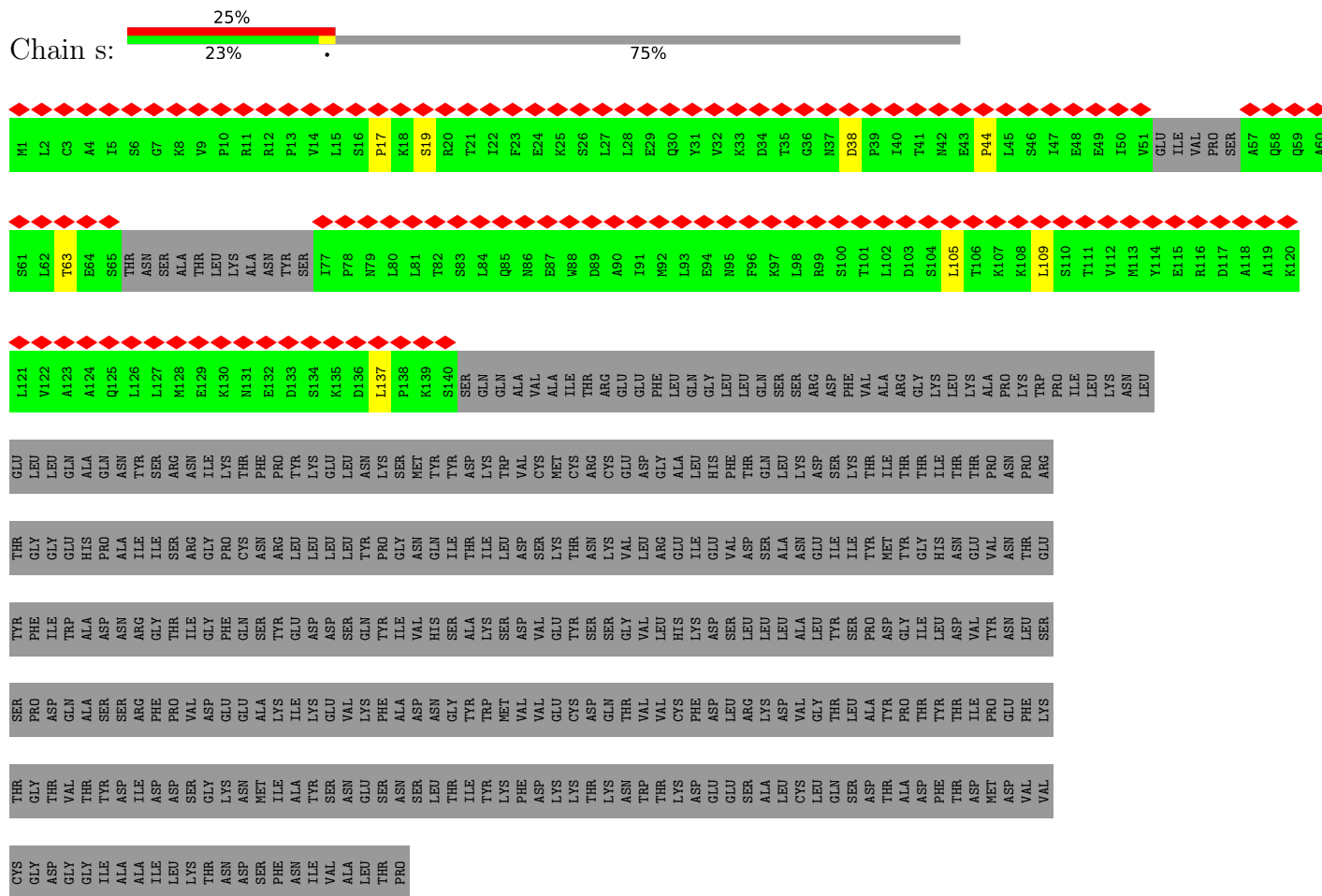


- Molecule 27: Pre-mRNA-splicing factor CEF1

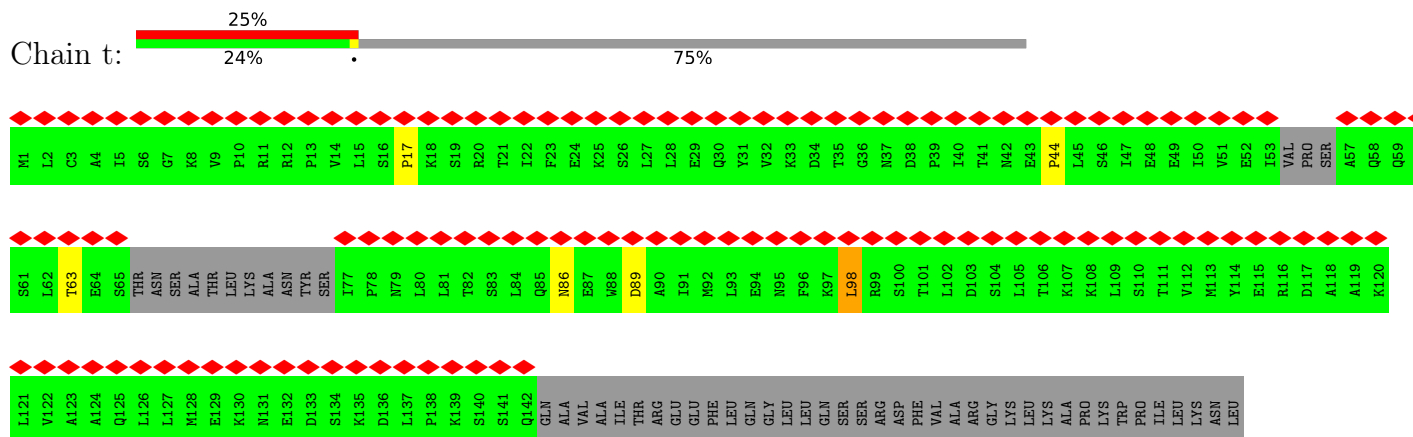


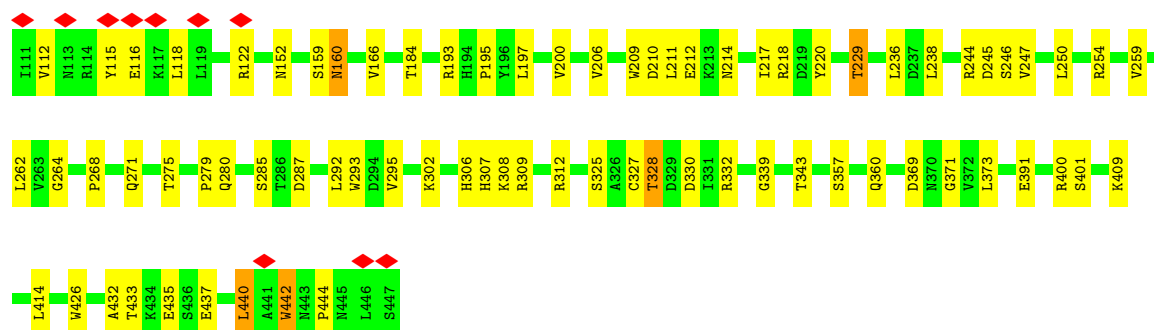


• Molecule 28: Pre-mRNA-processing factor 19

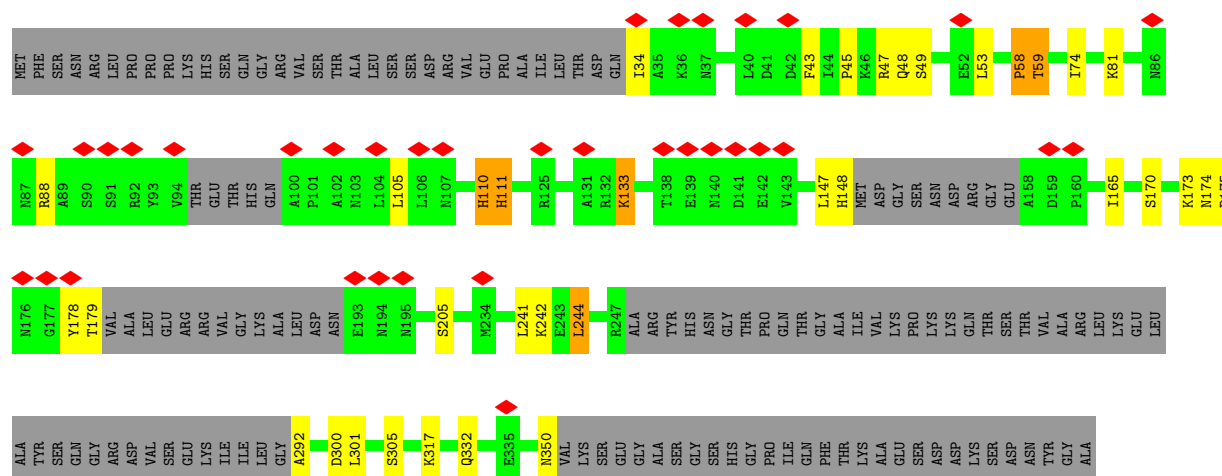


• Molecule 28: Pre-mRNA-processing factor 19

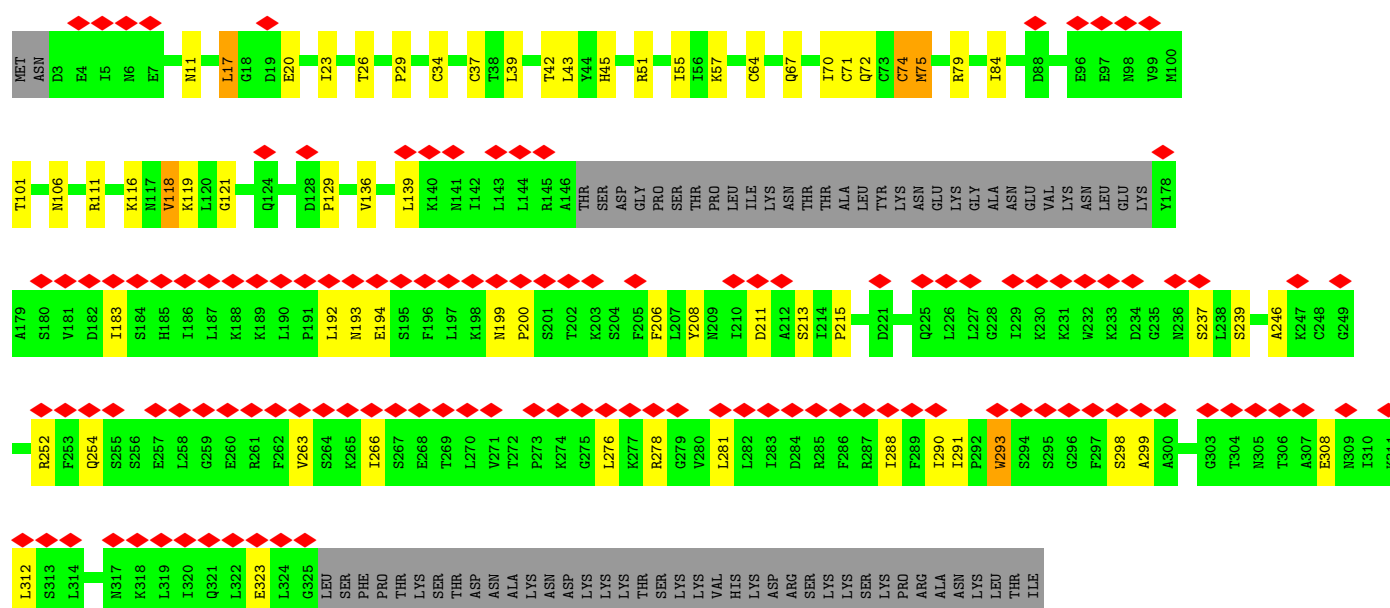




• Molecule 32: Pre-mRNA-processing protein 45

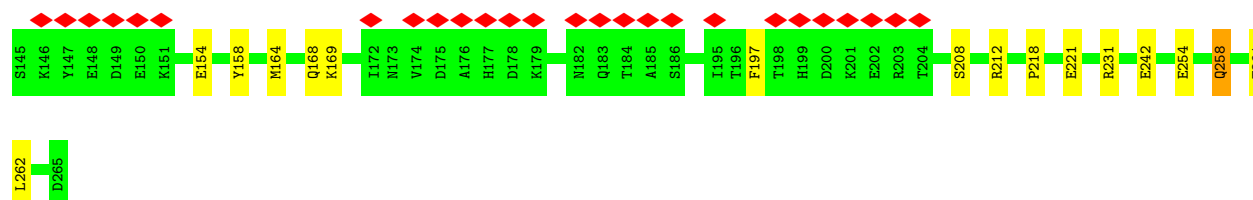
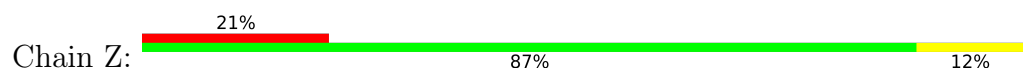


• Molecule 33: Pre-mRNA-splicing factor SLT11

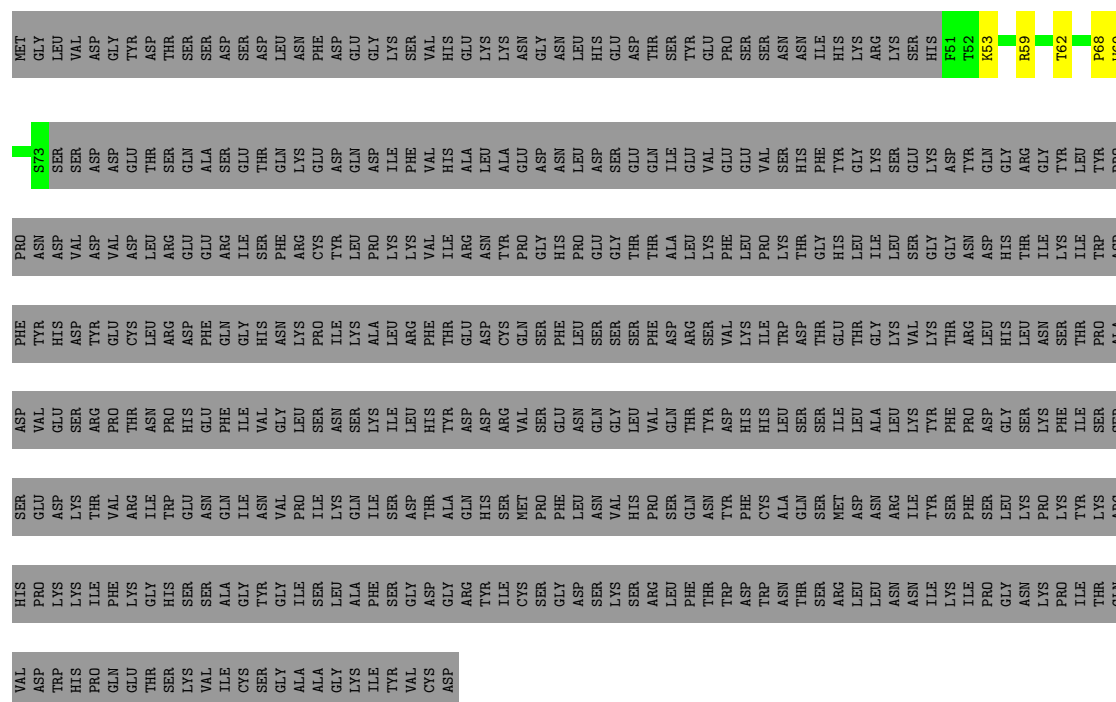




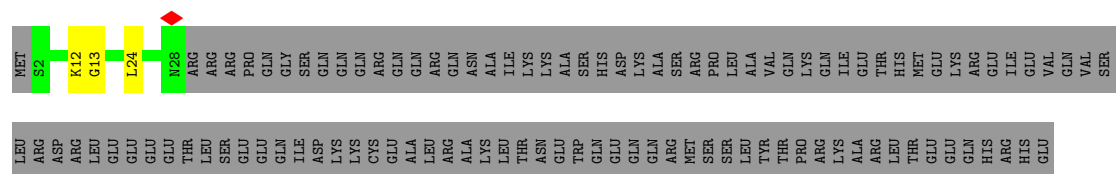
• Molecule 38: Pre-mRNA-splicing factor CWC26



• Molecule 39: CDC40 isoform 1

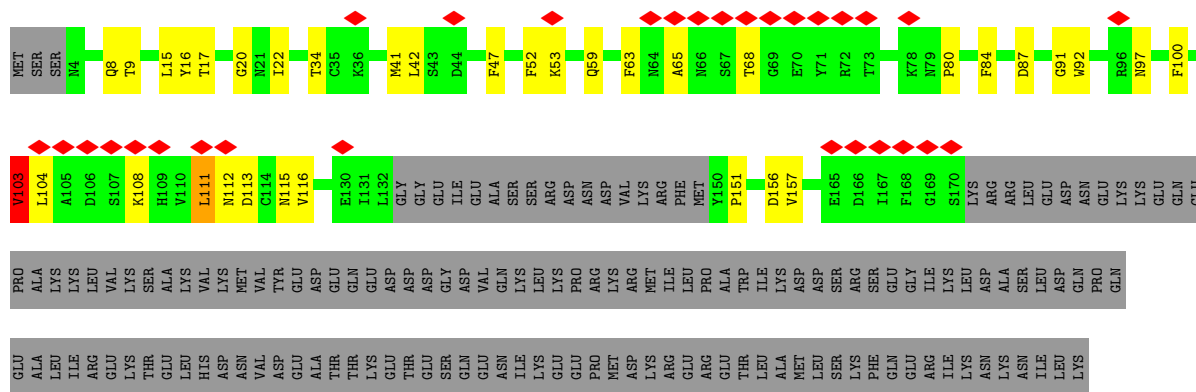


• Molecule 40: Pre-mRNA-splicing factor CWC21

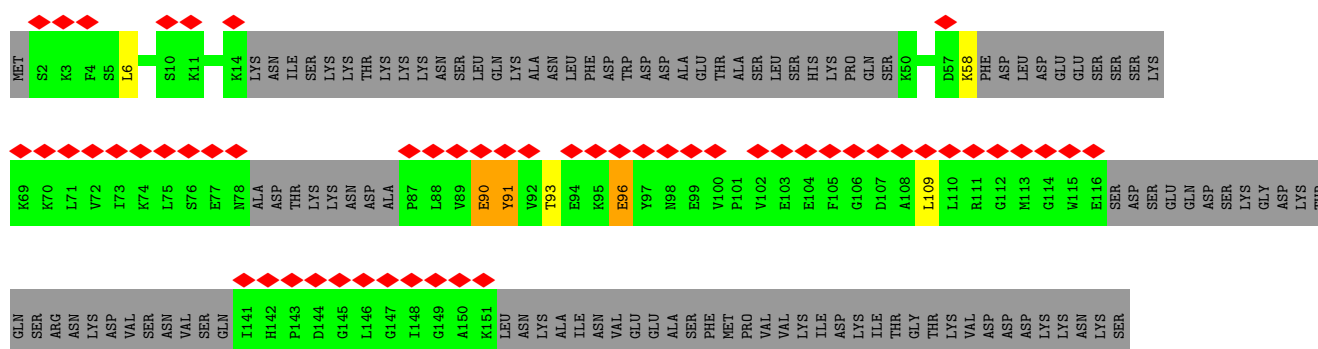


• Molecule 41: CWC22 isoform 1

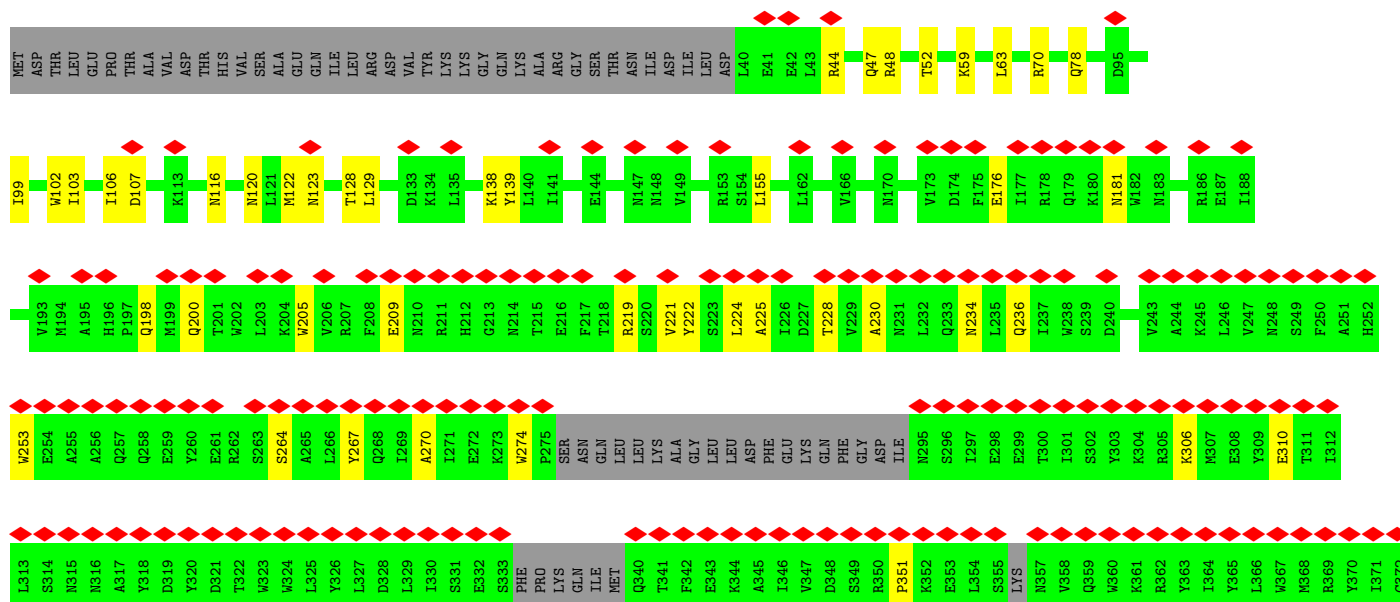




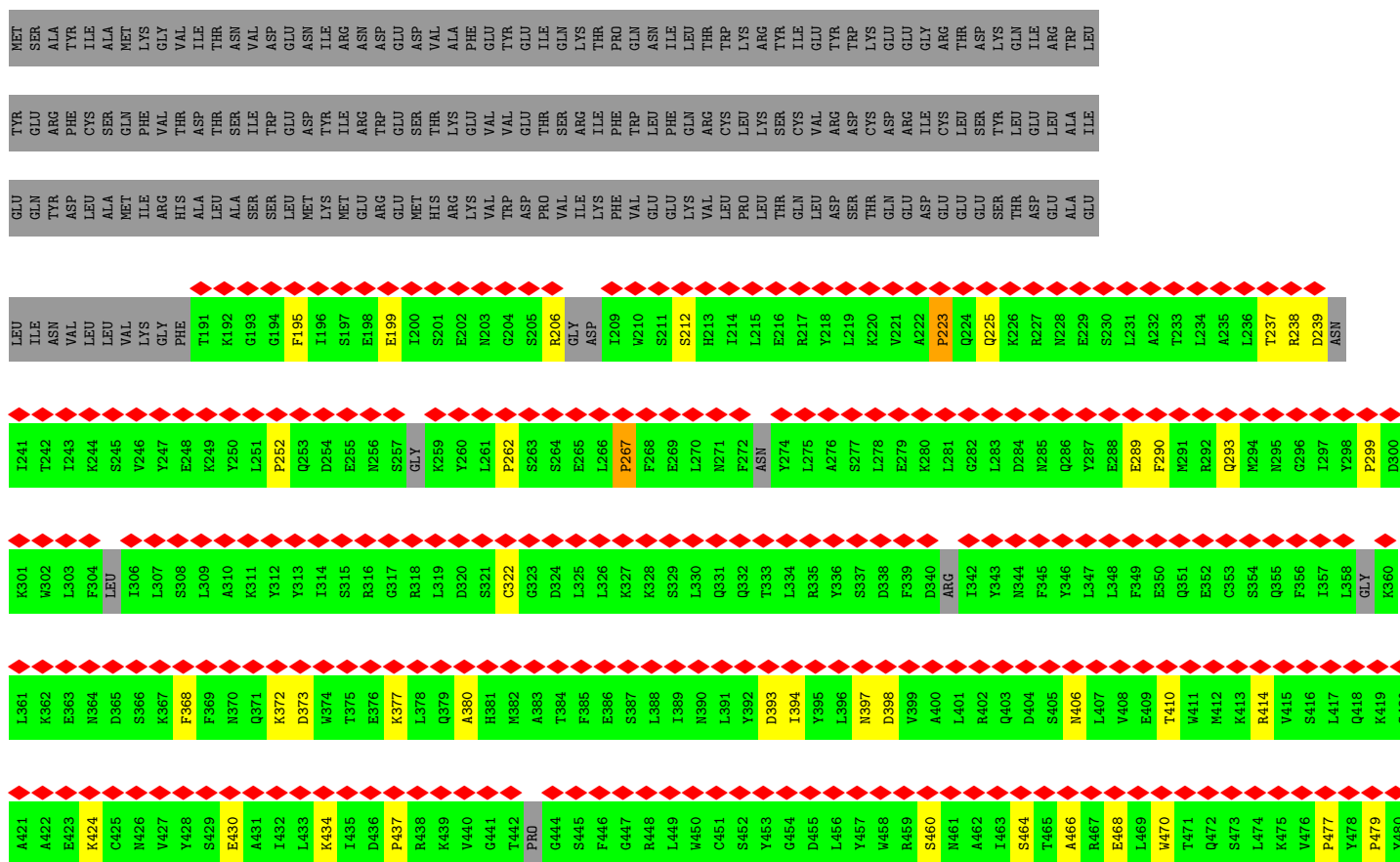
• Molecule 44: Pre-mRNA-splicing factor SPP2



• Molecule 45: CLF1 isoform 1



- Molecule 46: SYF1 isoform 1



R800	S801	S802	L805	R806	V807	T812	S813	I814	W817	N818	H819	K820	E821	Q824	Y832	Q833	Q834	L835	R836	L837	T838	S839	K840	E841	F842	I843	R844	D845	K851	E852	E853	W854	W858	V859	I862	F863	K864	D865	L866	I867	ASP	ASP	LYS	THR	ASN	ARG	GLY	ARG	ARG													
C724	Q725	Q725	D726	H727	K728	I729	Q730	F731	K732	T733	T733	W734	L735	R736	W739			I740	R741	W742	Q743	Q743	L744	F745	R746	C747	S748	E749	K750	V751	G752	L753	V754	E755	K756	N757	D758	Q759	A760	R761	M762	K763	I764	G765	N766	I767	A768	G769	Y770	I771	N772	A773	R774	R777		Y784	M785	T793		W796	G799	
E662	Q663	C664	Q665	G666	V667	L668	E669	E670	C671	L672	T673	S676			M677	L678	H679	E680	T681	F682	S683	L684	F685	I686	G687	Q688	K689	R690	D691	A692	A693	A694	S695	V696	L697	S698	E699	V700	E701	S702	D703	L706			Y707	L708	E709	C647	E648	P649	E650	Q713	W714	R715	N716	S717	K718	F719	S720	R721	S722	W723
L602	I603	K604	F605	P606	L607	M608	D609	K610	P611	S612	I613	P614	T615	L616	R617	K618	S619	L620	E621	N622	L623	Y624	I625	L626	G627	A628	L629	N630	S631	K632	G633	T634	I635	T636	R637	L638	G639	K640	M641	M642	C643	E644	F645	P646	C647	E648	P649	E650	F651	A652	K653	V654	L655	Y656	T657	A658	A659	T660	H661			
S542	R543	A544	S545	V546	D547	Q548	R549	A550	G551	R552	A553	G554	R555	V556	G557	P558	G559	K560	C561	F562	R563	I564	F565	T566	K567	W568	S569	Y570	L571	H572	E573	L574	E575	L576	M577	P578	K579	P580	E581	I582	T583	R584	T585	N586	L587	S588	N589	T590	V591	L592	L593	L594	L595	S596	L597	G598	V599	T600	D601			
E481	Q482	Q483	L484	K485	I486	F487	Q488	P489	T490	P491	E492	M493	C494	R495	K496	V497	V498	L499	A500	T501	N502	I503	A504	E505	T506	S507	L508	T509	I510	D511	G512	I513	R514	Y515	V516	I517	D518	P519	G520	F521	V522	K523	E524	N525	S526	Y527	S530			T531	G532	M533	T534	Q535	L536	L537	T538	V539	P540	C541		
A421	I422	T423	T424	I425	F426	Q427	I428	H429	T430	T431	Q432	Q432	L434	P435	G436	D437	I438	L439	V440	F441	L442	T443	G444	Q445	E446	E447	I448	E449	R450	T451	K452	T453	K454	L455	E456	E457	I458	M459	S460	K461	L462	G463	S464	R465	T466	K467	Q468	M469	I470	I471	T472	P473	I474	Y475	A476	N477	L478	P479	Q480			

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	705371	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.251	Depositor
Minimum map value	-0.119	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.58	0/18595	0.72	4/25207 (0.0%)
2	B	0.37	0/4239	0.52	3/6598 (0.0%)
3	C	0.36	0/7484	0.64	5/10135 (0.0%)
4	D	0.26	0/14978	0.52	1/20302 (0.0%)
5	d	0.15	0/315	0.37	0/392
6	a	0.16	0/290	0.34	0/359
6	h	0.24	0/615	0.62	0/829
7	b	0.14	0/305	0.34	0/376
7	m	0.24	0/649	0.49	0/880
8	c	0.14	0/358	0.31	0/444
8	n	0.27	0/535	0.60	0/717
9	e	0.14	0/285	0.31	0/351
9	i	0.27	0/585	0.58	0/795
10	f	0.16	0/278	0.50	0/344
10	j	0.28	0/564	0.68	0/761
11	g	0.14	0/277	0.38	0/341
11	k	0.23	0/532	0.53	0/715
12	F	0.37	0/2452	0.54	0/3817
13	G	0.35	0/2338	0.57	1/3621 (0.0%)
14	H	0.29	0/3969	0.45	0/6159
15	o	0.20	0/839	0.57	1/1127 (0.1%)
16	p	0.20	0/478	0.58	1/640 (0.2%)
17	l	0.27	0/620	0.58	0/841
18	u	0.26	0/3976	0.56	0/5327
19	w	0.21	0/1105	0.46	0/1475
20	v	0.47	0/1647	0.69	0/2213
21	1	0.58	0/7522	0.79	5/10203 (0.0%)
22	2	0.51	0/1840	0.67	0/2484
23	3	0.55	1/9789 (0.0%)	0.77	5/13273 (0.0%)
24	4	0.27	0/1457	0.55	0/1959
25	5	0.65	0/827	0.84	1/1105 (0.1%)
26	6	0.70	0/702	0.81	0/939

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
27	L	0.38	0/2924	0.75	14/3954 (0.4%)
28	q	0.21	0/856	0.55	0/1155
28	r	0.19	0/828	0.47	1/1117 (0.1%)
28	s	0.18	0/824	0.43	0/1111
28	t	0.19	0/848	0.42	0/1143
29	K	0.20	0/918	0.54	0/1236
30	N	0.52	0/1315	0.73	2/1759 (0.1%)
31	T	0.54	0/2704	0.73	0/3676
32	P	0.44	0/2008	0.72	5/2703 (0.2%)
33	Q	0.35	0/2339	0.79	4/3154 (0.1%)
34	R	0.37	0/2135	0.66	2/2871 (0.1%)
35	S	0.40	0/592	0.76	0/790
36	Y	0.28	0/1408	0.58	0/1900
37	X	0.52	0/1071	0.79	1/1445 (0.1%)
38	Z	0.47	0/936	0.63	0/1264
39	W	0.33	0/200	0.64	0/264
40	U	0.46	0/191	0.69	0/254
41	V	0.40	0/3720	0.63	0/5016
42	M	0.48	0/1385	0.68	3/1862 (0.2%)
43	z	0.35	0/1252	0.65	0/1692
44	y	0.36	0/577	0.65	0/765
45	J	0.31	0/3635	0.68	8/4962 (0.2%)
46	I	0.31	0/3095	0.82	23/4242 (0.5%)
47	x	0.49	0/5290	0.59	0/7155
All	All	0.43	1/131496 (0.0%)	0.65	90/180219 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	3	528	PRO	CA-C	5.21	1.54	1.51

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	L	417	PRO	N-CA-CB	8.57	111.40	103.08
23	3	435	ASN	N-CA-C	7.84	120.43	110.24
2	B	27	G	C2'-C3'-O3'	7.81	121.21	109.50
46	I	773	PRO	N-CA-CB	7.75	110.60	103.08
27	L	432	PRO	N-CA-CB	7.74	110.55	103.20
27	L	418	PRO	N-CA-CB	7.60	111.23	103.25
15	o	69	ASP	N-CA-C	7.45	121.95	111.52
46	I	515	PRO	N-CA-CB	7.37	110.20	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	J	397	PRO	N-CA-CB	7.13	109.98	103.20
33	Q	75	MET	N-CA-C	-7.10	104.57	113.23
27	L	334	PRO	N-CA-CB	7.09	110.69	103.25
23	3	980	VAL	N-CA-C	-7.08	103.95	110.82
45	J	435	PRO	N-CA-CB	7.07	110.30	103.51
46	I	252	PRO	N-CA-CB	7.01	109.98	103.46
46	I	774	PRO	N-CA-CB	6.87	110.47	103.25
46	I	477	PRO	N-CA-CB	6.87	110.46	103.25
46	I	267	PRO	N-CA-CB	6.84	110.44	103.25
46	I	557	PRO	N-CA-CB	6.84	110.77	103.52
45	J	559	PRO	N-CA-CB	6.83	110.52	103.00
46	I	479	PRO	N-CA-CB	6.77	110.36	103.25
27	L	467	PRO	N-CA-CB	6.75	110.33	103.25
27	L	439	PRO	N-CA-CB	6.74	110.33	103.25
25	5	37	VAL	N-CA-C	6.73	118.84	109.29
27	L	374	PRO	N-CA-CB	6.68	110.26	103.25
46	I	223	PRO	N-CA-CB	6.66	110.25	103.25
23	3	434	ASN	N-CA-C	6.64	117.82	108.00
46	I	796	THR	N-CA-C	6.63	118.50	111.28
46	I	533	PRO	N-CA-CB	6.53	110.11	103.25
45	J	421	PRO	N-CA-CB	6.53	110.10	103.25
45	J	545	PRO	N-CA-CB	6.48	110.46	103.33
27	L	447	PRO	N-CA-CB	6.47	110.38	103.52
27	L	376	PRO	N-CA-CB	6.44	110.41	103.33
27	L	441	PRO	N-CA-CB	6.42	110.39	103.33
46	I	299	PRO	N-CA-CB	6.41	110.31	103.52
32	P	110	HIS	CA-C-N	6.37	133.71	121.54
32	P	110	HIS	C-N-CA	6.37	133.71	121.54
45	J	351	PRO	N-CA-CB	6.30	110.50	103.44
27	L	339	PRO	N-CA-CB	6.29	110.19	103.52
46	I	795	GLU	N-CA-C	6.24	118.08	111.28
46	I	437	PRO	N-CA-CB	6.21	110.11	103.52
45	J	412	LYS	N-CA-C	6.20	118.04	111.28
27	L	80	LEU	CA-C-N	6.19	127.58	119.84
27	L	80	LEU	C-N-CA	6.19	127.58	119.84
45	J	468	PRO	N-CA-CB	6.19	109.85	103.23
37	X	107	THR	N-CA-C	6.10	118.12	108.79
46	I	262	PRO	N-CA-CB	5.93	110.09	103.44
46	I	487	ILE	N-CA-C	-5.89	104.77	110.72
21	1	152	PRO	N-CA-CB	5.86	110.00	103.44
46	I	518	PRO	N-CA-CB	5.83	109.70	103.52
1	A	1092	PHE	CA-C-N	5.81	132.63	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1092	PHE	C-N-CA	5.81	132.63	121.54
34	R	54	GLN	CA-C-N	5.79	127.08	119.84
34	R	54	GLN	C-N-CA	5.79	127.08	119.84
3	C	88	THR	CA-C-N	5.78	125.91	119.32
3	C	88	THR	C-N-CA	5.78	125.91	119.32
46	I	509	GLU	N-CA-C	5.78	117.09	108.31
21	1	427	ASP	CA-C-N	5.77	127.05	119.84
21	1	427	ASP	C-N-CA	5.77	127.05	119.84
42	M	232	LYS	N-CA-C	5.72	118.58	109.65
33	Q	74	CYS	CB-CA-C	-5.64	101.26	110.85
16	p	58	VAL	N-CA-C	5.61	116.55	108.48
3	C	443	TYR	N-CA-C	5.60	117.23	107.49
33	Q	118	VAL	CA-C-N	5.59	132.22	121.54
33	Q	118	VAL	C-N-CA	5.59	132.22	121.54
3	C	975	GLY	CA-C-N	5.57	127.79	120.60
3	C	975	GLY	C-N-CA	5.57	127.79	120.60
32	P	58	PRO	CA-C-N	5.56	132.16	121.54
32	P	58	PRO	C-N-CA	5.56	132.16	121.54
1	A	1346	PHE	CA-C-N	5.55	132.15	121.54
1	A	1346	PHE	C-N-CA	5.55	132.15	121.54
13	G	109	A	C4'-C3'-O3'	5.52	117.67	109.40
21	1	830	MET	CA-C-N	5.51	127.93	120.38
21	1	830	MET	C-N-CA	5.51	127.93	120.38
32	P	59	THR	N-CA-CB	5.51	119.80	110.49
42	M	119	LYS	CA-C-N	5.47	129.03	120.82
42	M	119	LYS	C-N-CA	5.47	129.03	120.82
2	B	130	A	C4'-C3'-O3'	5.47	117.60	109.40
46	I	509	GLU	CB-CA-C	-5.42	110.30	116.54
23	3	554	PHE	N-CA-C	-5.36	102.21	110.58
46	I	322	CYS	N-CA-C	-5.36	105.35	111.14
27	L	424	PRO	N-CA-CB	5.30	109.24	103.30
28	r	5	ILE	N-CA-C	-5.30	107.43	111.62
30	N	149	GLY	N-CA-C	-5.28	105.78	114.76
2	B	78	A	C2'-C3'-O3'	5.18	121.47	113.70
46	I	508	LEU	N-CA-C	5.13	117.05	108.99
23	3	743	VAL	N-CA-C	5.11	115.26	108.11
4	D	1646	SER	N-CA-C	5.10	117.50	111.33
46	I	372	LYS	CA-C-N	5.10	131.29	121.54
46	I	372	LYS	C-N-CA	5.10	131.29	121.54
30	N	146	VAL	N-CA-C	5.03	117.34	111.05

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	A	18135	0	18054	199	0
2	B	3795	0	1919	67	0
3	C	7328	0	7505	105	0
4	D	14666	0	14661	122	0
5	d	316	0	86	0	0
6	a	292	0	78	0	0
6	h	610	0	640	26	0
7	b	308	0	78	1	0
7	m	644	0	686	13	0
8	c	360	0	89	1	0
8	n	528	0	573	12	0
9	e	288	0	74	0	0
9	i	575	0	597	20	0
10	f	280	0	77	0	0
10	j	554	0	556	8	0
11	g	280	0	79	0	0
11	k	529	0	557	17	0
12	F	2192	0	1106	20	0
13	G	2099	0	1055	43	0
14	H	3566	0	1809	56	0
15	o	841	0	614	2	0
16	p	476	0	378	11	0
17	l	611	0	627	22	0
18	u	3899	0	3826	63	0
19	w	1084	0	1081	9	0
20	v	1621	0	1596	20	0
21	1	7376	0	7521	83	0
22	2	1793	0	1827	18	0
23	3	9599	0	9679	158	0
24	4	1433	0	1461	16	0
25	5	814	0	809	5	0
26	6	693	0	705	12	0
27	L	2901	0	2325	29	0
28	q	850	0	682	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	r	823	0	654	2	0
28	s	819	0	657	3	0
28	t	843	0	672	2	0
29	K	920	0	603	5	0
30	N	1291	0	1312	8	0
31	T	2646	0	2639	54	0
32	P	1978	0	1981	37	0
33	Q	2301	0	2366	46	0
34	R	2089	0	2053	52	0
35	S	578	0	565	26	0
36	Y	1386	0	1353	27	0
37	X	1051	0	1015	23	0
38	Z	920	0	841	15	0
39	W	195	0	198	3	0
40	U	190	0	186	3	0
41	V	3660	0	3706	40	0
42	M	1360	0	1280	18	0
43	z	1224	0	1217	28	0
44	y	572	0	597	9	0
45	J	3595	0	2639	39	0
46	I	3101	0	1639	32	0
47	x	5193	0	5347	60	0
48	A	36	0	6	2	0
49	C	32	0	12	2	0
50	3	1	0	0	0	0
50	C	1	0	0	0	0
50	F	4	0	0	0	0
51	C	1	0	0	0	0
52	5	3	0	0	0	0
52	M	3	0	0	0	0
52	N	3	0	0	0	0
52	Q	2	0	0	0	0
52	R	1	0	0	0	0
52	u	2	0	0	0	0
52	v	1	0	0	0	0
53	1	185	0	0	4	0
53	2	51	0	0	1	0
53	3	218	0	0	7	0
53	5	53	0	0	0	0
53	6	42	0	0	1	0
53	A	582	0	0	9	0
53	B	127	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	C	8	0	0	0	0
53	D	2	0	0	0	0
53	F	109	0	0	2	0
53	G	56	0	0	1	0
53	H	70	0	0	0	0
53	L	18	0	0	0	0
53	M	21	0	0	0	0
53	N	12	0	0	0	0
53	P	26	0	0	2	0
53	R	8	0	0	0	0
53	S	9	0	0	0	0
53	T	39	0	0	0	0
53	U	6	0	0	0	0
53	V	21	0	0	1	0
53	X	13	0	0	1	0
53	Z	9	0	0	0	0
53	v	29	0	0	0	0
All	All	129875	0	116948	1450	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (1450) 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)
1:A:784:GLN:HG2	14:H:19:U:C5	1.67	1.28
18:u:506:LEU:CD2	18:u:518:LYS:HD2	1.64	1.26
46:I:466:ALA:CB	46:I:470:TRP:CB	2.20	1.19
27:L:224:MET:SD	27:L:225:PRO:HD3	1.82	1.19
27:L:224:MET:SD	27:L:225:PRO:CD	2.33	1.17
46:I:466:ALA:HB3	46:I:470:TRP:CB	1.76	1.14
1:A:784:GLN:CG	14:H:19:U:C5	2.33	1.12
27:L:230:THR:CG2	45:J:116:ASN:HB2	1.80	1.11
18:u:506:LEU:HD21	18:u:518:LYS:HD2	1.29	1.09
27:L:230:THR:HG22	45:J:116:ASN:HB2	1.11	1.08
18:u:506:LEU:HD23	18:u:518:LYS:HA	1.40	1.02
27:L:230:THR:HG22	45:J:116:ASN:CB	1.89	1.02
3:C:438:ALA:O	3:C:442:CYS:HB2	1.57	1.01
23:3:1011:ASN:ND2	23:3:1016:SER:HB3	1.75	1.01
13:G:504:C:H5"	13:G:504:C:H6	1.25	1.01
43:z:87:ASP:HB3	43:z:103:VAL:O	1.62	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:L:224:MET:SD	27:L:225:PRO:HD2	2.02	1.00
46:I:468:GLU:CB	46:I:511:ALA:CB	2.43	0.97
47:x:630:ASN:HD22	47:x:636:THR:HG22	1.26	0.97
23:3:985:ILE:CD1	23:3:1041:LEU:HD23	1.96	0.96
1:A:784:GLN:HG2	14:H:19:U:H5	1.19	0.95
42:M:232:LYS:HB3	42:M:238:LYS:O	1.68	0.94
2:B:26:A:N6	2:B:141:G:H8	1.67	0.92
23:3:433:MET:CE	26:6:62:ILE:HD11	1.99	0.91
11:k:71:LEU:HD21	17:l:63:PHE:CD2	2.05	0.91
3:C:441:ARG:HG2	3:C:441:ARG:HH21	1.34	0.91
32:P:133:LYS:NZ	35:S:16:LYS:HE2	1.86	0.90
3:C:183:GLN:NE2	3:C:187:ARG:HH11	1.69	0.90
14:H:20:G:HO2'	35:S:3:THR:N	1.71	0.88
47:x:630:ASN:HD22	47:x:636:THR:CG2	1.86	0.88
1:A:1028:TRP:HA	1:A:1145:MET:HE1	1.56	0.88
13:G:495:A:H62	14:H:40:U:H3	1.15	0.88
33:Q:75:MET:HE1	34:R:130:PHE:CE1	2.08	0.88
23:3:433:MET:HE1	26:6:62:ILE:HD11	1.53	0.88
37:X:85:THR:CG2	37:X:106:HIS:CE1	2.58	0.87
23:3:1011:ASN:HD22	23:3:1016:SER:HB3	1.36	0.87
34:R:165:SER:HA	34:R:170:ILE:HD12	1.57	0.86
43:z:84:PHE:CD2	43:z:111:LEU:HD13	2.09	0.86
18:u:506:LEU:HD22	18:u:518:LYS:HD2	1.56	0.86
2:B:26:A:C6	2:B:141:G:H8	1.94	0.85
34:R:54:GLN:HB2	34:R:58:HIS:CD2	2.11	0.85
37:X:85:THR:HG22	37:X:106:HIS:HE1	1.39	0.85
46:I:466:ALA:HB1	46:I:470:TRP:CB	2.06	0.85
43:z:87:ASP:CB	43:z:103:VAL:O	2.24	0.85
9:i:18:PHE:CZ	9:i:46:PHE:CE2	2.64	0.85
1:A:1794:LEU:HD22	1:A:1798:ILE:HD12	1.57	0.84
37:X:85:THR:HG22	37:X:106:HIS:CE1	2.13	0.83
1:A:784:GLN:HG2	14:H:19:U:C6	2.13	0.83
13:G:490:A:H61	14:H:44:U:H3	1.23	0.83
13:G:495:A:N6	14:H:40:U:H3	1.77	0.83
31:T:206:VAL:HB	31:T:220:TYR:HB2	1.59	0.83
18:u:508:GLU:HB3	18:u:513:GLY:HA3	1.62	0.82
23:3:938:SER:HB3	23:3:957:ILE:CD1	2.09	0.82
46:I:468:GLU:CB	46:I:511:ALA:HB2	2.08	0.82
23:3:1096:LEU:HD13	23:3:1187:PHE:HZ	1.43	0.81
2:B:26:A:C5	2:B:141:G:C8	2.69	0.81
43:z:84:PHE:HD2	43:z:111:LEU:HD13	1.45	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:A:H61	2:B:164:C:N4	1.80	0.80
29:K:86:LEU:O	29:K:86:LEU:HD22	1.81	0.79
3:C:190:SER:HB2	49:C:1101:GTP:O1G	1.81	0.79
18:u:514:ASN:ND2	23:3:1058:GLN:HG2	1.98	0.79
46:I:468:GLU:CB	46:I:511:ALA:HB1	2.12	0.79
32:P:244:LEU:HD12	36:Y:202:MET:HE1	1.65	0.79
13:G:497:A:H5''	13:G:497:A:H8	1.47	0.78
33:Q:11:ASN:H	33:Q:72:GLN:HE21	1.30	0.78
27:L:484:ARG:CG	29:K:86:LEU:HG	2.14	0.78
40:U:24:LEU:H	41:V:310:HIS:HD2	1.30	0.78
47:x:777:ARG:NH2	47:x:854:TRP:CE2	2.51	0.78
47:x:630:ASN:ND2	47:x:636:THR:HG22	1.99	0.78
2:B:96:U:H3	13:G:99:G:H1	1.30	0.78
18:u:506:LEU:CD2	18:u:518:LYS:HA	2.14	0.77
18:u:63:LYS:HE3	18:u:378:ASP:C	2.09	0.77
21:1:838:ILE:HD11	21:1:864:LEU:HD21	1.65	0.77
3:C:84:GLN:HE21	3:C:88:THR:HG21	1.49	0.76
47:x:777:ARG:NH2	47:x:854:TRP:NE1	2.33	0.76
23:3:1125:ASP:HB2	23:3:1128:THR:HG22	1.67	0.76
2:B:141:G:H3'	2:B:141:G:N3	2.01	0.75
45:J:391:LEU:CB	45:J:425:LYS:O	2.35	0.75
21:1:117:LYS:O	21:1:117:LYS:HD3	1.85	0.75
2:B:26:A:C6	2:B:141:G:C8	2.75	0.74
21:1:117:LYS:HD3	21:1:117:LYS:C	2.12	0.74
47:x:271:LEU:N	47:x:271:LEU:HD13	2.01	0.74
46:I:510:ASP:O	46:I:512:LEU:N	2.20	0.74
46:I:468:GLU:CA	46:I:511:ALA:HB1	2.16	0.74
18:u:506:LEU:HD21	18:u:518:LYS:CD	2.16	0.73
23:3:781:ARG:HG3	23:3:782:GLU:HG2	1.69	0.73
2:B:151:A:N3	2:B:151:A:H2'	2.04	0.73
11:k:71:LEU:HD21	17:l:63:PHE:HD2	1.52	0.73
3:C:441:ARG:HG2	3:C:441:ARG:NH2	2.01	0.73
13:G:504:C:H5''	13:G:504:C:C6	2.18	0.73
34:R:165:SER:HA	34:R:170:ILE:CD1	2.18	0.73
1:A:1228:TRP:CH2	35:S:135:ARG:NH2	2.56	0.72
23:3:1084:ARG:HE	23:3:1126:GLU:HG3	1.52	0.72
23:3:433:MET:HG3	23:3:486:PRO:HD3	1.71	0.72
9:i:21:LEU:CD1	9:i:44:VAL:O	2.38	0.71
46:I:468:GLU:HA	46:I:511:ALA:HB1	1.72	0.71
1:A:784:GLN:CB	14:H:19:U:C5	2.74	0.71
23:3:102:GLU:OE2	23:3:116:LYS:HE2	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:26:A:N7	2:B:141:G:C8	2.59	0.70
3:C:183:GLN:HE21	3:C:187:ARG:HH11	1.35	0.70
6:h:15:LEU:HD12	6:h:15:LEU:O	1.90	0.70
46:I:468:GLU:CA	46:I:511:ALA:CB	2.70	0.70
23:3:938:SER:HB3	23:3:957:ILE:HD11	1.71	0.70
38:Z:258:GLN:HA	38:Z:261:THR:HG22	1.74	0.69
18:u:274:ARG:HG2	18:u:280:ILE:HG12	1.72	0.69
1:A:784:GLN:HB3	14:H:19:U:C4	2.27	0.69
2:B:26:A:N6	2:B:141:G:C8	2.57	0.69
3:C:208:ARG:NH1	3:C:440:THR:OG1	2.26	0.69
1:A:1631:GLY:HA3	1:A:1694:MET:HE3	1.75	0.68
16:p:55:PHE:CG	16:p:85:ALA:HB2	2.28	0.68
1:A:784:GLN:HB3	14:H:19:U:C5	2.29	0.68
4:D:638:LEU:O	4:D:638:LEU:HG	1.94	0.68
1:A:1051:GLU:HG2	1:A:1167:ARG:HH11	1.56	0.68
16:p:55:PHE:CG	16:p:85:ALA:HA	2.29	0.68
3:C:183:GLN:HE21	3:C:187:ARG:NH1	1.91	0.68
1:A:2188:ASN:HD21	1:A:2346:THR:HG23	1.58	0.68
21:1:435:THR:HG23	21:1:464:CYS:SG	2.34	0.68
36:Y:76:THR:HG23	36:Y:204:VAL:HG22	1.76	0.68
34:R:164:PHE:O	34:R:170:ILE:HD11	1.94	0.68
1:A:784:GLN:CD	14:H:19:U:C6	2.72	0.68
36:Y:26:ILE:HG22	36:Y:28:ILE:H	1.58	0.68
46:I:394:ILE:O	46:I:398:ASP:CB	2.42	0.68
1:A:1185:GLU:OE1	35:S:128:ARG:NH2	2.26	0.67
46:I:393:ASP:O	46:I:397:ASN:CB	2.42	0.67
47:x:837:LEU:C	47:x:837:LEU:HD12	2.19	0.67
1:A:733:GLN:NE2	53:A:3101:HOH:O	2.21	0.67
2:B:26:A:H62	2:B:141:G:H8	1.42	0.67
18:u:506:LEU:CD2	18:u:518:LYS:CD	2.59	0.67
21:1:885:ILE:HG22	21:1:886:PRO:HD3	1.76	0.67
23:3:1040:PHE:HB3	23:3:1052:TYR:O	1.92	0.67
42:M:199:CYS:SG	42:M:202:CYS:HB2	2.34	0.67
44:y:90:GLU:HA	44:y:90:GLU:OE1	1.93	0.67
34:R:46:ARG:HH22	34:R:222:LEU:HG	1.59	0.67
1:A:1028:TRP:CE3	1:A:1145:MET:HE3	2.29	0.67
11:k:71:LEU:HD12	11:k:71:LEU:O	1.95	0.67
46:I:765:LEU:O	46:I:768:GLY:N	2.27	0.67
1:A:936:GLU:HG2	1:A:986:PRO:HB3	1.76	0.67
3:C:126:MET:HE1	3:C:132:ARG:HH11	1.59	0.67
32:P:174:ASN:OD1	32:P:175:PRO:HD2	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:M:219:CYS:HB2	42:M:222:CYS:SG	2.34	0.66
1:A:1845:ASN:OD1	1:A:1849:LYS:NZ	2.29	0.66
1:A:784:GLN:HE22	14:H:19:U:H5''	1.59	0.66
23:3:155:GLY:O	23:3:179:LEU:HB2	1.96	0.66
32:P:133:LYS:HZ1	35:S:16:LYS:HE2	1.58	0.66
8:n:45:ILE:HG12	8:n:55:ILE:HG12	1.76	0.65
33:Q:75:MET:HE1	34:R:130:PHE:CD1	2.32	0.65
46:I:460:SER:O	46:I:464:SER:CB	2.43	0.65
3:C:90:LEU:HD11	31:T:166:VAL:HG11	1.77	0.65
6:h:12:LEU:O	6:h:15:LEU:HG	1.96	0.65
4:D:446:VAL:HG13	4:D:905:GLN:HG3	1.78	0.65
21:1:971:LEU:HD23	26:6:52:TYR:CD1	2.31	0.65
17:l:20:SER:HB2	17:l:73:VAL:HB	1.79	0.65
23:3:691:LEU:HB3	23:3:703:MET:HB2	1.77	0.65
23:3:938:SER:HB3	23:3:957:ILE:HD13	1.77	0.65
23:3:1039:ASN:ND2	53:3:1506:HOH:O	2.28	0.65
10:j:51:LEU:HB2	10:j:73:ILE:HB	1.78	0.65
23:3:558:THR:HB	23:3:583:LEU:HA	1.77	0.65
33:Q:192:LEU:O	33:Q:278:ARG:NH2	2.30	0.65
11:k:71:LEU:CD2	17:l:63:PHE:HD2	2.10	0.65
33:Q:239:SER:HB3	33:Q:252:ARG:HB3	1.79	0.65
1:A:273:ASP:HA	1:A:310:ASN:HD21	1.61	0.65
4:D:509:ALA:O	4:D:666:ARG:NH2	2.30	0.65
34:R:46:ARG:HH12	34:R:222:LEU:HD11	1.60	0.65
43:z:42:LEU:HB3	43:z:157:VAL:HG11	1.79	0.64
14:H:36:A:H8	14:H:36:A:H5''	1.62	0.64
23:3:985:ILE:HD13	23:3:1041:LEU:HD23	1.77	0.64
27:L:230:THR:CG2	45:J:116:ASN:CB	2.60	0.64
18:u:5:GLU:HB2	19:w:101:ARG:HH21	1.63	0.64
13:G:504:C:H6	13:G:504:C:C5'	2.05	0.64
23:3:165:HIS:HB3	23:3:170:ARG:HD3	1.78	0.64
23:3:433:MET:HE3	26:6:62:ILE:HD11	1.76	0.64
41:V:408:THR:HG22	41:V:410:GLU:H	1.62	0.64
47:x:509:THR:HA	47:x:552:ARG:HH22	1.63	0.64
1:A:784:GLN:CD	14:H:19:U:C5	2.76	0.64
47:x:664:CYS:SG	47:x:777:ARG:HG2	2.37	0.64
1:A:605:LEU:H	42:M:140:GLN:HE22	1.46	0.64
33:Q:194:GLU:O	33:Q:278:ARG:NH1	2.30	0.64
47:x:505:GLU:HG3	47:x:506:THR:HG23	1.80	0.64
4:D:2052:GLU:HB3	4:D:2076:THR:HB	1.79	0.63
23:3:638:SER:HB3	23:3:641:GLN:HB3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:361:THR:HG23	3:C:362:LYS:HG3	1.78	0.63
33:Q:215:PRO:HB3	34:R:171:ASP:OD2	1.97	0.63
1:A:1051:GLU:OE2	1:A:1204:ARG:NH2	2.29	0.63
9:i:21:LEU:HD12	9:i:44:VAL:O	1.99	0.63
23:3:985:ILE:HD11	23:3:1041:LEU:HD23	1.81	0.63
31:T:360:GLN:NE2	31:T:409:LYS:O	2.32	0.63
43:z:59:GLN:C	43:z:103:VAL:HG23	2.24	0.63
2:B:150:U:O5'	2:B:150:U:H6	1.81	0.63
2:B:147:C:H2'	2:B:148:G:H8	1.64	0.63
4:D:1204:VAL:HG12	4:D:1222:ILE:HG12	1.81	0.63
23:3:181:ARG:NH2	53:3:1518:HOH:O	2.32	0.63
1:A:784:GLN:CG	14:H:19:U:C6	2.79	0.63
27:L:228:TYR:HB2	45:J:120:ASN:HB3	1.81	0.62
46:I:510:ASP:C	46:I:512:LEU:H	2.07	0.62
37:X:97:ILE:O	37:X:97:ILE:HG22	2.00	0.62
14:H:54:U:H3	14:H:61:A:H61	1.46	0.62
4:D:1137:THR:HG21	4:D:1148:GLN:HE21	1.65	0.62
27:L:224:MET:CE	27:L:225:PRO:HD2	2.29	0.62
43:z:92:TRP:HB3	43:z:115:ASN:HB3	1.82	0.62
2:B:26:A:C5	2:B:141:G:H8	2.14	0.62
8:n:53:LYS:HB2	8:n:75:LEU:HB2	1.81	0.62
18:u:514:ASN:ND2	23:3:1057:LYS:HB2	2.14	0.62
30:N:132:GLU:HA	30:N:135:LYS:HD3	1.82	0.62
1:A:263:PRO:HD2	30:N:7:ARG:HH11	1.64	0.62
2:B:1:A:H61	2:B:164:C:H42	1.48	0.62
1:A:2398:LEU:HA	4:D:1147:ARG:HH12	1.65	0.62
34:R:202:GLN:O	34:R:220:GLY:HA2	2.00	0.62
45:J:387:LEU:C	45:J:389:GLN:H	2.08	0.62
4:D:433:LYS:HE2	4:D:914:SER:HA	1.82	0.62
23:3:704:SER:HB3	23:3:716:ILE:HD11	1.80	0.62
1:A:543:ASN:ND2	53:A:3132:HOH:O	2.32	0.61
32:P:133:LYS:HZ2	35:S:16:LYS:HE2	1.62	0.61
21:1:253:ASP:O	21:1:259:ARG:NH2	2.29	0.61
23:3:192:TYR:HB2	23:3:205:SER:HB3	1.82	0.61
14:H:38:U:OP2	21:1:186:ARG:NH1	2.33	0.61
23:3:600:ILE:HD11	23:3:607:LEU:HD23	1.82	0.61
2:B:149:U:H6	2:B:149:U:O5'	1.84	0.61
9:i:90:ILE:HB	11:k:62:VAL:HB	1.82	0.61
22:2:285:MET:HE2	24:4:23:GLU:HG3	1.82	0.61
3:C:707:SER:HB3	3:C:824:SER:HB3	1.83	0.61
2:B:43:G:H2'	2:B:45:A:H5'	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1982:MET:HE3	4:D:1988:TRP:HA	1.82	0.60
1:A:254:HIS:HE2	43:z:80:PRO:HB2	1.67	0.60
16:p:55:PHE:CG	16:p:85:ALA:CA	2.84	0.60
3:C:183:GLN:HE22	3:C:654:CYS:HA	1.66	0.60
4:D:1455:LEU:O	4:D:1462:ARG:NH1	2.33	0.60
12:F:84:C:H5''	12:F:84:C:H6	1.66	0.60
31:T:197:LEU:HB3	31:T:209:TRP:HB2	1.83	0.60
32:P:34:ILE:HG13	45:J:123:ASN:HA	1.84	0.60
44:y:96:GLU:HG2	47:x:631:SER:OG	2.01	0.60
1:A:1486:ARG:NH2	41:V:379:ASP:OD2	2.35	0.60
1:A:2207:ILE:HG22	1:A:2224:VAL:HG22	1.84	0.60
12:F:50:G:O2'	12:F:51:A:N7	2.33	0.60
23:3:406:GLN:HG2	23:3:456:THR:HG22	1.83	0.60
34:R:123:ASP:O	34:R:224:LYS:HD2	2.02	0.60
36:Y:83:TYR:HB3	36:Y:88:LYS:HG2	1.84	0.60
6:h:12:LEU:HD12	6:h:15:LEU:HD11	1.83	0.60
21:1:855:GLN:NE2	53:1:1005:HOH:O	2.30	0.60
32:P:81:LYS:HG3	35:S:21:THR:HG22	1.83	0.60
1:A:586:LYS:NZ	53:F:304:HOH:O	2.34	0.60
18:u:503:GLU:HG2	23:3:1061:ARG:HH11	1.67	0.60
1:A:1145:MET:HE2	1:A:1160:LEU:HD13	1.83	0.59
2:B:8:U:H3	2:B:157:G:H1	1.48	0.59
2:B:96:U:H5'	20:v:4:LEU:HD12	1.83	0.59
23:3:1126:GLU:HG2	23:3:1126:GLU:O	2.01	0.59
44:y:90:GLU:HB3	44:y:91:TYR:HD1	1.67	0.59
18:u:174:GLU:HG2	18:u:180:MET:HA	1.83	0.59
23:3:435:ASN:N	23:3:435:ASN:HD22	2.00	0.59
31:T:115:TYR:HD1	31:T:118:LEU:HD12	1.67	0.59
1:A:207:ARG:NH1	1:A:297:SER:O	2.35	0.59
3:C:91:VAL:HG12	3:C:91:VAL:O	2.01	0.59
1:A:376:ARG:NH2	3:C:910:GLU:OE2	2.36	0.59
34:R:124:MET:HE3	34:R:227:ASN:HD21	1.66	0.59
23:3:370:VAL:HG22	23:3:379:VAL:HG22	1.85	0.59
42:M:76:LEU:HD23	43:z:9:THR:HG23	1.84	0.59
3:C:347:ARG:HD2	3:C:352:VAL:HG21	1.83	0.59
12:F:39:G:N1	34:R:120:TYR:O	2.36	0.59
18:u:508:GLU:HB3	18:u:513:GLY:CA	2.32	0.59
23:3:337:VAL:HG22	23:3:346:LEU:HB2	1.83	0.59
33:Q:39:LEU:HD11	33:Q:111:ARG:HG3	1.83	0.59
46:I:237:THR:C	46:I:239:ASP:H	2.11	0.59
1:A:1861:THR:HG1	1:A:1863:HIS:HE2	1.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:90:LEU:HD23	3:C:90:LEU:O	2.03	0.59
21:1:962:GLU:O	26:6:36:ARG:NH2	2.36	0.59
31:T:307:HIS:NE2	31:T:325:SER:OG	2.31	0.59
32:P:305:SER:HB2	38:Z:221:GLU:HG2	1.85	0.59
1:A:389:HIS:HD2	3:C:660:ARG:HD2	1.66	0.59
1:A:1156:HIS:HD2	1:A:1158:ILE:H	1.51	0.59
9:i:18:PHE:CZ	9:i:46:PHE:CD2	2.90	0.59
18:u:150:PRO:HG3	18:u:154:THR:H	1.67	0.59
20:v:178:PRO:HB3	20:v:203:TYR:HB2	1.83	0.59
33:Q:246:ALA:HB1	33:Q:312:LEU:HD22	1.85	0.59
1:A:1004:ASP:OD2	1:A:1506:ARG:NH2	2.34	0.58
47:x:337:LEU:O	47:x:369:ARG:NH1	2.36	0.58
4:D:2139:ASN:HA	4:D:2159:GLU:HA	1.85	0.58
20:v:229:ASN:ND2	24:4:117:ASP:OD2	2.36	0.58
23:3:985:ILE:CD1	23:3:1041:LEU:CD2	2.78	0.58
34:R:159:ARG:NH1	34:R:209:ASP:OD2	2.36	0.58
47:x:508:LEU:O	47:x:552:ARG:NH2	2.36	0.58
4:D:1822:ILE:HG12	4:D:1844:ILE:HG12	1.83	0.58
23:3:719:GLN:HG2	23:3:762:PHE:HD2	1.67	0.58
23:3:1134:ARG:NH1	53:3:1520:HOH:O	2.33	0.58
37:X:85:THR:CG2	37:X:106:HIS:ND1	2.66	0.58
43:z:34:THR:OG1	43:z:115:ASN:ND2	2.36	0.58
1:A:425:ASP:HB3	1:A:428:LEU:HG	1.85	0.58
7:m:93:ARG:HD3	8:n:48:LEU:HD21	1.85	0.58
18:u:514:ASN:CG	23:3:1058:GLN:HG2	2.27	0.58
31:T:285:SER:OG	31:T:287:ASP:OD1	2.20	0.58
3:C:183:GLN:NE2	3:C:187:ARG:NH1	2.46	0.58
3:C:348:LEU:HD13	3:C:372:THR:HG22	1.86	0.58
1:A:1030:GLN:HE22	1:A:1289:VAL:H	1.50	0.58
3:C:143:HIS:CE1	3:C:189:LEU:HD12	2.39	0.58
4:D:699:ARG:NH1	4:D:701:CYS:O	2.37	0.58
45:J:393:ASP:C	45:J:395:ILE:H	2.12	0.58
1:A:1228:TRP:CH2	35:S:135:ARG:CZ	2.86	0.58
1:A:2294:PHE:HB3	1:A:2301:SER:HB2	1.84	0.58
23:3:517:VAL:HG21	23:3:828:VAL:HG21	1.86	0.58
23:3:651:LEU:HB3	23:3:670:PRO:HG2	1.85	0.58
23:3:955:LEU:C	23:3:955:LEU:HD12	2.29	0.58
31:T:275:THR:OG1	31:T:279:PRO:O	2.22	0.58
1:A:585:ARG:NH1	53:A:3101:HOH:O	2.32	0.58
1:A:1047:ALA:HB3	1:A:1251:TYR:HB3	1.84	0.58
1:A:2393:LEU:HD21	4:D:1161:GLU:HB3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:501:ILE:HG12	3:C:567:ILE:HG23	1.86	0.58
31:T:229:THR:HG21	31:T:271:GLN:HA	1.85	0.58
45:J:391:LEU:CB	45:J:425:LYS:CB	2.82	0.58
1:A:1159:ARG:NH1	53:A:3156:HOH:O	2.37	0.58
1:A:1881:THR:O	1:A:1889:LEU:HD23	2.03	0.58
3:C:191:ILE:HG22	3:C:192:LYS:HG2	1.86	0.58
21:1:885:ILE:CG2	21:1:886:PRO:HD3	2.33	0.58
23:3:156:ASN:HD22	23:3:178:PRO:HA	1.68	0.57
38:Z:254:GLU:HG2	38:Z:258:GLN:HE22	1.67	0.57
41:V:101:MET:O	41:V:105:GLN:NE2	2.37	0.57
4:D:1159:ARG:NH1	4:D:1183:ILE:O	2.35	0.57
4:D:1494:ARG:NH2	4:D:1757:GLU:OE2	2.37	0.57
21:1:867:ASN:HD21	25:5:38:ARG:HH12	1.52	0.57
41:V:454:ASP:HB3	41:V:457:HIS:HD2	1.68	0.57
3:C:731:GLY:HA2	13:G:74:A:H1'	1.85	0.57
1:A:2403:GLU:OE1	4:D:813:ARG:NH2	2.35	0.57
12:F:85:C:N4	14:H:20:G:O6	2.38	0.57
13:G:497:A:O2'	20:v:65:LYS:NZ	2.38	0.57
34:R:161:ARG:HG2	34:R:173:ILE:HD13	1.85	0.57
1:A:954:ILE:HG23	1:A:991:THR:HG23	1.86	0.57
32:P:88:ARG:NH2	53:P:401:HOH:O	2.38	0.57
43:z:52:PHE:HA	43:z:63:PHE:HB3	1.87	0.57
47:x:837:LEU:HD12	47:x:837:LEU:O	2.05	0.57
1:A:1747:ASP:OD1	1:A:1747:ASP:N	2.37	0.57
21:1:971:LEU:HB3	26:6:52:TYR:CZ	2.39	0.57
3:C:190:SER:O	3:C:216:PRO:HB3	2.05	0.56
34:R:26:THR:HB	34:R:37:TRP:HB2	1.87	0.56
3:C:438:ALA:O	3:C:442:CYS:CB	2.43	0.56
4:D:749:GLU:OE1	4:D:752:ARG:NH1	2.37	0.56
4:D:962:SER:O	4:D:968:LYS:NZ	2.36	0.56
20:v:33:LEU:HD11	27:L:39:LEU:HD13	1.86	0.56
22:2:296:GLN:NE2	22:2:306:GLU:OE2	2.39	0.56
28:s:137:LEU:HD23	28:r:137:LEU:HD23	1.87	0.56
32:P:133:LYS:NZ	35:S:16:LYS:CE	2.66	0.56
16:p:55:PHE:CG	16:p:85:ALA:CB	2.88	0.56
19:w:148:PHE:HB2	19:w:151:GLN:HB2	1.86	0.56
21:1:117:LYS:HE2	21:1:121:ASP:HB3	1.88	0.56
23:3:246:ASN:HD22	23:3:303:ARG:HH22	1.53	0.56
2:B:96:U:O2	13:G:99:G:N2	2.27	0.56
16:p:52:PHE:HB2	16:p:58:VAL:HG11	1.88	0.56
36:Y:132:PRO:HD2	36:Y:197:TYR:HE2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:968:ASP:OD2	27:L:46:ARG:NH2	2.39	0.56
23:3:293:ASN:HB2	26:6:67:ILE:HD13	1.87	0.56
36:Y:41:GLU:OE2	37:X:98:GLY:N	2.38	0.56
1:A:420:PRO:HG2	1:A:423:PHE:HB2	1.88	0.56
2:B:152:C:H6	2:B:152:C:O5'	1.87	0.56
12:F:41:A:H1'	34:R:34:TYR:CZ	2.40	0.56
42:M:251:GLN:O	42:M:255:ASN:ND2	2.39	0.56
13:G:94:U:H2'	13:G:94:U:O2	2.04	0.56
21:1:767:LEU:HD22	21:1:804:GLU:HG2	1.86	0.56
34:R:54:GLN:HB2	34:R:58:HIS:HD2	1.65	0.56
1:A:978:ILE:HG13	35:S:174:VAL:HG13	1.88	0.56
18:u:508:GLU:CB	18:u:513:GLY:HA3	2.34	0.56
3:C:156:ASP:OD2	3:C:432:GLN:NE2	2.34	0.55
13:G:497:A:H5''	13:G:497:A:C8	2.35	0.55
18:u:204:LEU:HD23	18:u:207:LEU:HD12	1.88	0.55
20:v:69:LYS:O	22:2:186:ARG:NH1	2.38	0.55
23:3:105:ASP:HB2	23:3:114:ILE:HD11	1.88	0.55
34:R:164:PHE:C	34:R:170:ILE:HD11	2.31	0.55
18:u:172:ARG:O	18:u:175:GLN:NE2	2.39	0.55
22:2:364:PHE:H	23:3:1125:ASP:CG	2.14	0.55
24:4:44:LYS:O	24:4:47:GLN:NE2	2.39	0.55
1:A:1442:ARG:NH2	53:A:3172:HOH:O	2.40	0.55
1:A:2225:VAL:HG22	1:A:2350:ILE:HB	1.88	0.55
13:G:486:A:C5	20:v:96:ARG:HD2	2.41	0.55
23:3:579:SER:OG	23:3:580:ALA:N	2.39	0.55
23:3:611:VAL:HG21	23:3:621:LYS:HE2	1.87	0.55
32:P:110:HIS:O	32:P:111:HIS:ND1	2.39	0.55
1:A:244:ASP:OD1	1:A:596:ASN:ND2	2.31	0.55
23:3:568:MET:HB3	44:y:6:LEU:HB3	1.87	0.55
37:X:82:GLN:H	38:Z:168:GLN:HE22	1.54	0.55
3:C:632:VAL:HG21	3:C:655:LEU:HD21	1.87	0.55
23:3:1011:ASN:ND2	23:3:1016:SER:CB	2.62	0.55
23:3:1080:TRP:CD1	23:3:1126:GLU:HB2	2.42	0.55
34:R:46:ARG:NH2	34:R:222:LEU:HG	2.22	0.55
36:Y:80:LEU:HD21	36:Y:199:LEU:HD23	1.88	0.55
1:A:220:THR:HG22	1:A:224:MET:HE2	1.87	0.55
1:A:1028:TRP:CE3	1:A:1145:MET:CE	2.89	0.55
1:A:1362:LYS:NZ	40:U:13:GLY:O	2.40	0.55
1:A:1595:ARG:NH1	53:A:3169:HOH:O	2.39	0.55
1:A:2070:ASN:OD1	32:P:350:ASN:ND2	2.34	0.55
4:D:679:ASP:OD1	4:D:682:ARG:NH1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:2102:VAL:HB	4:D:2143:TRP:HB2	1.88	0.55
18:u:506:LEU:HD22	18:u:518:LYS:CD	2.32	0.55
23:3:318:ASP:OD1	23:3:318:ASP:N	2.36	0.55
33:Q:281:LEU:HB2	33:Q:288:ILE:HB	1.89	0.55
34:R:83:LEU:HB2	34:R:87:CYS:HB2	1.88	0.55
45:J:198:GLN:OE1	45:J:200:GLN:NE2	2.39	0.55
4:D:2011:ILE:HD11	4:D:2030:ILE:HD11	1.89	0.55
23:3:736:ILE:HG23	23:3:738:GLN:H	1.71	0.55
45:J:176:GLU:OE1	45:J:181:ASN:ND2	2.31	0.55
25:5:18:GLN:OE1	25:5:50:SER:OG	2.24	0.55
45:J:103:ILE:HA	45:J:106:ILE:HD12	1.89	0.55
1:A:1717:LEU:O	1:A:1799:GLN:NE2	2.36	0.55
4:D:636:ILE:C	4:D:638:LEU:H	2.14	0.55
11:k:71:LEU:CD1	17:l:63:PHE:HB3	2.37	0.55
2:B:10:U:O4	2:B:12:C:N4	2.40	0.55
23:3:1239:MET:HE3	23:3:1243:ILE:HD11	1.88	0.55
4:D:788:VAL:O	4:D:794:ARG:NH2	2.37	0.54
12:F:84:C:H5"	12:F:84:C:C6	2.42	0.54
28:t:98:LEU:HD12	28:q:98:LEU:HG	1.87	0.54
1:A:228:LYS:NZ	1:A:698:GLY:O	2.40	0.54
1:A:908:ASP:HB2	1:A:951:LEU:HD11	1.90	0.54
2:B:136:G:N2	2:B:142:C:C4	2.75	0.54
9:i:25:THR:OG1	9:i:92:SER:OG	2.24	0.54
21:1:412:LEU:HD22	21:1:412:LEU:C	2.31	0.54
32:P:133:LYS:HZ2	35:S:16:LYS:CE	2.19	0.54
34:R:124:MET:O	34:R:224:LYS:HB3	2.07	0.54
1:A:188:GLU:HG3	30:N:2:PRO:HD2	1.88	0.54
2:B:102:C:O2	40:U:12:LYS:NZ	2.39	0.54
3:C:941:PRO:HD2	3:C:962:LEU:HD23	1.90	0.54
16:p:58:VAL:HG12	16:p:74:ILE:CG1	2.38	0.54
9:i:18:PHE:CE2	9:i:46:PHE:CE2	2.95	0.54
23:3:68:GLN:HE21	23:3:97:THR:HB	1.72	0.54
47:x:784:PRO:HB3	47:x:859:VAL:HG21	1.89	0.54
3:C:463:THR:HG22	3:C:465:GLU:H	1.72	0.54
12:F:38:U:O2	34:R:196:LYS:NZ	2.40	0.54
8:n:55:ILE:HB	8:n:73:LYS:HB3	1.90	0.54
18:u:319:TYR:OH	18:u:323:ARG:NH1	2.41	0.54
21:1:379:SER:HB3	21:1:418:ALA:HA	1.89	0.54
32:P:43:PHE:HE1	32:P:147:LEU:HD22	1.72	0.54
1:A:2257:GLY:HA2	1:A:2288:CYS:HB3	1.90	0.54
21:1:27:GLN:OE1	21:1:30:ARG:NH2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:6:23:ASP:O	26:6:25:SER:N	2.33	0.54
29:K:86:LEU:HD22	29:K:86:LEU:C	2.32	0.54
33:Q:75:MET:HE1	34:R:130:PHE:HE1	1.71	0.54
41:V:475:GLU:OE2	41:V:478:ARG:NH1	2.40	0.54
45:J:230:ALA:O	45:J:234:ASN:ND2	2.41	0.54
4:D:1499:ALA:HB2	4:D:1506:ILE:HD12	1.88	0.54
23:3:1355:GLU:HG3	23:3:1359:ASN:HD22	1.72	0.54
33:Q:199:ASN:HB3	33:Q:200:PRO:HD2	1.89	0.54
34:R:149:LYS:NZ	34:R:209:ASP:O	2.40	0.54
4:D:1173:LEU:HD22	4:D:1178:GLU:HG2	1.89	0.54
8:n:72:VAL:HG11	8:n:94:LEU:HD13	1.90	0.54
21:1:138:PRO:HA	21:1:141:HIS:HD2	1.72	0.54
32:P:170:SER:OG	32:P:173:LYS:O	2.25	0.54
43:z:53:LYS:HE3	43:z:65:ALA:H	1.72	0.54
1:A:1465:ARG:HG3	32:P:301:LEU:HD22	1.89	0.54
9:i:21:LEU:HD11	9:i:44:VAL:O	2.07	0.54
7:m:17:ILE:HD12	7:m:40:LEU:HD11	1.90	0.54
21:1:595:LYS:NZ	21:1:634:CYS:O	2.40	0.54
32:P:317:LYS:HE3	38:Z:262:LEU:HD11	1.88	0.54
1:A:467:GLU:O	3:C:387:TYR:OH	2.25	0.54
1:A:724:ARG:NH1	53:A:3157:HOH:O	2.37	0.54
6:h:96:VAL:HG22	7:m:85:ILE:HG12	1.89	0.54
31:T:432:ALA:HB1	31:T:437:GLU:HG3	1.89	0.54
41:V:10:ASP:OD2	41:V:244:LYS:NZ	2.41	0.54
45:J:270:ALA:O	45:J:274:TRP:N	2.36	0.54
1:A:1722:ASP:OD2	1:A:1795:LYS:NZ	2.40	0.54
4:D:765:ASN:HB2	23:3:166:ALA:HB2	1.90	0.54
23:3:607:LEU:HB2	23:3:624:TRP:HB3	1.89	0.54
46:I:237:THR:O	46:I:239:ASP:N	2.41	0.54
47:x:268:GLN:NE2	47:x:268:GLN:HA	2.21	0.54
1:A:185:GLN:HE21	1:A:263:PRO:HD3	1.73	0.53
3:C:722:ASP:OD2	3:C:755:TYR:OH	2.26	0.53
34:R:63:ARG:HD3	34:R:86:LYS:HA	1.88	0.53
13:G:108:U:O5'	13:G:108:U:H6	1.92	0.53
23:3:639:LYS:HB3	23:3:686:GLN:HA	1.89	0.53
47:x:409:TYR:HE1	47:x:563:ARG:HD2	1.73	0.53
1:A:1315:ARG:HH12	1:A:1524:PRO:HB3	1.73	0.53
13:G:512:U:H2'	13:G:512:U:O2	2.06	0.53
6:h:11:ARG:O	6:h:15:LEU:HD23	2.07	0.53
23:3:522:LEU:HD21	23:3:875:ARG:HH11	1.73	0.53
3:C:468:LEU:HA	3:C:491:GLY:HA3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:2140:LEU:N	4:D:2158:PHE:O	2.41	0.53
6:h:31:ILE:HD11	6:h:49:ILE:HD12	1.89	0.53
6:h:91:GLN:HG3	17:l:70:LYS:HA	1.90	0.53
37:X:43:THR:OG1	37:X:44:GLU:N	2.40	0.53
46:I:206:ARG:CB	46:I:212:SER:CB	2.87	0.53
23:3:435:ASN:HD21	23:3:482:LEU:HD12	1.74	0.53
24:4:119:ILE:O	24:4:149:LYS:NZ	2.41	0.53
4:D:1246:THR:OG1	4:D:1287:ASN:O	2.27	0.53
20:v:190:ASP:HB2	20:v:192:LYS:HE3	1.90	0.53
47:x:252:LYS:HA	47:x:256:LEU:HD23	1.90	0.53
3:C:772:ASN:OD1	3:C:816:VAL:N	2.34	0.53
4:D:133:ASN:ND2	4:D:1090:GLU:O	2.42	0.53
36:Y:80:LEU:HB2	36:Y:98:LEU:HD11	1.91	0.53
37:X:91:ASN:ND2	38:Z:242:GLU:HB2	2.23	0.53
1:A:1472:ASN:HB3	38:Z:218:PRO:HD3	1.91	0.53
2:B:25:G:N2	2:B:146:C:C2	2.74	0.53
4:D:1005:ALA:HB2	4:D:1015:MET:HG3	1.91	0.53
13:G:473:A:H61	22:2:315:LYS:HE3	1.73	0.53
23:3:649:TYR:HB3	23:3:672:LEU:HB2	1.91	0.53
41:V:84:ASN:ND2	41:V:220:TYR:OH	2.41	0.53
4:D:1057:LEU:HD21	4:D:1089:PHE:HE1	1.74	0.53
18:u:131:GLU:O	19:w:89:SER:N	2.41	0.53
20:v:219:LEU:O	20:v:219:LEU:HG	2.08	0.53
21:1:339:GLN:NE2	53:1:1027:HOH:O	2.42	0.53
23:3:518:ASN:HB3	23:3:877:SER:HB2	1.90	0.53
35:S:12:ARG:O	35:S:16:LYS:NZ	2.36	0.53
1:A:1286:TRP:HB2	1:A:1300:ALA:HB3	1.89	0.53
3:C:629:TYR:OH	3:C:658:ASP:OD2	2.27	0.53
9:i:77:LEU:HD21	9:i:80:ILE:HD12	1.91	0.53
11:k:71:LEU:HD11	17:l:63:PHE:HB3	1.91	0.53
23:3:556:LYS:O	23:3:584:SER:O	2.27	0.53
23:3:741:LEU:HB3	23:3:753:PHE:HB2	1.90	0.53
34:R:78:LYS:NZ	34:R:197:GLU:OE1	2.42	0.53
4:D:1476:ALA:HB3	4:D:1512:SER:HB2	1.91	0.52
20:v:180:ILE:HG22	20:v:201:ILE:HG12	1.90	0.52
21:1:675:LEU:HD13	21:1:715:ALA:HB2	1.90	0.52
24:4:64:GLN:HA	24:4:67:ILE:HD12	1.91	0.52
31:T:244:ARG:HG2	35:S:7:PRO:HG3	1.92	0.52
36:Y:66:ASP:OD1	36:Y:75:ARG:NH2	2.42	0.52
45:J:530:ALA:O	45:J:534:TYR:N	2.34	0.52
46:I:377:LYS:O	46:I:380:ALA:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:LEU:HB2	1:A:254:HIS:ND1	2.24	0.52
1:A:765:ASP:OD1	31:T:312:ARG:NH2	2.42	0.52
14:H:51:C:H2'	14:H:52:A:H8	1.74	0.52
21:1:412:LEU:HD22	21:1:412:LEU:O	2.09	0.52
23:3:746:GLU:HA	23:3:774:PRO:HB3	1.91	0.52
23:3:1328:ARG:NH2	53:3:1535:HOH:O	2.41	0.52
31:T:244:ARG:HA	31:T:268:PRO:HB3	1.92	0.52
34:R:46:ARG:NH1	34:R:222:LEU:HD11	2.24	0.52
23:3:979:CYS:HB2	23:3:996:ILE:HG23	1.91	0.52
34:R:139:VAL:HG13	34:R:221:LEU:HD13	1.92	0.52
1:A:141:LYS:NZ	30:N:35:LYS:O	2.41	0.52
2:B:90:C:H5''	2:B:90:C:H6	1.73	0.52
3:C:905:GLN:HE22	13:G:79:A:H1'	1.74	0.52
4:D:1653:LYS:NZ	4:D:1673:PHE:O	2.42	0.52
35:S:6:ARG:HH21	45:J:63:LEU:HD21	1.74	0.52
45:J:219:ARG:HA	45:J:222:TYR:HD2	1.74	0.52
1:A:1679:GLU:HG2	1:A:1706:VAL:HA	1.92	0.52
3:C:352:VAL:O	3:C:372:THR:OG1	2.22	0.52
23:3:183:THR:HB	23:3:1310:TYR:OH	2.09	0.52
34:R:54:GLN:CB	34:R:58:HIS:CD2	2.91	0.52
4:D:1624:LEU:HD21	4:D:1629:LEU:HB2	1.92	0.52
23:3:986:ASP:OD1	23:3:1036:LYS:HE3	2.10	0.52
31:T:306:HIS:HB3	31:T:332:ARG:HH11	1.73	0.52
1:A:400:ILE:CG2	3:C:187:ARG:HG2	2.40	0.52
1:A:1028:TRP:HE3	1:A:1145:MET:HE3	1.74	0.52
2:B:25:G:N2	2:B:146:C:O2	2.42	0.52
9:i:27:VAL:HG22	9:i:92:SER:HB2	1.91	0.52
27:L:27:LYS:HE2	27:L:28:TYR:CZ	2.44	0.52
31:T:152:ASN:HD21	31:T:409:LYS:HB3	1.74	0.52
37:X:2:ASN:N	53:X:203:HOH:O	2.42	0.52
45:J:221:VAL:O	45:J:225:ALA:N	2.43	0.52
47:x:271:LEU:HD13	47:x:271:LEU:H	1.74	0.52
13:G:506:U:C5'	13:G:506:U:H6	2.23	0.52
8:n:69:LEU:HD11	8:n:96:LEU:HD22	1.91	0.52
1:A:1361:VAL:HG22	1:A:1403:SER:HB2	1.92	0.52
4:D:589:THR:HG21	4:D:595:SER:HB2	1.91	0.52
6:h:21:ARG:HG2	6:h:31:ILE:HG22	1.92	0.52
29:K:86:LEU:C	29:K:86:LEU:HD13	2.35	0.52
33:Q:67:GLN:NE2	33:Q:116:LYS:O	2.42	0.52
33:Q:206:PHE:N	33:Q:291:ILE:O	2.39	0.52
45:J:264:SER:HA	45:J:267:TYR:HD2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:x:268:GLN:NE2	47:x:268:GLN:CA	2.73	0.52
3:C:760:LEU:O	3:C:764:ASN:ND2	2.43	0.52
13:G:490:A:H2'	13:G:491:C:C6	2.45	0.52
23:3:776:SER:HB3	23:3:822:HIS:HB2	1.92	0.52
47:x:256:LEU:HB3	47:x:344:MET:HE1	1.91	0.52
3:C:374:VAL:HA	3:C:378:LEU:HB2	1.92	0.51
17:l:21:LEU:O	17:l:29:TYR:N	2.44	0.51
21:1:197:PRO:HB3	21:1:232:LEU:HD22	1.92	0.51
24:4:116:ALA:HB2	24:4:176:ASN:HB2	1.92	0.51
36:Y:45:LYS:HB2	36:Y:50:LEU:HD23	1.91	0.51
36:Y:65:MET:HE3	36:Y:76:THR:H	1.73	0.51
44:y:91:TYR:CD1	44:y:91:TYR:N	2.77	0.51
2:B:22:G:H1	2:B:149:U:H3	1.57	0.51
3:C:134:ILE:HB	3:C:210:ILE:HG12	1.93	0.51
3:C:331:TYR:OH	3:C:428:ILE:O	2.27	0.51
3:C:345:THR:HA	3:C:348:LEU:HD23	1.92	0.51
23:3:132:LEU:HD13	23:3:218:TYR:HB2	1.90	0.51
31:T:327:CYS:SG	31:T:328:THR:N	2.84	0.51
42:M:199:CYS:HB2	42:M:203:LYS:H	1.76	0.51
1:A:1684:GLU:OE2	1:A:1702:THR:OG1	2.28	0.51
2:B:161:U:H2'	2:B:162:G:H8	1.75	0.51
3:C:765:VAL:HG22	3:C:775:ILE:HG12	1.92	0.51
4:D:1236:LEU:HD11	4:D:1258:PHE:HB3	1.93	0.51
28:t:86:ASN:HA	28:t:89:ASP:HB2	1.92	0.51
46:I:781:TRP:O	46:I:784:PHE:N	2.43	0.51
47:x:777:ARG:HG3	47:x:858:MET:HG3	1.92	0.51
2:B:109:A:N7	53:B:309:HOH:O	2.34	0.51
3:C:88:THR:O	31:T:214:ASN:ND2	2.40	0.51
4:D:536:LEU:HD23	4:D:539:LEU:HD12	1.93	0.51
6:h:12:LEU:HA	6:h:15:LEU:HD21	1.92	0.51
30:N:144:GLN:HB3	30:N:149:GLY:HA2	1.92	0.51
3:C:636:VAL:HG22	3:C:642:HIS:HD1	1.76	0.51
23:3:417:HIS:CE1	23:3:432:GLU:HA	2.46	0.51
41:V:102:PHE:HZ	41:V:142:LEU:HD21	1.74	0.51
41:V:166:SER:HG	41:V:169:THR:HG1	1.57	0.51
3:C:319:GLY:HA3	3:C:426:GLN:HE21	1.75	0.51
33:Q:211:ASP:OD1	33:Q:213:SER:OG	2.28	0.51
37:X:89:VAL:HG22	37:X:104:ILE:HG22	1.93	0.51
41:V:63:PHE:O	41:V:69:ASN:ND2	2.36	0.51
4:D:1536:SER:HB3	4:D:1539:GLU:HG2	1.92	0.51
13:G:486:A:N7	20:v:96:ARG:HD2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:h:21:ARG:N	6:h:96:VAL:O	2.44	0.51
2:B:14:G:H1	2:B:152:C:N4	2.09	0.51
4:D:1424:ILE:HG12	4:D:1444:VAL:HB	1.93	0.51
1:A:1840:TYR:HB3	1:A:1961:LEU:HD11	1.93	0.51
3:C:968:MET:HE1	3:C:986:GLY:HA2	1.92	0.51
12:F:66:C:H2'	12:F:66:C:O2	2.09	0.51
20:v:199:LEU:HB3	20:v:211:ILE:HB	1.91	0.51
23:3:432:GLU:HB3	26:6:62:ILE:HD12	1.93	0.51
23:3:585:GLN:OE1	23:3:585:GLN:HA	2.10	0.51
23:3:953:ILE:HD12	23:3:974:LEU:HD13	1.92	0.51
24:4:33:ASN:ND2	24:4:62:ASP:O	2.43	0.51
41:V:148:LEU:HB2	41:V:190:LEU:HD11	1.93	0.51
18:u:514:ASN:HD21	23:3:1057:LYS:HB2	1.74	0.51
28:q:105:LEU:O	28:q:109:LEU:N	2.44	0.51
31:T:302:LYS:HE2	31:T:339:GLY:HA3	1.93	0.51
43:z:41:MET:SD	43:z:68:THR:OG1	2.61	0.51
1:A:928:ARG:NH1	1:A:1583:ASP:OD2	2.43	0.50
1:A:1750:ARG:HH11	42:M:91:GLU:HB2	1.76	0.50
12:F:68:C:OP2	32:P:133:LYS:HD2	2.10	0.50
13:G:488:A:H1'	18:u:414:LEU:HD22	1.93	0.50
6:h:85:THR:HG22	17:l:73:VAL:HG22	1.93	0.50
18:u:28:ASN:HD21	18:u:72:ILE:HG12	1.76	0.50
21:1:550:THR:OG1	21:1:590:LEU:HD23	2.11	0.50
23:3:514:THR:HG21	23:3:842:LYS:HD3	1.91	0.50
31:T:193:ARG:NH2	31:T:236:LEU:O	2.44	0.50
32:P:88:ARG:NH1	53:P:404:HOH:O	2.44	0.50
23:3:600:ILE:HD13	23:3:642:LEU:HD13	1.93	0.50
2:B:19:A:O5'	2:B:19:A:H8	1.94	0.50
26:6:66:ARG:NH2	53:6:104:HOH:O	2.44	0.50
47:x:474:ILE:HD11	47:x:486:ILE:HG21	1.93	0.50
1:A:421:ALA:HB3	1:A:469:ILE:HD12	1.93	0.50
2:B:141:G:N3	2:B:141:G:C3'	2.73	0.50
28:r:14:VAL:HG12	28:r:52:GLU:HA	1.93	0.50
31:T:115:TYR:HA	31:T:118:LEU:HG	1.94	0.50
2:B:123:U:H2'	2:B:124:C:C6	2.47	0.50
8:c:55:ILE:O	8:c:73:LYS:N	2.41	0.50
14:H:35:U:H2'	14:H:36:A:H5''	1.93	0.50
8:n:46:ILE:HG12	8:n:104:VAL:HG22	1.93	0.50
18:u:19:ASN:OD1	19:w:167:ARG:NH1	2.45	0.50
7:m:101:LEU:HD11	7:m:106:LEU:HD11	1.94	0.50
21:1:850:ASP:HB3	21:1:853:HIS:HD2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:3:742:HIS:HD2	23:3:752:LYS:HG3	1.77	0.50
33:Q:67:GLN:HA	33:Q:119:LYS:HG2	1.92	0.50
1:A:301:TRP:HB3	1:A:493:MET:HE2	1.94	0.50
1:A:1051:GLU:HG3	1:A:1167:ARG:HD2	1.94	0.50
2:B:14:G:H1	2:B:152:C:H42	1.60	0.50
21:1:495:ASP:OD1	21:1:495:ASP:N	2.41	0.50
28:q:84:LEU:HA	28:q:87:GLU:HG2	1.94	0.50
33:Q:194:GLU:HA	33:Q:276:LEU:HD22	1.93	0.50
47:x:777:ARG:HH22	47:x:854:TRP:NE1	2.08	0.50
1:A:173:LEU:HD13	1:A:715:LEU:HB3	1.94	0.50
2:B:65:U:H2'	2:B:66:A:H8	1.76	0.50
4:D:1990:VAL:HG12	4:D:1992:ASN:H	1.77	0.50
4:D:2103:LEU:HD11	4:D:2140:LEU:HD23	1.92	0.50
45:J:387:LEU:C	45:J:389:GLN:N	2.70	0.50
1:A:1403:SER:OG	1:A:1429:MET:SD	2.67	0.50
23:3:435:ASN:N	23:3:435:ASN:ND2	2.60	0.50
23:3:1140:THR:OG1	23:3:1190:LEU:HB3	2.12	0.50
33:Q:11:ASN:H	33:Q:72:GLN:NE2	2.02	0.50
45:J:107:ASP:OD1	45:J:138:LYS:NZ	2.44	0.50
4:D:2073:ILE:HD12	4:D:2128:LEU:HD13	1.93	0.49
12:F:80:U:OP1	20:v:10:LYS:NZ	2.43	0.49
9:i:53:VAL:HA	9:i:81:LEU:HA	1.94	0.49
21:1:412:LEU:C	21:1:412:LEU:CD2	2.85	0.49
28:s:19:SER:OG	28:s:38:ASP:OD2	2.27	0.49
31:T:246:SER:HB2	35:S:9:LEU:HG	1.94	0.49
1:A:1863:HIS:HB2	1:A:1871:ALA:HB3	1.95	0.49
2:B:143:U:H2'	2:B:144:G:H8	1.77	0.49
3:C:470:ALA:HB3	3:C:577:LEU:HD22	1.95	0.49
18:u:424:GLU:H	18:u:465:THR:HB	1.76	0.49
23:3:400:ARG:HB2	23:3:402:ARG:HG2	1.94	0.49
27:L:361:ARG:O	27:L:365:PHE:HA	2.12	0.49
32:P:105:LEU:HD11	33:Q:17:LEU:HD13	1.95	0.49
3:C:91:VAL:HG12	31:T:212:GLU:HG2	1.94	0.49
4:D:706:GLN:HB3	4:D:887:ILE:HG12	1.94	0.49
4:D:1619:PRO:O	4:D:1623:LYS:NZ	2.38	0.49
4:D:1936:ARG:NE	4:D:1986:GLY:O	2.45	0.49
17:l:28:THR:HG1	17:l:50:THR:HG1	1.42	0.49
21:1:843:GLU:OE2	22:2:262:HIS:NE2	2.34	0.49
37:X:102:LEU:HD13	37:X:104:ILE:HD11	1.94	0.49
43:z:59:GLN:C	43:z:103:VAL:CG2	2.84	0.49
1:A:282:ASP:HB2	1:A:285:PRO:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:G:109:A:OP2	13:G:109:A:H2'	2.12	0.49
14:H:143:G:H2'	14:H:144:G:H8	1.77	0.49
6:h:89:GLY:HA2	6:h:92:ILE:HD12	1.94	0.49
34:R:48:VAL:HG12	34:R:220:GLY:N	2.28	0.49
38:Z:154:GLU:O	38:Z:158:TYR:N	2.43	0.49
41:V:118:LEU:HB3	41:V:154:VAL:HG22	1.93	0.49
46:I:237:THR:C	46:I:239:ASP:N	2.69	0.49
46:I:628:LEU:HD11	46:I:665:ILE:HG23	1.94	0.49
3:C:105:ILE:O	3:C:180:ASN:ND2	2.40	0.49
7:b:20:LYS:N	7:b:91:THR:O	2.46	0.49
12:F:67:C:OP1	45:J:59:LYS:HE2	2.12	0.49
21:1:288:ASN:HD22	21:1:293:VAL:HG11	1.78	0.49
21:1:695:ASN:HD22	21:1:696:LYS:N	2.11	0.49
23:3:126:SER:HB2	23:3:151:THR:OG1	2.11	0.49
47:x:638:LEU:HG	47:x:642:MET:HE3	1.94	0.49
1:A:953:ARG:NH2	53:A:3171:HOH:O	2.40	0.49
1:A:1272:ARG:HA	1:A:1275:MET:HE3	1.94	0.49
4:D:966:LEU:O	4:D:970:ARG:NE	2.35	0.49
10:j:77:ASN:OD1	8:n:49:ARG:NH1	2.46	0.49
7:m:27:GLY:HA3	7:m:40:LEU:HD13	1.95	0.49
18:u:194:LYS:HE2	18:u:228:ARG:HH12	1.76	0.49
43:z:104:LEU:C	43:z:104:LEU:HD12	2.37	0.49
4:D:265:ILE:O	4:D:265:ILE:HG22	2.11	0.49
14:H:17:U:O2	14:H:17:U:H2'	2.12	0.49
21:1:181:ARG:NH1	53:1:1019:HOH:O	2.36	0.49
23:3:726:SER:OG	23:3:775:VAL:O	2.29	0.49
27:L:379:ASP:C	27:L:381:GLU:H	2.20	0.49
46:I:726:ARG:NH1	46:I:761:ALA:HB1	2.28	0.49
3:C:918:LEU:HD23	3:C:928:CYS:HB2	1.95	0.49
4:D:656:TRP:HE1	4:D:928:ASN:HB3	1.77	0.49
13:G:111:U:O4	34:R:44:ASN:ND2	2.45	0.49
23:3:557:LYS:HG3	23:3:584:SER:HA	1.95	0.49
47:x:278:PRO:HG3	47:x:350:GLU:HG3	1.93	0.49
1:A:784:GLN:HB3	14:H:19:U:O4	2.12	0.49
1:A:1228:TRP:CZ3	35:S:135:ARG:NH2	2.81	0.49
1:A:1570:TRP:HA	1:A:1573:LEU:HD13	1.94	0.49
3:C:889:TYR:OH	13:G:79:A:O2'	2.30	0.49
20:v:237:ASN:O	20:v:241:THR:OG1	2.29	0.49
21:1:675:LEU:HD11	21:1:714:LEU:HB3	1.94	0.49
23:3:1258:TYR:HB2	23:3:1292:ILE:HD13	1.95	0.49
1:A:1324:GLY:HA2	1:A:1598:LEU:HG	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2405:GLU:OE1	4:D:833:THR:OG1	2.29	0.48
2:B:143:U:H2'	2:B:144:G:C8	2.48	0.48
3:C:713:GLU:HB2	3:C:817:GLN:HB3	1.95	0.48
4:D:2075:LEU:HD22	4:D:2119:LEU:HD21	1.93	0.48
38:Z:197:PHE:CE2	41:V:463:ASN:HB3	2.48	0.48
41:V:77:SER:HA	41:V:80:ILE:HD12	1.95	0.48
2:B:87:G:H2'	2:B:88:U:C6	2.48	0.48
2:B:159:C:H5'	3:C:401:ARG:HH21	1.77	0.48
4:D:1076:VAL:HG13	4:D:1101:ILE:HD12	1.94	0.48
4:D:1430:ASN:ND2	4:D:2091:TYR:OH	2.46	0.48
4:D:1707:VAL:HG22	4:D:1720:VAL:HG11	1.95	0.48
13:G:504:C:OP2	53:G:601:HOH:O	2.20	0.48
21:1:237:LYS:HG3	21:1:238:PRO:HD3	1.94	0.48
21:1:682:ILE:HB	21:1:718:TYR:HD2	1.78	0.48
23:3:230:ILE:HD11	23:3:280:ILE:HG21	1.93	0.48
23:3:961:CYS:CB	23:3:970:LEU:HD23	2.43	0.48
34:R:55:PRO:HB3	34:R:93:ILE:HD11	1.95	0.48
41:V:115:GLY:HA2	41:V:118:LEU:HB2	1.94	0.48
1:A:1809:ASN:HD22	1:A:1811:ALA:H	1.61	0.48
1:A:2259:ILE:HD11	1:A:2293:ILE:HD11	1.95	0.48
2:B:27:G:OP1	2:B:141:G:O5'	2.31	0.48
3:C:495:ARG:HH21	3:C:542:ILE:H	1.61	0.48
4:D:1217:ARG:HG2	4:D:1273:THR:HG22	1.95	0.48
31:T:115:TYR:OH	31:T:444:PRO:O	2.32	0.48
31:T:116:GLU:HG2	45:J:236:GLN:HB2	1.96	0.48
18:u:192:VAL:HG12	18:u:222:MET:HE1	1.95	0.48
23:3:609:HIS:HD2	23:3:621:LYS:HB2	1.77	0.48
23:3:1080:TRP:NE1	23:3:1126:GLU:HB2	2.28	0.48
45:J:47:GLN:NE2	45:J:78:GLN:OE1	2.40	0.48
3:C:652:MET:HA	3:C:655:LEU:HD12	1.95	0.48
14:H:84:C:H2'	14:H:85:A:H8	1.77	0.48
9:i:86:ASN:OD1	10:j:32:LYS:NZ	2.39	0.48
12:F:56:A:H2'	12:F:57:U:C6	2.49	0.48
17:l:22:GLU:HB2	17:l:28:THR:HG22	1.95	0.48
21:1:722:LYS:NZ	22:2:235:PRO:O	2.46	0.48
31:T:160:ASN:ND2	31:T:184:THR:OG1	2.47	0.48
6:h:12:LEU:HA	6:h:15:LEU:CD2	2.44	0.48
21:1:935:TRP:CD1	26:6:24:GLU:H	2.32	0.48
23:3:567:SER:OG	44:y:6:LEU:O	2.28	0.48
45:J:393:ASP:C	45:J:395:ILE:N	2.70	0.48
47:x:625:ILE:HD13	47:x:862:ILE:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:x:836:MET:SD	47:x:838:THR:HG23	2.53	0.48
2:B:5:A:C6	2:B:162:G:O6	2.67	0.48
3:C:264:CYS:HB3	3:C:442:CYS:HG	1.78	0.48
9:i:83:LYS:NZ	10:j:75:CYS:O	2.40	0.48
21:1:337:VAL:HG13	21:1:355:LEU:HD22	1.96	0.48
23:3:553:THR:HG21	23:3:588:THR:HB	1.96	0.48
27:L:224:MET:HE3	27:L:225:PRO:HD2	1.94	0.48
27:L:513:ILE:O	27:L:517:VAL:N	2.42	0.48
4:D:1707:VAL:HG13	4:D:1720:VAL:HG21	1.96	0.48
14:H:115:U:H5'	14:H:116:U:H5'	1.96	0.48
17:l:19:VAL:HG21	17:l:33:LEU:HD12	1.96	0.48
22:2:297:GLU:OE2	24:4:24:GLN:NE2	2.38	0.48
43:z:52:PHE:HB2	43:z:151:PRO:HB3	1.95	0.48
1:A:391:TYR:OH	3:C:649:GLU:OE2	2.29	0.48
1:A:1145:MET:HB3	21:1:19:LEU:HD23	1.96	0.48
1:A:1893:ILE:HD12	1:A:1985:GLN:HE21	1.79	0.48
4:D:1935:SER:OG	4:D:1988:TRP:NE1	2.39	0.48
13:G:487:A:H3'	13:G:487:A:C8	2.49	0.48
23:3:484:LEU:HD11	23:3:511:ILE:HG21	1.96	0.48
27:L:28:TYR:HE2	27:L:39:LEU:HD11	1.78	0.48
33:Q:281:LEU:HG	33:Q:290:ILE:HD11	1.95	0.48
47:x:384:LYS:NZ	47:x:388:GLU:OE2	2.47	0.48
4:D:1426:ASN:HB3	4:D:1446:LEU:HB2	1.95	0.47
8:n:102:ILE:HG22	8:n:103:VAL:HG23	1.95	0.47
21:1:694:ARG:NH2	53:1:1033:HOH:O	2.47	0.47
33:Q:37:CYS:HB3	33:Q:64:CYS:SG	2.53	0.47
41:V:366:GLU:HG2	41:V:404:ILE:HD13	1.96	0.47
18:u:295:PHE:O	18:u:298:HIS:ND1	2.45	0.47
21:1:945:TYR:HB3	21:1:948:ALA:HB3	1.96	0.47
23:3:881:THR:OG1	23:3:882:LEU:N	2.47	0.47
1:A:1091:ASN:OD1	1:A:1096:SER:OG	2.23	0.47
13:G:531:U:O4	47:x:525:ASN:ND2	2.47	0.47
6:h:22:VAL:HG22	6:h:95:THR:HG22	1.97	0.47
6:h:88:ARG:HG2	6:h:90:GLU:H	1.80	0.47
21:1:887:ASN:HB3	21:1:899:ILE:HD13	1.95	0.47
31:T:210:ASP:HB2	31:T:217:ILE:HD13	1.95	0.47
46:I:410:THR:O	46:I:414:ARG:N	2.47	0.47
47:x:777:ARG:NH2	47:x:854:TRP:CZ2	2.82	0.47
1:A:431:ILE:HA	3:C:895:ALA:HB1	1.97	0.47
1:A:2330:GLU:HB3	1:A:2332:THR:HG22	1.95	0.47
3:C:89:PRO:O	31:T:211:LEU:O	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:u:507:GLU:O	18:u:507:GLU:HG3	2.13	0.47
21:1:399:PRO:HA	21:1:402:LYS:HG2	1.96	0.47
23:3:1074:ILE:HG21	23:3:1077:MET:HE3	1.96	0.47
34:R:27:GLY:H	34:R:37:TRP:HB3	1.77	0.47
43:z:111:LEU:C	43:z:113:ASP:H	2.23	0.47
46:I:430:GLU:O	46:I:434:LYS:N	2.39	0.47
1:A:473:THR:O	1:A:477:MET:HG3	2.14	0.47
3:C:727:THR:OG1	3:C:734:CYS:SG	2.64	0.47
4:D:1229:ASP:HB3	4:D:1232:VAL:HG12	1.94	0.47
23:3:416:SER:HA	23:3:431:SER:HA	1.96	0.47
23:3:580:ALA:O	23:3:608:ARG:NH2	2.39	0.47
36:Y:26:ILE:HG12	37:X:117:LYS:HB3	1.96	0.47
41:V:412:SER:O	41:V:417:ARG:NH1	2.48	0.47
1:A:1051:GLU:CG	1:A:1167:ARG:HD2	2.45	0.47
4:D:109:TYR:CZ	4:D:192:ILE:HD11	2.50	0.47
9:i:13:PRO:HD2	11:k:33:ASP:HB3	1.97	0.47
20:v:179:LEU:HD13	20:v:233:VAL:HG21	1.97	0.47
30:N:36:ASP:OD1	30:N:36:ASP:N	2.46	0.47
45:J:224:LEU:O	45:J:228:THR:N	2.37	0.47
1:A:681:LYS:NZ	48:A:3000:IHP:O33	2.47	0.47
2:B:27:G:OP1	2:B:141:G:H5''	2.15	0.47
4:D:817:GLU:HG2	4:D:840:LEU:HD22	1.97	0.47
4:D:933:ASN:O	4:D:937:ASN:ND2	2.47	0.47
4:D:945:TYR:HE1	4:D:966:LEU:HB2	1.80	0.47
4:D:1546:ILE:HD13	4:D:1736:LEU:HD13	1.97	0.47
4:D:1820:ILE:HG22	4:D:1846:THR:HG22	1.97	0.47
14:H:15:C:H6	14:H:15:C:O5'	1.97	0.47
21:1:632:LYS:HD2	21:1:672:VAL:HG13	1.96	0.47
23:3:1361:MET:HE2	23:3:1361:MET:HB3	1.78	0.47
24:4:120:ASP:H	24:4:123:GLN:HB2	1.80	0.47
25:5:41:ARG:NH1	25:5:82:ASP:OD2	2.42	0.47
33:Q:43:LEU:HD21	33:Q:57:LYS:HG3	1.95	0.47
33:Q:71:CYS:HB3	33:Q:74:CYS:HB2	1.97	0.47
34:R:170:ILE:HG21	34:R:173:ILE:HD11	1.96	0.47
45:J:614:ILE:HA	45:J:617:ALA:HB3	1.97	0.47
46:I:806:VAL:O	46:I:810:ASN:N	2.46	0.47
1:A:2189:LEU:HD13	1:A:2224:VAL:HG23	1.97	0.47
6:h:21:ARG:HB2	6:h:96:VAL:HB	1.96	0.47
18:u:16:ILE:O	18:u:20:ALA:N	2.46	0.47
24:4:108:ALA:HB3	24:4:155:PHE:HB2	1.96	0.47
31:T:327:CYS:HB3	31:T:330:ASP:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1368:VAL:HA	4:D:1533:TYR:HB2	1.97	0.47
14:H:36:A:H8	14:H:36:A:C5'	2.28	0.47
6:h:49:ILE:HG12	6:h:81:VAL:HG22	1.96	0.47
17:l:50:THR:HG22	17:l:56:VAL:HG12	1.96	0.47
27:L:213:TYR:HD2	45:J:52:THR:HG22	1.79	0.47
33:Q:237:SER:O	33:Q:254:GLN:N	2.48	0.47
37:X:82:GLN:O	37:X:85:THR:HB	2.15	0.47
41:V:113:SER:HA	41:V:116:ASN:HD22	1.79	0.47
1:A:137:GLU:HG3	30:N:34:GLN:HE21	1.79	0.47
1:A:1122:ASP:OD1	1:A:1161:TYR:OH	2.27	0.47
13:G:506:U:H5''	13:G:506:U:C6	2.50	0.47
10:j:56:ALA:HB3	10:j:68:LEU:HB2	1.96	0.47
19:w:120:ALA:O	19:w:123:ASN:ND2	2.48	0.47
21:1:67:ARG:HD2	21:1:292:TYR:HB2	1.97	0.47
23:3:198:ASN:ND2	53:3:1541:HOH:O	2.48	0.47
23:3:678:LYS:NZ	23:3:727:ASP:OD1	2.48	0.47
47:x:225:VAL:HG12	47:x:398:VAL:HG11	1.97	0.47
1:A:901:PRO:HD3	1:A:1078:ILE:HD11	1.97	0.46
1:A:1795:LYS:CB	1:A:1796:PRO:HD3	2.45	0.46
16:p:55:PHE:CB	16:p:85:ALA:HB2	2.45	0.46
23:3:488:ILE:HD12	23:3:489:LYS:HB2	1.95	0.46
23:3:718:LEU:HB2	42:M:244:ALA:HB3	1.98	0.46
24:4:138:PRO:HB3	24:4:153:VAL:HG22	1.96	0.46
35:S:128:ARG:HH21	35:S:135:ARG:HH22	1.62	0.46
38:Z:208:SER:HB3	38:Z:212:ARG:H	1.80	0.46
1:A:1067:ASN:HD21	27:L:82:ASN:HD22	1.62	0.46
1:A:2182:VAL:HG23	1:A:2338:GLN:HB3	1.97	0.46
18:u:90:GLN:HE21	19:w:153:ILE:HG13	1.80	0.46
21:1:803:ASN:HD22	22:2:205:ILE:HG13	1.79	0.46
21:1:881:MET:HE2	21:1:918:TYR:CD2	2.50	0.46
47:x:271:LEU:N	47:x:271:LEU:CD1	2.73	0.46
1:A:1748:ILE:HD13	1:A:1778:ASP:HB2	1.96	0.46
2:B:1:A:N6	2:B:164:C:H42	2.13	0.46
4:D:1260:THR:OG1	4:D:1262:ASP:OD1	2.26	0.46
13:G:497:A:H1'	20:v:76:MET:SD	2.55	0.46
23:3:854:ASN:HB2	23:3:857:VAL:H	1.81	0.46
41:V:181:LEU:HB2	41:V:194:LEU:HD12	1.98	0.46
1:A:1941:LEU:HD21	1:A:1958:PRO:HD3	1.98	0.46
3:C:869:HIS:CD2	3:C:925:LEU:HD22	2.51	0.46
4:D:682:ARG:HD2	4:D:946:VAL:HG13	1.98	0.46
4:D:896:GLN:HG2	44:y:58:LYS:HD3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:2075:LEU:HD11	4:D:2101:LEU:HD21	1.98	0.46
14:H:114:U:H3	11:k:37:ASN:HD21	1.63	0.46
46:I:468:GLU:N	46:I:511:ALA:HB3	2.31	0.46
1:A:697:LYS:CG	48:A:3000:IHP:O46	2.63	0.46
1:A:856:TRP:CD1	35:S:174:VAL:HG11	2.50	0.46
1:A:2149:LYS:HE3	1:A:2151:GLU:HB3	1.96	0.46
2:B:25:G:H2'	2:B:26:A:H8	1.79	0.46
4:D:1585:LEU:HD21	4:D:1683:LEU:HD23	1.97	0.46
9:i:21:LEU:C	9:i:21:LEU:HD23	2.41	0.46
11:k:36:LEU:HD23	17:l:65:ARG:HH11	1.81	0.46
18:u:67:ARG:HH12	18:u:370:GLU:HB3	1.80	0.46
36:Y:144:GLN:NE2	36:Y:145:PHE:O	2.46	0.46
1:A:598:ASN:OD1	1:A:627:LYS:NZ	2.49	0.46
1:A:1156:HIS:CD2	1:A:1158:ILE:H	2.32	0.46
27:L:212:ASP:H	33:Q:106:ASN:ND2	2.14	0.46
41:V:55:ILE:O	41:V:59:ASN:ND2	2.48	0.46
46:I:393:ASP:O	46:I:397:ASN:N	2.45	0.46
47:x:601:ASP:OD1	47:x:601:ASP:N	2.44	0.46
1:A:1932:GLN:HG2	1:A:1955:ALA:HB3	1.98	0.46
3:C:143:HIS:CE1	3:C:189:LEU:CD1	2.98	0.46
6:h:22:VAL:N	6:h:30:TYR:O	2.45	0.46
23:3:194:GLU:HB2	23:3:240:MET:HE3	1.97	0.46
31:T:245:ASP:HB3	35:S:10:GLU:HB2	1.98	0.46
37:X:104:ILE:N	37:X:104:ILE:HD12	2.30	0.46
41:V:180:ILE:HG22	41:V:186:LEU:HD11	1.98	0.46
47:x:608:MET:HE3	47:x:608:MET:HB2	1.85	0.46
1:A:468:LEU:HD12	1:A:469:ILE:HG12	1.98	0.46
1:A:1573:LEU:HG	1:A:1825:ILE:HD11	1.97	0.46
4:D:502:ILE:HD11	4:D:698:PHE:HB3	1.97	0.46
23:3:1061:ARG:NH2	53:3:1542:HOH:O	2.48	0.46
31:T:262:LEU:HD13	31:T:293:TRP:CD2	2.50	0.46
32:P:292:ALA:HB3	36:Y:39:GLU:HG2	1.98	0.46
44:y:90:GLU:HB3	44:y:91:TYR:CD1	2.49	0.46
3:C:208:ARG:HH12	3:C:440:THR:CG2	2.28	0.46
12:F:28:U:H1'	33:Q:51:ARG:HH21	1.81	0.46
14:H:83:U:H2'	14:H:84:C:C6	2.51	0.46
16:p:40:ASN:O	16:p:44:LEU:N	2.41	0.46
21:1:971:LEU:HB2	26:6:56:SER:HB3	1.98	0.46
23:3:881:THR:HG23	23:3:884:ASN:H	1.80	0.46
41:V:408:THR:HG23	41:V:457:HIS:HE1	1.80	0.46
47:x:351:ARG:NH2	47:x:609:ASP:OD2	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:780:ARG:HE	35:S:3:THR:HG21	1.80	0.46
1:A:862:GLU:OE2	1:A:866:GLN:NE2	2.49	0.46
1:A:1859:ARG:HH22	1:A:1969:MET:HE2	1.81	0.46
2:B:121:U:H2'	2:B:122:C:C6	2.51	0.46
3:C:91:VAL:HG11	31:T:195:PRO:HB3	1.98	0.46
3:C:625:ILE:HG23	3:C:629:TYR:HD2	1.81	0.46
14:H:68:U:H2'	14:H:69:G:H8	1.81	0.46
33:Q:20:GLU:HB3	33:Q:23:ILE:HD11	1.98	0.46
43:z:16:TYR:HD2	43:z:156:ASP:HB3	1.81	0.46
1:A:1145:MET:HG2	1:A:1160:LEU:HD22	1.98	0.45
1:A:1794:LEU:HD23	1:A:1794:LEU:HA	1.84	0.45
2:B:60:U:H5''	2:B:60:U:O2	2.16	0.45
4:D:727:TYR:HE1	4:D:761:PHE:CE1	2.34	0.45
6:h:50:GLU:N	6:h:80:ARG:O	2.46	0.45
18:u:75:GLN:HE21	18:u:156:ILE:HG21	1.81	0.45
21:1:855:GLN:HG2	21:1:895:ALA:HA	1.97	0.45
23:3:427:LEU:HB3	23:3:439:PHE:HB2	1.98	0.45
31:T:440:LEU:HD22	31:T:440:LEU:HA	1.82	0.45
33:Q:101:THR:HG22	33:Q:121:GLY:HA3	1.98	0.45
42:M:216:HIS:CE1	42:M:235:ILE:HB	2.51	0.45
1:A:2247:LEU:HD21	1:A:2375:LYS:HA	1.98	0.45
4:D:2146:CYS:SG	4:D:2147:ASP:N	2.89	0.45
23:3:553:THR:HG22	23:3:558:THR:HG23	1.97	0.45
23:3:839:ARG:HG3	23:3:880:PRO:HG2	1.99	0.45
1:A:148:ASP:OD1	1:A:148:ASP:N	2.50	0.45
3:C:683:ASN:ND2	3:C:684:GLU:OE1	2.49	0.45
14:H:56:U:O2'	14:H:58:A:N7	2.46	0.45
14:H:143:G:H2'	14:H:144:G:C8	2.51	0.45
4:D:803:THR:HG22	4:D:808:LEU:HD11	1.99	0.45
18:u:419:ARG:HE	18:u:434:ARG:HH21	1.64	0.45
27:L:507:GLU:HA	27:L:510:LEU:HB2	1.98	0.45
33:Q:136:VAL:HA	33:Q:139:LEU:HD12	1.99	0.45
33:Q:263:VAL:HA	33:Q:266:ILE:HD12	1.98	0.45
34:R:145:ALA:HB2	34:R:221:LEU:HB3	1.96	0.45
41:V:152:ILE:HG23	41:V:197:LEU:HB2	1.98	0.45
53:A:3134:HOH:O	32:P:332:GLN:NE2	2.42	0.45
2:B:147:C:H2'	2:B:148:G:C8	2.50	0.45
14:H:28:U:H2'	14:H:29:C:C6	2.51	0.45
9:i:91:THR:HB	11:k:61:THR:HG22	1.98	0.45
33:Q:206:PHE:HB2	33:Q:293:TRP:CD1	2.52	0.45
45:J:122:MET:HG3	45:J:139:TYR:CD1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1347:ARG:NH1	1:A:1445:THR:O	2.43	0.45
4:D:116:ASN:HD21	4:D:193:THR:H	1.64	0.45
4:D:770:LEU:O	4:D:826:GLN:HG2	2.16	0.45
9:i:90:ILE:O	11:k:62:VAL:N	2.43	0.45
10:j:53:LEU:HB2	10:j:71:ILE:HD11	1.99	0.45
21:1:763:LEU:HD11	21:1:797:VAL:HG22	1.99	0.45
21:1:916:MET:SD	21:1:941:MET:HG2	2.56	0.45
22:2:167:LYS:NZ	53:2:412:HOH:O	2.49	0.45
23:3:1091:HIS:HD2	23:3:1117:HIS:CD2	2.34	0.45
33:Q:70:ILE:HG21	33:Q:84:ILE:HD11	1.97	0.45
36:Y:76:THR:HG23	36:Y:204:VAL:CG2	2.45	0.45
45:J:99:ILE:HA	45:J:102:TRP:HD1	1.81	0.45
1:A:814:ARG:HH11	1:A:815:TYR:HE2	1.65	0.45
4:D:626:GLU:O	4:D:662:GLN:NE2	2.50	0.45
4:D:1269:THR:O	4:D:1694:LYS:NZ	2.36	0.45
13:G:495:A:C2'	13:G:496:U:H5'	2.46	0.45
18:u:377:VAL:HB	18:u:378:ASP:H	1.66	0.45
18:u:418:ASP:N	18:u:432:ASN:O	2.50	0.45
21:1:383:GLU:HG3	21:1:421:SER:HB3	1.99	0.45
21:1:719:ALA:O	42:M:172:TRP:NE1	2.39	0.45
32:P:110:HIS:CD2	33:Q:17:LEU:HD22	2.52	0.45
47:x:807:VAL:HG11	47:x:835:LEU:HD11	1.99	0.45
1:A:394:ARG:NH1	3:C:667:GLU:OE1	2.49	0.45
1:A:757:GLU:HA	31:T:244:ARG:HH12	1.82	0.45
1:A:901:PRO:HA	1:A:902:PRO:HD3	1.70	0.45
1:A:1734:PHE:CZ	1:A:1798:ILE:HD11	2.52	0.45
2:B:27:G:OP1	2:B:141:G:C5'	2.65	0.45
2:B:28:G:N2	2:B:126:A:H1'	2.32	0.45
17:l:69:ILE:HD13	17:l:72:ILE:HD11	1.97	0.45
21:1:365:ASP:O	21:1:371:ARG:NH2	2.48	0.45
23:3:582:LYS:HE2	23:3:585:GLN:CB	2.46	0.45
41:V:313:LEU:HG	41:V:350:MET:CE	2.47	0.45
42:M:128:PRO:HB2	42:M:131:ILE:HG12	1.99	0.45
1:A:835:LYS:HD2	35:S:173:HIS:CE1	2.52	0.45
1:A:1817:GLU:OE1	21:1:646:ILE:HG23	2.16	0.45
4:D:139:LEU:HG	4:D:715:SER:HB2	1.98	0.45
4:D:444:THR:HA	44:y:58:LYS:HE3	1.99	0.45
14:H:44:U:H2'	14:H:45:U:H6	1.82	0.45
15:o:132:ASN:HB3	15:o:134:VAL:HG12	1.99	0.45
7:m:26:TRP:HB2	7:m:44:LYS:HB3	1.99	0.45
21:1:558:GLU:OE2	21:1:593:ARG:NH2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:3:169:LEU:HD23	23:3:169:LEU:HA	1.85	0.45
23:3:499:SER:HB3	23:3:514:THR:HG23	1.98	0.45
23:3:943:ASP:HB2	23:3:952:ARG:HG2	1.99	0.45
36:Y:25:TYR:HB3	37:X:117:LYS:HG2	1.98	0.45
1:A:1585:MET:HG3	21:1:695:ASN:HA	1.98	0.45
7:m:19:LEU:HD12	7:m:23:THR:HB	1.99	0.45
1:A:351:LYS:NZ	13:G:91:A:OP1	2.41	0.44
1:A:1054:LEU:HB3	1:A:1239:THR:HG21	1.99	0.44
14:H:56:U:H1'	14:H:59:C:H5	1.80	0.44
18:u:517:SER:OG	18:u:518:LYS:N	2.48	0.44
21:1:798:LEU:HD13	21:1:823:MET:HE1	2.00	0.44
32:P:242:LYS:NZ	36:Y:92:PRO:HG3	2.33	0.44
34:R:205:LEU:HD11	34:R:215:ARG:HB3	1.98	0.44
47:x:273:ILE:HG23	47:x:342:CYS:O	2.17	0.44
1:A:1419:ASP:OD1	1:A:1419:ASP:N	2.43	0.44
3:C:264:CYS:CB	3:C:442:CYS:HG	2.30	0.44
4:D:531:ALA:HB1	4:D:632:ILE:HD13	1.99	0.44
4:D:891:ASP:OD1	4:D:892:GLN:N	2.50	0.44
4:D:1457:ARG:HG2	4:D:1756:ASN:HD21	1.82	0.44
12:F:68:C:H2'	12:F:69:C:C6	2.52	0.44
13:G:497:A:C8	13:G:497:A:C5'	3.00	0.44
23:3:1029:SER:HB3	23:3:1045:MET:HB2	2.00	0.44
31:T:112:VAL:O	31:T:116:GLU:N	2.46	0.44
33:Q:17:LEU:HD23	33:Q:23:ILE:HD12	2.00	0.44
33:Q:183:ILE:HG22	33:Q:308:GLU:HG3	1.99	0.44
33:Q:208:TYR:OH	33:Q:323:GLU:OE1	2.29	0.44
39:W:59:ARG:O	39:W:62:THR:OG1	2.32	0.44
1:A:1233:ARG:HD3	35:S:131:THR:HG21	1.99	0.44
1:A:2262:GLN:OE1	1:A:2292:SER:OG	2.32	0.44
4:D:562:PRO:HD2	4:D:566:LEU:HD23	1.98	0.44
12:F:42:A:H3'	53:F:379:HOH:O	2.17	0.44
8:n:73:LYS:HB2	8:n:90:PHE:HE1	1.83	0.44
20:v:233:VAL:HB	20:v:237:ASN:HD22	1.82	0.44
23:3:697:GLU:HG2	23:3:699:MET:HE3	1.98	0.44
23:3:1077:MET:HA	23:3:1086:ALA:O	2.17	0.44
31:T:254:ARG:NE	35:S:35:THR:O	2.51	0.44
1:A:1717:LEU:HB2	1:A:1786:ALA:HB3	2.00	0.44
2:B:151:A:N3	2:B:151:A:C2'	2.78	0.44
4:D:170:GLN:NE2	4:D:176:ASN:OD1	2.51	0.44
23:3:63:LEU:HD12	23:3:1361:MET:HE1	1.99	0.44
23:3:1084:ARG:HH21	23:3:1084:ARG:CG	2.29	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Q:34:CYS:HB3	33:Q:37:CYS:SG	2.57	0.44
34:R:169:ASP:OD1	34:R:169:ASP:N	2.46	0.44
41:V:428:VAL:HG21	41:V:470:LEU:HD21	2.00	0.44
4:D:112:LYS:NZ	4:D:194:ASP:OD2	2.37	0.44
18:u:167:ASN:ND2	18:u:176:TYR:OH	2.51	0.44
21:1:422:MET:HB3	21:1:426:MET:HE3	2.00	0.44
23:3:642:LEU:HD21	23:3:644:ILE:HG23	1.99	0.44
34:R:12:GLN:HE21	34:R:58:HIS:HB3	1.81	0.44
43:z:17:THR:OG1	43:z:20:GLY:O	2.34	0.44
1:A:1815:LEU:HD22	1:A:1815:LEU:O	2.17	0.44
2:B:142:C:H6	2:B:142:C:O5'	2.01	0.44
2:B:153:U:O2	2:B:153:U:H2'	2.17	0.44
3:C:141:PRO:O	3:C:146:LYS:NZ	2.51	0.44
14:H:120:G:H5'	8:n:49:ARG:HH21	1.81	0.44
21:1:790:LYS:HD2	21:1:826:TYR:HB3	2.00	0.44
21:1:885:ILE:N	21:1:886:PRO:CD	2.81	0.44
22:2:301:ILE:HG21	24:4:20:ILE:HD11	2.00	0.44
33:Q:11:ASN:HB3	33:Q:72:GLN:HG3	1.99	0.44
2:B:158:G:H2'	2:B:159:C:C6	2.52	0.44
3:C:156:ASP:HB3	3:C:431:GLN:HE22	1.83	0.44
4:D:637:HIS:O	4:D:637:HIS:CD2	2.70	0.44
21:1:884:LEU:O	21:1:884:LEU:HD22	2.18	0.44
23:3:316:ASP:CG	47:x:770:TYR:HH	2.25	0.44
31:T:292:LEU:HD12	31:T:302:LYS:HB3	2.00	0.44
31:T:442:TRP:O	31:T:442:TRP:CG	2.70	0.44
32:P:47:ARG:NH2	32:P:53:LEU:O	2.50	0.44
32:P:178:TYR:CD1	32:P:178:TYR:O	2.70	0.44
47:x:305:GLN:HG2	47:x:326:MET:HE2	1.98	0.44
3:C:142:LEU:HD11	3:C:218:HIS:HD2	1.82	0.44
4:D:487:CYS:HB2	4:D:536:LEU:HD13	2.00	0.44
4:D:1512:SER:OG	4:D:1513:ASN:N	2.51	0.44
16:p:58:VAL:CG1	16:p:74:ILE:CG1	2.95	0.44
18:u:30:GLU:HA	18:u:33:TYR:HB2	1.98	0.44
22:2:179:LYS:HE3	22:2:179:LYS:HB3	1.40	0.44
24:4:115:LEU:HD13	24:4:149:LYS:HE2	1.98	0.44
28:q:94:GLU:OE2	29:K:50:ALA:N	2.51	0.44
36:Y:51:LYS:HG3	36:Y:52:HIS:H	1.82	0.44
37:X:89:VAL:O	37:X:93:ASN:HB2	2.18	0.44
41:V:52:GLY:HA2	41:V:55:ILE:HD12	2.00	0.44
42:M:201:LEU:HD12	42:M:222:CYS:HB3	2.00	0.44
47:x:406:ASP:OD1	47:x:406:ASP:N	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:633:ILE:HB	3:C:645:LEU:HB2	2.00	0.44
12:F:85:C:C4	14:H:20:G:O6	2.71	0.44
21:1:689:LEU:HD21	21:1:707:PHE:CD2	2.53	0.44
1:A:930:ASN:HA	14:H:30:A:OP1	2.18	0.43
11:k:27:GLY:HA3	11:k:40:LEU:HD13	2.00	0.43
23:3:455:LEU:HD11	23:3:464:LEU:HB3	1.99	0.43
23:3:1031:ILE:HG21	23:3:1034:MET:HE3	2.00	0.43
36:Y:105:LEU:HD23	36:Y:127:ALA:HA	2.01	0.43
47:x:345:ILE:HD11	47:x:358:LEU:HD12	1.99	0.43
2:B:127:U:O2	2:B:127:U:H2'	2.18	0.43
23:3:956:GLN:HG2	23:3:956:GLN:O	2.18	0.43
25:5:32:ILE:HG21	25:5:81:LYS:HD3	1.99	0.43
33:Q:193:ASN:HA	33:Q:278:ARG:HH22	1.83	0.43
37:X:56:VAL:HG23	37:X:80:GLU:HB3	2.00	0.43
37:X:91:ASN:HD21	38:Z:242:GLU:HB2	1.82	0.43
1:A:705:GLN:O	1:A:709:ARG:HG3	2.18	0.43
3:C:299:THR:HG21	3:C:304:PHE:HE2	1.83	0.43
13:G:506:U:C5'	13:G:506:U:C6	3.00	0.43
18:u:213:ASP:OD1	18:u:322:HIS:NE2	2.45	0.43
21:1:158:LYS:O	21:1:161:LYS:N	2.51	0.43
23:3:957:ILE:HD13	23:3:957:ILE:HA	1.76	0.43
34:R:26:THR:HG23	34:R:42:ALA:HA	1.99	0.43
47:x:807:VAL:HG12	47:x:841:GLU:HB3	2.00	0.43
3:C:183:GLN:HE21	3:C:187:ARG:CZ	2.31	0.43
14:H:68:U:H2'	14:H:69:G:C8	2.53	0.43
9:i:36:GLY:HA2	9:i:62:VAL:HB	1.99	0.43
21:1:305:ALA:HA	21:1:313:LEU:HD13	2.00	0.43
45:J:128:THR:HG22	45:J:129:LEU:HG	2.00	0.43
1:A:1890:PHE:HB3	1:A:1986:MET:HE1	2.01	0.43
2:B:129:G:H4'	2:B:130:A:H3'	2.00	0.43
3:C:796:ILE:HD12	3:C:796:ILE:HA	1.87	0.43
4:D:1858:VAL:HG21	4:D:1960:VAL:HG21	2.00	0.43
14:H:2:C:H2'	14:H:3:G:C8	2.54	0.43
22:2:240:LEU:HB3	22:2:242:LEU:HD23	2.00	0.43
23:3:316:ASP:OD1	47:x:770:TYR:OH	2.36	0.43
33:Q:45:HIS:HB3	33:Q:55:ILE:HD11	2.01	0.43
36:Y:186:LEU:HB2	36:Y:199:LEU:HB2	2.00	0.43
47:x:832:TYR:CE1	47:x:835:LEU:HB2	2.53	0.43
3:C:706:LEU:HD23	3:C:825:VAL:HA	2.01	0.43
3:C:922:THR:OG1	3:C:925:LEU:O	2.27	0.43
4:D:1808:GLU:O	4:D:1812:ASN:ND2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1936:ARG:NH2	4:D:1985:GLN:O	2.48	0.43
4:D:2057:LEU:HD23	4:D:2060:SER:HA	1.99	0.43
27:L:57:ASN:HB3	27:L:60:LEU:HG	2.00	0.43
37:X:82:GLN:H	38:Z:168:GLN:NE2	2.16	0.43
41:V:73:ILE:HG22	41:V:123:ILE:HD12	1.99	0.43
4:D:1212:THR:HB	4:D:1215:VAL:H	1.84	0.43
34:R:95:ASP:OD1	34:R:95:ASP:N	2.51	0.43
42:M:236:CYS:HB3	42:M:238:LYS:HG3	2.00	0.43
1:A:1093:LYS:O	14:H:25:A:C2	2.72	0.43
1:A:2307:LEU:HD11	1:A:2311:GLY:HA3	2.01	0.43
13:G:504:C:C6	13:G:504:C:C5'	2.91	0.43
6:h:15:LEU:HB2	6:h:18:TYR:CD2	2.54	0.43
18:u:226:ASN:HB3	18:u:229:TYR:HB3	1.99	0.43
23:3:433:MET:CG	23:3:486:PRO:HD3	2.44	0.43
23:3:938:SER:CB	23:3:957:ILE:HD13	2.46	0.43
34:R:176:VAL:HG12	34:R:179:LYS:H	1.84	0.43
41:V:41:HIS:CE1	41:V:82:LEU:HB3	2.54	0.43
41:V:228:ILE:HD12	41:V:230:SER:HB2	2.01	0.43
43:z:42:LEU:HD23	43:z:47:PHE:HD2	1.83	0.43
43:z:84:PHE:CE2	43:z:116:VAL:HG22	2.53	0.43
4:D:804:HIS:NE2	4:D:817:GLU:OE2	2.52	0.43
17:l:21:LEU:HD21	17:l:64:VAL:HG11	2.00	0.43
22:2:364:PHE:N	23:3:1125:ASP:OD2	2.33	0.43
33:Q:75:MET:CE	34:R:130:PHE:CD1	3.01	0.43
34:R:121:ARG:HD3	34:R:125:GLY:H	1.84	0.43
1:A:715:LEU:HD12	1:A:715:LEU:HA	1.86	0.43
3:C:100:LEU:HD13	3:C:108:GLN:NE2	2.34	0.43
3:C:713:GLU:O	3:C:817:GLN:N	2.39	0.43
4:D:1883:LEU:HD21	4:D:1954:VAL:HG23	1.99	0.43
4:D:2031:LEU:HB3	4:D:2038:LEU:HD21	2.01	0.43
12:F:87:U:O2	45:J:70:ARG:NH1	2.47	0.43
14:H:51:C:H2'	14:H:52:A:C8	2.53	0.43
7:m:43:VAL:HG11	7:m:85:ILE:HD12	2.00	0.43
21:1:144:PHE:O	21:1:146:ASP:N	2.51	0.43
21:1:158:LYS:O	21:1:161:LYS:HB2	2.19	0.43
22:2:180:LYS:HB3	22:2:181:GLU:H	1.47	0.43
23:3:253:VAL:HG21	23:3:327:VAL:HG11	2.00	0.43
23:3:393:VAL:HG22	23:3:405:VAL:HG22	2.00	0.43
28:q:52:GLU:HB2	28:q:53:ILE:H	1.73	0.43
33:Q:79:ARG:HH12	33:Q:129:PRO:HA	1.83	0.43
47:x:271:LEU:HA	47:x:339:LYS:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:H:49:U:H3'	14:H:49:U:H6	1.84	0.42
18:u:506:LEU:HD13	18:u:506:LEU:HA	1.74	0.42
23:3:630:ILE:HG23	23:3:647:SER:HB2	2.00	0.42
27:L:22:LYS:HE3	27:L:56:LEU:HD22	2.00	0.42
27:L:79:GLU:OE1	32:P:205:SER:OG	2.36	0.42
31:T:433:THR:OG1	31:T:435:GLU:OE1	2.28	0.42
36:Y:77:MET:SD	36:Y:99:ASN:ND2	2.92	0.42
42:M:199:CYS:HB2	42:M:203:LYS:N	2.34	0.42
1:A:270:SER:HA	1:A:277:LYS:HE2	2.02	0.42
1:A:1706:VAL:O	4:D:1184:ARG:NH2	2.52	0.42
1:A:1830:VAL:HG13	21:1:611:HIS:CD2	2.54	0.42
3:C:776:ASN:ND2	3:C:781:ASP:OD2	2.47	0.42
36:Y:105:LEU:HA	36:Y:142:VAL:HG12	2.01	0.42
42:M:148:LYS:O	42:M:165:ARG:NH1	2.52	0.42
1:A:1125:LEU:O	1:A:1233:ARG:NH1	2.51	0.42
1:A:1746:HIS:CD2	42:M:88:LEU:HB3	2.55	0.42
2:B:102:C:C2'	2:B:103:A:H5'	2.49	0.42
3:C:269:LYS:HG2	49:C:1101:GTP:C6	2.54	0.42
4:D:585:VAL:HG12	4:D:604:VAL:HB	2.01	0.42
7:m:17:ILE:HG23	7:m:92:ILE:HG23	2.01	0.42
8:n:48:LEU:HD22	8:n:54:ILE:HD11	2.01	0.42
18:u:233:LEU:HB3	18:u:314:PHE:HE1	1.83	0.42
21:1:46:ASP:OD1	21:1:47:VAL:N	2.52	0.42
21:1:117:LYS:HE2	21:1:121:ASP:CB	2.49	0.42
23:3:1077:MET:HE2	23:3:1087:VAL:HG22	2.01	0.42
41:V:319:ASN:HA	41:V:322:LYS:HD3	2.02	0.42
47:x:337:LEU:HD13	47:x:343:ILE:HD11	2.02	0.42
11:k:71:LEU:CD2	17:l:63:PHE:CD2	2.85	0.42
23:3:1151:MET:HE1	23:3:1159:LEU:HD11	2.00	0.42
23:3:1233:SER:HB2	23:3:1236:ASN:HB2	2.00	0.42
36:Y:140:HIS:NE2	36:Y:165:THR:OG1	2.43	0.42
4:D:739:GLN:NE2	4:D:823:GLY:HA2	2.34	0.42
4:D:1016:ASP:OD2	4:D:1020:ARG:NH1	2.49	0.42
4:D:1031:LEU:HD22	4:D:1128:LEU:HD21	2.00	0.42
12:F:88:U:O4	14:H:17:U:H6	2.01	0.42
14:H:44:U:H2'	14:H:45:U:C6	2.55	0.42
21:1:732:LEU:HD12	21:1:732:LEU:HA	1.79	0.42
23:3:1084:ARG:HH21	23:3:1084:ARG:HG3	1.84	0.42
32:P:81:LYS:HE2	32:P:81:LYS:HB2	1.89	0.42
34:R:48:VAL:HG13	34:R:218:GLY:C	2.45	0.42
46:I:553:GLU:O	46:I:557:PRO:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:x:296:VAL:HG11	47:x:301:GLU:HB2	2.02	0.42
47:x:777:ARG:HE	47:x:777:ARG:HB2	1.51	0.42
3:C:802:ALA:HB2	3:C:843:LYS:HA	2.02	0.42
3:C:889:TYR:HH	13:G:79:A:HO2'	1.61	0.42
4:D:463:ILE:HB	4:D:707:PHE:HB2	2.01	0.42
13:G:487:A:N3	18:u:411:LEU:HD22	2.35	0.42
14:H:1096:C:H2'	14:H:1097:G:H8	1.85	0.42
18:u:24:ARG:HA	18:u:27:ARG:HG2	2.01	0.42
18:u:81:ILE:HD11	18:u:161:ALA:HB2	2.02	0.42
23:3:380:LEU:HD12	23:3:380:LEU:HA	1.84	0.42
23:3:955:LEU:HD12	23:3:956:GLN:N	2.35	0.42
31:T:160:ASN:HA	31:T:184:THR:HG23	2.02	0.42
31:T:369:ASP:HA	31:T:401:SER:HB2	2.01	0.42
45:J:205:TRP:CE2	45:J:209:GLU:HG3	2.54	0.42
46:I:511:ALA:O	46:I:514:VAL:N	2.44	0.42
47:x:709:GLU:OE2	47:x:713:GLN:NE2	2.52	0.42
1:A:476:ALA:HB1	3:C:389:LEU:HB3	2.01	0.42
2:B:1:A:N6	2:B:164:C:N4	2.58	0.42
3:C:183:GLN:HE22	3:C:187:ARG:HH11	1.58	0.42
4:D:912:PHE:HB3	4:D:944:LEU:HD22	2.01	0.42
4:D:1342:VAL:O	4:D:1415:ARG:NH1	2.48	0.42
12:F:3:U:O4	39:W:53:LYS:NZ	2.53	0.42
10:j:56:ALA:HB2	10:j:71:ILE:HG12	2.02	0.42
18:u:53:LEU:HD23	18:u:58:LYS:HE3	2.02	0.42
21:1:519:ILE:HG21	21:1:561:LEU:HG	2.01	0.42
21:1:550:THR:CB	21:1:590:LEU:HD23	2.50	0.42
27:L:214:ASN:HD21	45:J:44:ARG:HD2	1.85	0.42
31:T:247:VAL:HG21	35:S:10:GLU:HG2	2.02	0.42
33:Q:29:PRO:HA	33:Q:42:THR:HG22	2.02	0.42
41:V:9:GLU:HA	41:V:12:LYS:HB3	2.02	0.42
41:V:408:THR:HG23	41:V:457:HIS:CE1	2.53	0.42
1:A:909:THR:HG21	21:1:49:GLN:HG3	2.00	0.42
4:D:1921:SER:OG	4:D:1922:VAL:N	2.52	0.42
13:G:504:C:H42	21:1:776:GLN:HE21	1.68	0.42
14:H:47:U:OP2	18:u:409:TYR:CE2	2.72	0.42
6:h:44:VAL:HG23	17:l:7:PRO:HG3	2.02	0.42
23:3:173:THR:CG2	23:3:1296:SER:HA	2.49	0.42
23:3:1096:LEU:HD13	23:3:1187:PHE:CZ	2.35	0.42
31:T:238:LEU:HD21	31:T:250:LEU:HD22	2.02	0.42
43:z:15:LEU:HB2	43:z:22:ILE:HB	2.01	0.42
47:x:550:ALA:HB2	47:x:563:ARG:HH21	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:60:U:O2	2:B:60:U:H3'	2.19	0.42
2:B:105:A:N6	53:B:326:HOH:O	2.52	0.42
3:C:397:LYS:NZ	3:C:408:LEU:O	2.52	0.42
3:C:500:ARG:NE	3:C:536:SER:OG	2.53	0.42
3:C:617:LYS:HE2	3:C:617:LYS:HB2	1.83	0.42
14:H:119:G:N7	7:m:20:LYS:NZ	2.62	0.42
6:h:23:LEU:HD23	6:h:29:VAL:HG22	2.02	0.42
17:l:21:LEU:HD13	17:l:72:ILE:HG12	2.02	0.42
18:u:22:ALA:HB2	19:w:164:CYS:HB3	2.02	0.42
18:u:512:GLU:O	18:u:512:GLU:HG2	2.19	0.42
21:1:371:ARG:HH11	21:1:371:ARG:HD2	1.72	0.42
32:P:241:LEU:CD1	36:Y:204:VAL:HG12	2.49	0.42
45:J:219:ARG:HG3	45:J:253:TRP:HE1	1.85	0.42
47:x:523:LYS:HD3	47:x:536:LEU:HD21	2.02	0.42
47:x:836:MET:HE3	47:x:842:PHE:HB2	2.01	0.42
1:A:1790:TRP:HE3	1:A:1794:LEU:HB3	1.84	0.42
3:C:190:SER:O	3:C:216:PRO:CB	2.68	0.42
14:H:47:U:H3'	14:H:47:U:O2	2.20	0.42
18:u:425:ILE:HG13	18:u:467:ILE:HG22	2.02	0.42
20:v:175:LYS:HE3	20:v:175:LYS:HB3	1.75	0.42
21:1:285:ASP:HB3	21:1:297:THR:HG21	2.01	0.42
23:3:368:GLY:HA2	23:3:380:LEU:O	2.20	0.42
23:3:1078:HIS:O	23:3:1085:LEU:HD23	2.19	0.42
31:T:218:ARG:NH2	35:S:34:HIS:O	2.53	0.42
31:T:302:LYS:HG2	31:T:339:GLY:HA3	2.02	0.42
31:T:373:LEU:HD11	31:T:426:TRP:CE2	2.55	0.42
1:A:1991:ILE:HA	1:A:2039:LEU:HD12	2.01	0.41
3:C:234:LEU:HD13	3:C:439:ILE:HG23	2.02	0.41
13:G:111:U:O4	34:R:44:ASN:CG	2.63	0.41
21:1:590:LEU:H	21:1:590:LEU:HG	1.74	0.41
31:T:159:SER:OG	31:T:160:ASN:N	2.52	0.41
33:Q:75:MET:SD	34:R:130:PHE:CD1	3.13	0.41
43:z:111:LEU:C	43:z:113:ASP:N	2.78	0.41
1:A:784:GLN:CG	14:H:19:U:H5	1.96	0.41
2:B:10:U:H2'	2:B:11:A:C8	2.55	0.41
3:C:274:ILE:HD13	3:C:385:PHE:HE2	1.85	0.41
4:D:1091:GLY:O	4:D:1095:ASN:ND2	2.53	0.41
4:D:1475:ASP:N	4:D:1511:LEU:O	2.54	0.41
13:G:487:A:C8	13:G:487:A:C3'	3.03	0.41
15:o:100:ASN:HA	15:o:126:ASN:HB2	2.01	0.41
22:2:323:THR:OG1	24:4:62:ASP:OD1	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:3:196:ASP:HA	23:3:197:PRO:HD3	1.96	0.41
38:Z:164:MET:HE3	38:Z:169:LYS:HG2	2.02	0.41
1:A:631:LEU:HD12	1:A:631:LEU:HA	1.94	0.41
1:A:675:HIS:NE2	2:B:102:C:OP1	2.52	0.41
1:A:893:ARG:NH2	1:A:1136:GLY:O	2.46	0.41
1:A:1486:ARG:NH2	53:V:602:HOH:O	2.54	0.41
4:D:460:TYR:OH	4:D:728:GLU:OE1	2.32	0.41
4:D:774:ASP:HB3	4:D:777:SER:HB3	2.02	0.41
7:m:102:ASN:ND2	18:u:343:LEU:O	2.47	0.41
20:v:241:THR:HG22	20:v:252:VAL:HG12	2.01	0.41
21:1:969:LEU:O	23:3:1134:ARG:NH2	2.43	0.41
30:N:80:TRP:HE3	30:N:81:LEU:HD12	1.85	0.41
41:V:84:ASN:HB3	41:V:220:TYR:HE1	1.85	0.41
1:A:770:MET:O	31:T:309:ARG:NH1	2.53	0.41
1:A:784:GLN:NE2	14:H:19:U:H5''	2.33	0.41
1:A:1797:LEU:O	1:A:1797:LEU:HD22	2.20	0.41
13:G:504:C:H42	21:1:776:GLN:NE2	2.17	0.41
19:w:200:PHE:HE2	20:v:189:SER:H	1.67	0.41
21:1:777:LEU:O	21:1:781:THR:HG22	2.21	0.41
23:3:70:ASN:ND2	53:3:1553:HOH:O	2.54	0.41
24:4:13:VAL:HG22	24:4:83:VAL:HG22	2.01	0.41
1:A:966:PRO:HB3	1:A:1089:VAL:HB	2.02	0.41
2:B:26:A:C6	2:B:141:G:H1'	2.56	0.41
2:B:131:A:H5''	2:B:132:A:N7	2.35	0.41
4:D:1388:TRP:HH2	4:D:1416:PHE:HB3	1.85	0.41
4:D:1889:PHE:HE1	4:D:1950:ILE:HG23	1.85	0.41
18:u:474:TRP:HA	18:u:477:MET:HB2	2.03	0.41
22:2:291:PRO:HG3	22:2:325:TYR:CZ	2.55	0.41
23:3:396:ASP:HB2	23:3:404:LEU:HB2	2.03	0.41
32:P:242:LYS:HZ3	36:Y:92:PRO:HG3	1.85	0.41
33:Q:26:THR:HB	33:Q:45:HIS:HB2	2.02	0.41
47:x:232:LEU:HD21	47:x:256:LEU:HD11	2.03	0.41
1:A:831:ARG:HD2	1:A:831:ARG:HA	1.68	0.41
1:A:878:GLU:HG2	35:S:133:PHE:HE1	1.85	0.41
1:A:1029:THR:HG23	1:A:1269:ILE:HD11	2.01	0.41
1:A:1731:LYS:HD3	1:A:1768:PRO:HB2	2.03	0.41
1:A:2208:TYR:HE1	1:A:2255:LEU:HD23	1.84	0.41
1:A:2356:VAL:HG13	1:A:2387:HIS:CD2	2.56	0.41
13:G:506:U:H4'	13:G:506:U:OP1	2.21	0.41
6:h:28:ARG:HB2	17:l:70:LYS:HZ1	1.86	0.41
10:j:80:TYR:HE1	10:j:82:ARG:HD2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:k:17:LEU:N	11:k:25:VAL:O	2.40	0.41
23:3:1056:LYS:HE3	23:3:1056:LYS:HB2	1.93	0.41
47:x:678:LEU:HA	47:x:681:THR:HG23	2.02	0.41
3:C:150:MET:HE3	3:C:150:MET:HB3	1.91	0.41
4:D:1542:GLU:OE1	4:D:1711:SER:OG	2.35	0.41
16:p:55:PHE:HB3	16:p:81:GLN:O	2.20	0.41
23:3:582:LYS:HE2	23:3:585:GLN:HB3	2.03	0.41
27:L:491:GLY:O	27:L:495:MET:N	2.45	0.41
46:I:195:PHE:O	46:I:199:GLU:N	2.52	0.41
1:A:237:MET:HG2	1:A:644:VAL:HG11	2.02	0.41
1:A:763:MET:HE3	1:A:763:MET:HB3	1.81	0.41
1:A:1879:ILE:HB	1:A:1892:LYS:HB3	2.03	0.41
3:C:124:LEU:HD13	3:C:124:LEU:HA	1.86	0.41
3:C:270:LEU:HD11	3:C:313:PHE:HB3	2.03	0.41
3:C:915:GLU:OE2	3:C:919:ARG:NH2	2.50	0.41
18:u:91:GLN:HG2	18:u:95:LYS:HE2	2.03	0.41
23:3:724:LYS:HE3	23:3:746:GLU:OE1	2.21	0.41
23:3:742:HIS:HE2	23:3:752:LYS:HE2	1.85	0.41
25:5:38:ARG:HA	25:5:39:PRO:HD2	1.91	0.41
34:R:50:PRO:HG2	34:R:51:PHE:CZ	2.56	0.41
34:R:53:LEU:HD22	34:R:54:GLN:H	1.85	0.41
34:R:54:GLN:HB3	34:R:57:LEU:HB3	2.02	0.41
41:V:148:LEU:HA	41:V:151:VAL:HG12	2.03	0.41
41:V:345:ILE:HD13	41:V:345:ILE:HA	1.88	0.41
43:z:92:TRP:CZ2	43:z:97:ASN:HA	2.56	0.41
1:A:2249:ASP:OD1	4:D:1792:ARG:NH2	2.49	0.41
2:B:6:G:N2	2:B:161:U:C2	2.88	0.41
2:B:142:C:H2'	2:B:143:U:C6	2.56	0.41
3:C:721:GLN:HE21	3:C:725:ARG:HH12	1.68	0.41
4:D:503:GLN:HG2	4:D:530:ILE:HG13	2.03	0.41
4:D:1010:ILE:HD12	4:D:1108:LEU:HD23	2.03	0.41
12:F:79:A:OP2	13:G:102:A:O2'	2.38	0.41
14:H:149:A:H2'	14:H:150:G:H8	1.85	0.41
7:m:16:THR:HB	7:m:96:ILE:HB	2.03	0.41
18:u:251:LEU:HD13	18:u:256:VAL:HG21	2.01	0.41
19:w:129:HIS:CD2	19:w:131:LEU:HB2	2.56	0.41
23:3:289:ASN:HB3	23:3:331:PHE:CE1	2.55	0.41
23:3:636:THR:HG22	23:3:643:ILE:HB	2.03	0.41
31:T:280:GLN:HG3	31:T:295:VAL:HG22	2.01	0.41
31:T:306:HIS:HB3	31:T:332:ARG:NH1	2.34	0.41
32:P:105:LEU:HD13	32:P:105:LEU:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:X:80:GLU:OE2	38:Z:208:SER:OG	2.39	0.41
41:V:471:GLY:O	41:V:474:THR:OG1	2.33	0.41
43:z:87:ASP:HB2	43:z:103:VAL:O	2.16	0.41
43:z:91:GLY:N	43:z:100:PHE:O	2.45	0.41
45:J:306:LYS:O	45:J:310:GLU:N	2.50	0.41
47:x:777:ARG:HG2	47:x:858:MET:SD	2.61	0.41
1:A:1335:TRP:HB2	1:A:1367:ILE:HD13	2.02	0.41
1:A:2014:ALA:HB3	1:A:2055:MET:HE3	2.02	0.41
3:C:863:GLU:HB2	3:C:931:TYR:CE1	2.56	0.41
14:H:12:U:H2'	14:H:13:G:C8	2.56	0.41
6:h:50:GLU:HB3	6:h:80:ARG:HB3	2.02	0.41
9:i:40:LYS:O	9:i:58:VAL:N	2.54	0.41
18:u:148:SER:HB2	18:u:158:SER:HA	2.03	0.41
18:u:174:GLU:OE2	18:u:239:TYR:OH	2.25	0.41
28:q:19:SER:OG	28:q:38:ASP:OD2	2.37	0.41
36:Y:64:TYR:OH	36:Y:150:GLY:O	2.30	0.41
39:W:68:PRO:HG2	39:W:69:TRP:CE3	2.56	0.41
42:M:78:VAL:HG13	43:z:8:GLN:HE22	1.87	0.41
47:x:474:ILE:HD13	47:x:474:ILE:HG21	1.91	0.41
1:A:1283:GLU:HG3	41:V:341:LYS:HB2	2.02	0.40
1:A:2041:PRO:HG2	1:A:2043:PHE:CE2	2.56	0.40
2:B:21:G:H2'	2:B:22:G:C8	2.56	0.40
3:C:133:ILE:HD13	3:C:560:GLN:HB3	2.03	0.40
4:D:1063:ILE:HA	4:D:1064:PRO:HD3	1.92	0.40
28:s:105:LEU:O	28:s:109:LEU:N	2.52	0.40
31:T:118:LEU:HD21	32:P:49:SER:HA	2.03	0.40
31:T:259:VAL:HG11	32:P:74:ILE:HG23	2.03	0.40
1:A:548:LEU:HD23	1:A:548:LEU:HA	1.92	0.40
1:A:2302:LEU:HD23	1:A:2339:LEU:HD21	2.03	0.40
3:C:493:LEU:HD21	3:C:539:VAL:HG21	2.02	0.40
3:C:683:ASN:HD22	3:C:683:ASN:HA	1.66	0.40
4:D:877:ARG:HA	4:D:878:PRO:HD3	1.96	0.40
11:k:71:LEU:HG	17:l:63:PHE:HB3	2.02	0.40
17:l:41:ASN:HD22	17:l:65:ARG:HA	1.86	0.40
18:u:150:PRO:HG3	18:u:155:ASN:H	1.85	0.40
22:2:181:GLU:HB3	22:2:184:SER:OG	2.21	0.40
32:P:300:ASP:N	32:P:300:ASP:OD1	2.53	0.40
43:z:59:GLN:N	43:z:103:VAL:HG21	2.35	0.40
1:A:173:LEU:HD13	1:A:715:LEU:CB	2.51	0.40
1:A:222:ILE:HD11	1:A:317:PRO:HG3	2.04	0.40
1:A:1608:LEU:HD11	1:A:1648:ILE:HD11	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:740:ILE:HD12	3:C:740:ILE:HA	1.92	0.40
4:D:567:VAL:HG13	4:D:606:VAL:HG12	2.02	0.40
6:h:42:ASN:ND2	6:h:89:GLY:H	2.20	0.40
9:i:32:PHE:HE1	11:k:67:SER:HA	1.86	0.40
18:u:170:PHE:CZ	18:u:246:LYS:HG2	2.56	0.40
21:1:864:LEU:HD12	21:1:864:LEU:HA	1.91	0.40
23:3:651:LEU:O	23:3:669:HIS:HB2	2.21	0.40
31:T:371:GLY:HA3	31:T:400:ARG:HG2	2.03	0.40
31:T:414:LEU:HB3	31:T:426:TRP:HB2	2.02	0.40
47:x:409:TYR:CE2	47:x:567:LYS:HD3	2.57	0.40
1:A:227:GLU:OE2	1:A:231:ARG:NE	2.54	0.40
1:A:770:MET:HE1	32:P:165:ILE:HD11	2.04	0.40
1:A:1067:ASN:HD22	27:L:81:PRO:HB2	1.86	0.40
3:C:693:ASN:HB2	3:C:841:LEU:HD13	2.03	0.40
4:D:2135:SER:OG	4:D:2163:LYS:OXT	2.34	0.40
23:3:1092:GLU:O	23:3:1116:ARG:N	2.37	0.40
24:4:67:ILE:HD13	24:4:85:GLN:HB3	2.03	0.40
27:L:214:ASN:HB2	45:J:48:ARG:HG3	2.02	0.40
31:T:308:LYS:HA	32:P:148:HIS:CE1	2.56	0.40
32:P:45:PRO:HG2	32:P:48:GLN:HB2	2.03	0.40
34:R:87:CYS:SG	34:R:91:HIS:HE1	2.45	0.40
37:X:129:ASP:OD2	38:Z:231:ARG:NH2	2.55	0.40
41:V:80:ILE:HA	41:V:83:LEU:HD12	2.04	0.40
1:A:1588:LYS:O	1:A:1590:LEU:N	2.55	0.40
1:A:2356:VAL:HG13	1:A:2387:HIS:HD2	1.87	0.40
4:D:1984:ILE:HG21	4:D:2148:SER:HB2	2.03	0.40
14:H:36:A:C5'	14:H:36:A:C8	3.04	0.40
14:H:47:U:O2	14:H:47:U:C3'	2.70	0.40
16:p:31:TYR:O	16:p:102:GLU:N	2.54	0.40
6:h:42:ASN:HD22	6:h:88:ARG:HA	1.86	0.40
7:m:17:ILE:HB	7:m:25:VAL:HB	2.04	0.40
21:1:677:LYS:HA	21:1:677:LYS:HD2	1.92	0.40
23:3:961:CYS:HB3	23:3:970:LEU:HD23	2.02	0.40
33:Q:75:MET:CE	34:R:130:PHE:CE1	2.94	0.40
36:Y:41:GLU:OE2	37:X:98:GLY:CA	2.70	0.40
41:V:322:LYS:HE3	41:V:357:TRP:CE2	2.57	0.40
45:J:155:LEU:HD23	45:J:155:LEU:HA	1.95	0.40
46:I:565:LYS:HA	46:I:570:THR:HG21	2.04	0.40
47:x:349:HIS:HA	47:x:382:ASN:HD22	1.86	0.40
47:x:585:THR:OG1	47:x:586:ASN:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2199/2413 (91%)	2127 (97%)	68 (3%)	4 (0%)	43	63
3	C	912/1008 (90%)	877 (96%)	33 (4%)	2 (0%)	43	63
4	D	1820/2163 (84%)	1759 (97%)	60 (3%)	1 (0%)	48	68
5	d	77/101 (76%)	69 (90%)	8 (10%)	0	100	100
6	a	69/196 (35%)	64 (93%)	5 (7%)	0	100	100
6	h	74/196 (38%)	70 (95%)	4 (5%)	0	100	100
7	b	71/146 (49%)	69 (97%)	2 (3%)	0	100	100
7	m	78/146 (53%)	77 (99%)	1 (1%)	0	100	100
8	c	86/110 (78%)	79 (92%)	7 (8%)	0	100	100
8	n	63/110 (57%)	57 (90%)	6 (10%)	0	100	100
9	e	66/94 (70%)	63 (96%)	3 (4%)	0	100	100
9	i	71/94 (76%)	70 (99%)	1 (1%)	0	100	100
10	f	66/86 (77%)	59 (89%)	7 (11%)	0	100	100
10	j	66/86 (77%)	65 (98%)	1 (2%)	0	100	100
11	g	64/77 (83%)	61 (95%)	3 (5%)	0	100	100
11	k	65/77 (84%)	64 (98%)	1 (2%)	0	100	100
15	o	125/238 (52%)	115 (92%)	8 (6%)	2 (2%)	7	14
16	p	73/111 (66%)	73 (100%)	0	0	100	100
17	l	79/81 (98%)	73 (92%)	6 (8%)	0	100	100
18	u	453/530 (86%)	423 (93%)	29 (6%)	1 (0%)	43	63
19	w	123/280 (44%)	117 (95%)	6 (5%)	0	100	100
20	v	201/266 (76%)	185 (92%)	16 (8%)	0	100	100
21	1	926/971 (95%)	898 (97%)	23 (2%)	5 (0%)	24	43
22	2	214/238 (90%)	208 (97%)	4 (2%)	2 (1%)	14	27
23	3	1193/1361 (88%)	1124 (94%)	65 (5%)	4 (0%)	36	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	4	166/213 (78%)	161 (97%)	5 (3%)	0	100	100
25	5	101/107 (94%)	99 (98%)	2 (2%)	0	100	100
26	6	82/84 (98%)	81 (99%)	0	1 (1%)	10	20
27	L	427/590 (72%)	391 (92%)	26 (6%)	10 (2%)	5	8
28	q	125/503 (25%)	116 (93%)	9 (7%)	0	100	100
28	r	119/503 (24%)	114 (96%)	5 (4%)	0	100	100
28	s	118/503 (24%)	114 (97%)	4 (3%)	0	100	100
28	t	122/503 (24%)	118 (97%)	4 (3%)	0	100	100
29	K	149/175 (85%)	140 (94%)	7 (5%)	2 (1%)	9	18
30	N	155/157 (99%)	148 (96%)	6 (4%)	1 (1%)	21	38
31	T	335/337 (99%)	317 (95%)	14 (4%)	4 (1%)	10	20
32	P	236/379 (62%)	228 (97%)	5 (2%)	3 (1%)	9	18
33	Q	288/364 (79%)	265 (92%)	20 (7%)	3 (1%)	12	24
34	R	259/261 (99%)	241 (93%)	17 (7%)	1 (0%)	30	49
35	S	65/175 (37%)	61 (94%)	4 (6%)	0	100	100
36	Y	170/204 (83%)	163 (96%)	6 (4%)	1 (1%)	21	38
37	X	126/128 (98%)	122 (97%)	4 (3%)	0	100	100
38	Z	119/121 (98%)	117 (98%)	2 (2%)	0	100	100
39	W	21/455 (5%)	20 (95%)	1 (5%)	0	100	100
40	U	25/135 (18%)	24 (96%)	1 (4%)	0	100	100
41	V	446/577 (77%)	427 (96%)	19 (4%)	0	100	100
42	M	172/259 (66%)	163 (95%)	8 (5%)	1 (1%)	21	38
43	z	146/301 (48%)	126 (86%)	18 (12%)	2 (1%)	9	17
44	y	63/185 (34%)	57 (90%)	6 (10%)	0	100	100
45	J	528/687 (77%)	493 (93%)	31 (6%)	4 (1%)	16	31
46	I	544/859 (63%)	491 (90%)	36 (7%)	17 (3%)	3	5
47	x	651/876 (74%)	617 (95%)	33 (5%)	1 (0%)	43	63
All	All	14992/20820 (72%)	14260 (95%)	660 (4%)	72 (0%)	26	43

All (72) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	91	VAL

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Mol	Chain	Res	Type
22	2	268	ASP
23	3	585	GLN
27	L	367	VAL
27	L	417	PRO
27	L	418	PRO
29	K	77	PRO
33	Q	118	VAL
33	Q	299	ALA
46	I	223	PRO
46	I	373	ASP
46	I	511	ALA
46	I	739	SER
15	o	68	PRO
21	1	158	LYS
23	3	958	ASP
27	L	374	PRO
31	T	442	TRP
33	Q	298	SER
42	M	234	PHE
43	z	103	VAL
45	J	539	GLU
46	I	238	ARG
46	I	293	GLN
46	I	368	PHE
46	I	507	ILE
1	A	510	PRO
21	1	157	ASN
23	3	584	SER
46	I	225	GLN
46	I	759	ILE
46	I	778	THR
1	A	771	PRO
1	A	1489	PRO
3	C	87	GLN
21	1	125	VAL
22	2	180	LYS
23	3	1039	ASN
26	6	24	GLU
27	L	223	PRO
27	L	415	ILE
29	K	82	ASP
31	T	391	GLU

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Mol	Chain	Res	Type
32	P	58	PRO
32	P	111	HIS
46	I	289	GLU
46	I	406	ASN
46	I	424	LYS
47	x	578	PRO
21	l	127	VAL
27	L	334	PRO
30	N	139	GLN
32	P	59	THR
34	R	24	ALA
43	z	112	ASN
45	J	388	PHE
45	J	467	GLN
1	A	547	LEU
15	o	67	ILE
21	l	145	ALA
46	I	290	PHE
4	D	265	ILE
18	u	377	VAL
45	J	464	ILE
27	L	225	PRO
27	L	440	ILE
31	T	122	ARG
36	Y	29	MET
46	I	267	PRO
46	I	773	PRO
27	L	81	PRO
31	T	264	GLY

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	
1	A	1997/2182 (92%)	1954 (98%)	43 (2%)	45	73
3	C	828/910 (91%)	815 (98%)	13 (2%)	55	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	1651/1955 (84%)	1646 (100%)	5 (0%)	86	94
6	h	67/176 (38%)	67 (100%)	0	100	100
7	m	77/129 (60%)	77 (100%)	0	100	100
8	n	59/103 (57%)	59 (100%)	0	100	100
9	i	65/83 (78%)	65 (100%)	0	100	100
10	j	61/77 (79%)	61 (100%)	0	100	100
11	k	58/66 (88%)	57 (98%)	1 (2%)	53	78
15	o	44/219 (20%)	42 (96%)	2 (4%)	24	49
16	p	23/100 (23%)	22 (96%)	1 (4%)	26	51
17	l	67/70 (96%)	67 (100%)	0	100	100
18	u	426/492 (87%)	422 (99%)	4 (1%)	70	87
19	w	118/259 (46%)	118 (100%)	0	100	100
20	v	182/236 (77%)	181 (100%)	1 (0%)	81	92
21	1	817/867 (94%)	785 (96%)	32 (4%)	28	55
22	2	197/212 (93%)	194 (98%)	3 (2%)	57	80
23	3	1113/1244 (90%)	1070 (96%)	43 (4%)	28	55
24	4	154/189 (82%)	153 (99%)	1 (1%)	78	91
25	5	93/97 (96%)	91 (98%)	2 (2%)	45	73
26	6	76/76 (100%)	76 (100%)	0	100	100
27	L	195/525 (37%)	186 (95%)	9 (5%)	24	48
28	q	65/451 (14%)	61 (94%)	4 (6%)	16	34
28	r	59/451 (13%)	56 (95%)	3 (5%)	21	43
28	s	61/451 (14%)	58 (95%)	3 (5%)	22	45
28	t	62/451 (14%)	58 (94%)	4 (6%)	15	32
29	K	37/165 (22%)	27 (73%)	10 (27%)	0	1
30	N	141/141 (100%)	137 (97%)	4 (3%)	38	66
31	T	295/295 (100%)	288 (98%)	7 (2%)	43	70
32	P	218/328 (66%)	215 (99%)	3 (1%)	59	81
33	Q	265/332 (80%)	263 (99%)	2 (1%)	73	88
34	R	224/224 (100%)	220 (98%)	4 (2%)	51	77
35	S	58/151 (38%)	58 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	Y	156/186 (84%)	156 (100%)	0	100	100
37	X	114/114 (100%)	107 (94%)	7 (6%)	17	35
38	Z	88/107 (82%)	87 (99%)	1 (1%)	65	84
39	W	20/413 (5%)	20 (100%)	0	100	100
40	U	21/121 (17%)	21 (100%)	0	100	100
41	V	416/538 (77%)	409 (98%)	7 (2%)	53	78
42	M	145/237 (61%)	143 (99%)	2 (1%)	59	81
43	z	134/273 (49%)	131 (98%)	3 (2%)	45	73
44	y	63/167 (38%)	58 (92%)	5 (8%)	11	24
45	J	215/633 (34%)	215 (100%)	0	100	100
46	I	58/786 (7%)	54 (93%)	4 (7%)	14	30
47	x	586/789 (74%)	575 (98%)	11 (2%)	50	76
All	All	11869/18071 (66%)	11625 (98%)	244 (2%)	46	74

All (244) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	461	LEU
1	A	479	LEU
1	A	593	LEU
1	A	631	LEU
1	A	632	ILE
1	A	712	LEU
1	A	715	LEU
1	A	737	ARG
1	A	738	SER
1	A	739	ASN
1	A	742	VAL
1	A	783	LEU
1	A	1087	ASN
1	A	1178	GLU
1	A	1180	GLU
1	A	1182	LEU
1	A	1222	LEU
1	A	1268	ARG
1	A	1301	TYR
1	A	1356	LEU
1	A	1457	VAL

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Mol	Chain	Res	Type
1	A	1475	LEU
1	A	1601	ILE
1	A	1608	LEU
1	A	1618	ASN
1	A	1619	VAL
1	A	1624	LEU
1	A	1728	ILE
1	A	1739	ARG
1	A	1742	ASP
1	A	1747	ASP
1	A	1782	ASN
1	A	1794	LEU
1	A	1797	LEU
1	A	1798	ILE
1	A	1801	SER
1	A	1809	ASN
1	A	1815	LEU
1	A	1889	LEU
1	A	1891	LEU
1	A	1892	LYS
1	A	2075	THR
1	A	2325	LEU
3	C	77	LEU
3	C	84	GLN
3	C	87	GLN
3	C	91	VAL
3	C	189	LEU
3	C	190	SER
3	C	191	ILE
3	C	264	CYS
3	C	441	ARG
3	C	442	CYS
3	C	634	ILE
3	C	683	ASN
3	C	945	LEU
4	D	265	ILE
4	D	763	GLU
4	D	764	GLU
4	D	1557	ILE
4	D	1799	ILE
15	o	4	THR
15	o	44	PRO

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Mol	Chain	Res	Type
16	p	58	VAL
11	k	20	ASN
18	u	377	VAL
18	u	506	LEU
18	u	508	GLU
18	u	515	VAL
20	v	219	LEU
21	1	117	LYS
21	1	122	SER
21	1	124	LEU
21	1	125	VAL
21	1	131	HIS
21	1	254	GLU
21	1	285	ASP
21	1	306	LYS
21	1	396	VAL
21	1	411	VAL
21	1	412	LEU
21	1	416	LEU
21	1	421	SER
21	1	422	MET
21	1	429	GLU
21	1	437	GLU
21	1	561	LEU
21	1	562	ILE
21	1	589	SER
21	1	590	LEU
21	1	615	LEU
21	1	672	VAL
21	1	698	ARG
21	1	732	LEU
21	1	734	LEU
21	1	736	LYS
21	1	864	LEU
21	1	884	LEU
21	1	885	ILE
21	1	923	LEU
21	1	967	LEU
21	1	971	LEU
22	2	179	LYS
22	2	180	LYS
22	2	181	GLU

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Mol	Chain	Res	Type
23	3	65	LEU
23	3	101	LEU
23	3	151	THR
23	3	152	SER
23	3	170	ARG
23	3	171	LEU
23	3	172	LYS
23	3	179	LEU
23	3	296	LEU
23	3	310	LEU
23	3	380	LEU
23	3	381	LEU
23	3	382	GLN
23	3	401	ASN
23	3	431	SER
23	3	433	MET
23	3	537	ILE
23	3	582	LYS
23	3	584	SER
23	3	644	ILE
23	3	765	ILE
23	3	954	SER
23	3	955	LEU
23	3	956	GLN
23	3	957	ILE
23	3	963	LYS
23	3	977	ILE
23	3	979	CYS
23	3	1011	ASN
23	3	1012	LYS
23	3	1035	LEU
23	3	1039	ASN
23	3	1041	LEU
23	3	1084	ARG
23	3	1085	LEU
23	3	1097	PHE
23	3	1124	LEU
23	3	1126	GLU
23	3	1171	ILE
23	3	1188	GLN
23	3	1217	ILE
23	3	1236	ASN

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Mol	Chain	Res	Type
23	3	1249	GLU
24	4	107	ILE
25	5	12	LEU
25	5	62	ASN
27	L	44	THR
27	L	224	MET
27	L	229	ASP
27	L	232	THR
27	L	501	THR
27	L	504	PRO
27	L	505	PRO
27	L	532	PRO
27	L	550	PRO
28	s	17	PRO
28	s	44	PRO
28	s	63	THR
28	t	17	PRO
28	t	44	PRO
28	t	63	THR
28	t	98	LEU
28	q	17	PRO
28	q	44	PRO
28	q	55	PRO
28	q	106	THR
28	r	17	PRO
28	r	44	PRO
28	r	63	THR
29	K	7	VAL
29	K	13	PRO
29	K	76	THR
29	K	86	LEU
29	K	96	PRO
29	K	100	THR
29	K	105	PRO
29	K	133	PRO
29	K	150	THR
29	K	152	THR
30	N	2	PRO
30	N	140	VAL
30	N	145	CYS
30	N	146	VAL
31	T	160	ASN

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Mol	Chain	Res	Type
31	T	200	VAL
31	T	229	THR
31	T	328	THR
31	T	343	THR
31	T	357	SER
31	T	440	LEU
32	P	133	LYS
32	P	179	THR
32	P	244	LEU
33	Q	17	LEU
33	Q	293	TRP
34	R	51	PHE
34	R	53	LEU
34	R	54	GLN
34	R	169	ASP
37	X	56	VAL
37	X	85	THR
37	X	87	LEU
37	X	97	ILE
37	X	100	ARG
37	X	102	LEU
37	X	103	LYS
38	Z	258	GLN
41	V	162	LEU
41	V	194	LEU
41	V	345	ILE
41	V	346	LEU
41	V	350	MET
41	V	420	ILE
41	V	445	LEU
42	M	134	THR
42	M	210	VAL
43	z	103	VAL
43	z	108	LYS
43	z	111	LEU
44	y	90	GLU
44	y	91	TYR
44	y	93	THR
44	y	96	GLU
44	y	109	LEU
46	I	616	PRO
46	I	617	PRO

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Mol	Chain	Res	Type
46	I	641	PRO
46	I	722	PRO
47	x	267	ASP
47	x	268	GLN
47	x	270	LYS
47	x	271	LEU
47	x	272	GLN
47	x	358	LEU
47	x	534	THR
47	x	630	ASN
47	x	777	ARG
47	x	836	MET
47	x	837	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (232) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	HIS
1	A	170	HIS
1	A	185	GLN
1	A	310	ASN
1	A	343	ASN
1	A	389	HIS
1	A	429	ASN
1	A	509	HIS
1	A	542	HIS
1	A	543	ASN
1	A	574	GLN
1	A	576	HIS
1	A	636	HIS
1	A	784	GLN
1	A	839	HIS
1	A	868	GLN
1	A	974	ASN
1	A	1030	GLN
1	A	1067	ASN
1	A	1086	ASN
1	A	1087	ASN
1	A	1128	GLN
1	A	1156	HIS
1	A	1173	HIS
1	A	1376	ASN

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Mol	Chain	Res	Type
1	A	1424	HIS
1	A	1529	ASN
1	A	1531	HIS
1	A	1635	HIS
1	A	1658	HIS
1	A	1746	HIS
1	A	1782	ASN
1	A	1809	ASN
1	A	1883	ASN
1	A	1895	HIS
1	A	1985	GLN
1	A	2018	ASN
1	A	2047	GLN
1	A	2232	HIS
1	A	2387	HIS
3	C	84	GLN
3	C	103	HIS
3	C	108	GLN
3	C	119	ASN
3	C	158	HIS
3	C	180	ASN
3	C	183	GLN
3	C	251	GLN
3	C	259	ASN
3	C	289	ASN
3	C	366	ASN
3	C	426	GLN
3	C	431	GLN
3	C	444	GLN
3	C	560	GLN
3	C	608	GLN
3	C	683	ASN
3	C	693	ASN
3	C	721	GLN
3	C	726	ASN
3	C	794	GLN
3	C	905	GLN
4	D	157	ASN
4	D	541	HIS
4	D	637	HIS
4	D	662	GLN
4	D	739	GLN

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Mol	Chain	Res	Type
4	D	826	GLN
4	D	892	GLN
4	D	919	ASN
4	D	937	ASN
4	D	1025	HIS
4	D	1086	GLN
4	D	1143	ASN
4	D	1148	GLN
4	D	1266	HIS
4	D	1278	GLN
4	D	1279	HIS
4	D	1283	ASN
4	D	1443	HIS
4	D	1481	GLN
4	D	1531	ASN
4	D	1549	GLN
4	D	1701	ASN
4	D	1760	ASN
4	D	1783	HIS
4	D	1812	ASN
4	D	1931	GLN
4	D	1968	ASN
4	D	2161	ASN
15	o	132	ASN
6	h	42	ASN
11	k	18	ASN
11	k	20	ASN
11	k	66	ASN
7	m	12	ASN
7	m	30	GLN
7	m	83	GLN
18	u	75	GLN
18	u	90	GLN
18	u	167	ASN
18	u	186	HIS
18	u	440	HIS
18	u	446	HIS
18	u	476	ASN
19	w	129	HIS
19	w	191	GLN
20	v	208	ASN
21	1	18	GLN

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Mol	Chain	Res	Type
21	1	65	HIS
21	1	141	HIS
21	1	219	HIS
21	1	339	GLN
21	1	607	ASN
21	1	695	ASN
21	1	776	GLN
21	1	853	HIS
21	1	867	ASN
21	1	873	HIS
21	1	882	ASN
21	1	894	HIS
22	2	136	GLN
22	2	248	HIS
23	3	68	GLN
23	3	70	ASN
23	3	156	ASN
23	3	176	ASN
23	3	198	ASN
23	3	246	ASN
23	3	333	ASN
23	3	360	HIS
23	3	382	GLN
23	3	385	HIS
23	3	401	ASN
23	3	417	HIS
23	3	435	ASN
23	3	453	ASN
23	3	547	ASN
23	3	590	HIS
23	3	601	GLN
23	3	609	HIS
23	3	696	ASN
23	3	719	GLN
23	3	754	HIS
23	3	887	HIS
23	3	1011	ASN
23	3	1023	HIS
23	3	1039	ASN
23	3	1081	ASN
23	3	1091	HIS
23	3	1188	GLN

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Mol	Chain	Res	Type
23	3	1191	ASN
23	3	1196	ASN
23	3	1222	GLN
23	3	1236	ASN
23	3	1304	HIS
24	4	9	ASN
24	4	187	ASN
24	4	191	ASN
25	5	62	ASN
25	5	64	ASN
26	6	11	GLN
27	L	214	ASN
27	L	249	ASN
30	N	112	ASN
30	N	115	ASN
30	N	116	ASN
30	N	144	GLN
31	T	138	HIS
31	T	152	ASN
31	T	160	ASN
31	T	181	HIS
32	P	37	ASN
32	P	110	HIS
32	P	148	HIS
32	P	322	GLN
32	P	331	GLN
32	P	332	GLN
33	Q	6	ASN
33	Q	54	ASN
33	Q	72	GLN
33	Q	81	HIS
33	Q	89	HIS
33	Q	106	ASN
33	Q	134	ASN
33	Q	244	HIS
34	R	54	GLN
34	R	69	GLN
34	R	91	HIS
34	R	147	ASN
34	R	227	ASN
34	R	248	ASN
35	S	34	HIS

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Mol	Chain	Res	Type
35	S	173	HIS
36	Y	99	ASN
37	X	2	ASN
37	X	72	GLN
38	Z	168	GLN
38	Z	258	GLN
40	U	4	ASN
40	U	19	HIS
41	V	84	ASN
41	V	105	GLN
41	V	116	ASN
41	V	182	GLN
41	V	223	HIS
41	V	279	GLN
41	V	310	HIS
41	V	354	HIS
41	V	429	ASN
41	V	457	HIS
42	M	79	ASN
42	M	126	ASN
42	M	140	GLN
42	M	179	ASN
42	M	237	HIS
42	M	241	HIS
42	M	255	ASN
43	z	8	GLN
43	z	115	ASN
44	y	98	ASN
45	J	117	HIS
45	J	147	ASN
45	J	170	ASN
47	x	234	GLN
47	x	268	GLN
47	x	502	ASN
47	x	630	ASN
47	x	661	HIS
47	x	727	HIS
47	x	757	ASN
47	x	833	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
12	F	102/112 (91%)	19 (18%)	1 (0%)
13	G	99/162 (61%)	45 (45%)	4 (4%)
14	H	161/1175 (13%)	40 (24%)	1 (0%)
2	B	177/214 (82%)	58 (32%)	6 (3%)
All	All	539/1663 (32%)	162 (30%)	12 (2%)

All (162) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	9	U
2	B	12	C
2	B	13	A
2	B	14	G
2	B	18	A
2	B	20	U
2	B	26	A
2	B	27	G
2	B	28	G
2	B	33	U
2	B	40	C
2	B	43	G
2	B	45	A
2	B	46	C
2	B	47	U
2	B	75	A
2	B	76	U
2	B	77	A
2	B	79	C
2	B	80	G
2	B	81	A
2	B	84	A
2	B	92	U
2	B	95	C
2	B	96	U
2	B	97	U
2	B	101	C
2	B	103	A
2	B	108	C
2	B	126	A
2	B	127	U
2	B	128	A
2	B	129	G
2	B	130	A

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Mol	Chain	Res	Type
2	B	131	A
2	B	135	G
2	B	139	A
2	B	141	G
2	B	142	C
2	B	149	U
2	B	151	A
2	B	152	C
2	B	157	G
2	B	158	G
2	B	160	U
2	B	161	U
2	B	162	G
2	B	163	C
2	B	164	C
2	B	165	A
2	B	166	U
2	B	167	A
2	B	168	U
2	B	170	U
2	B	171	U
2	B	172	U
2	B	174	G
2	B	176	A
12	F	14	C
12	F	36	U
12	F	41	A
12	F	42	A
12	F	43	C
12	F	48	C
12	F	51	A
12	F	53	A
12	F	54	U
12	F	60	G
12	F	66	C
12	F	74	U
12	F	81	G
12	F	82	A
12	F	85	C
12	F	86	G
12	F	88	U
12	F	91	A

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Mol	Chain	Res	Type
12	F	92	C
13	G	78	U
13	G	79	A
13	G	80	A
13	G	81	A
13	G	82	A
13	G	88	A
13	G	91	A
13	G	93	U
13	G	95	G
13	G	96	U
13	G	100	G
13	G	102	A
13	G	109	A
13	G	110	U
13	G	111	U
13	G	115	U
13	G	471	A
13	G	473	A
13	G	475	A
13	G	481	A
13	G	483	A
13	G	484	A
13	G	487	A
13	G	488	A
13	G	489	A
13	G	494	G
13	G	496	U
13	G	497	A
13	G	498	C
13	G	501	A
13	G	502	C
13	G	504	C
13	G	505	A
13	G	506	U
13	G	507	U
13	G	509	A
13	G	510	A
13	G	514	U
13	G	516	U
13	G	518	U
13	G	520	G

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Mol	Chain	Res	Type
13	G	521	U
13	G	529	U
13	G	530	U
13	G	533	U
14	H	17	U
14	H	18	U
14	H	19	U
14	H	25	A
14	H	26	G
14	H	30	A
14	H	32	G
14	H	36	A
14	H	37	G
14	H	45	U
14	H	47	U
14	H	48	U
14	H	49	U
14	H	59	C
14	H	66	A
14	H	67	A
14	H	68	U
14	H	82	C
14	H	83	U
14	H	111	C
14	H	115	U
14	H	116	U
14	H	118	U
14	H	119	G
14	H	1092	A
14	H	1094	G
14	H	1095	U
14	H	1096	C
14	H	1098	C
14	H	1101	C
14	H	1102	C
14	H	1103	C
14	H	1123	C
14	H	1124	U
14	H	1125	U
14	H	1142	G
14	H	1144	U
14	H	1145	U

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Mol	Chain	Res	Type
14	H	1146	G
14	H	1152	U

All (12) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	27	G
2	B	44	A
2	B	78	A
2	B	130	A
2	B	150	U
2	B	166	U
12	F	53	A
13	G	109	A
13	G	472	A
13	G	480	A
13	G	488	A
14	H	36	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 22 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
49	GTP	C	1101	50	33,34,34	0.90	1 (3%)	50,54,54	1.58	9 (18%)
48	IHP	A	3000	-	36,36,36	0.77	0	60,60,60	0.93	0

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
49	GTP	C	1101	50	-	7/22/38/38	0/3/3/3
48	IHP	A	3000	-	-	4/30/54/54	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	C	1101	GTP	C5-N7	-2.03	1.35	1.39

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	C	1101	GTP	C5-C4-N3	-4.51	121.22	128.39
49	C	1101	GTP	C2-N3-C4	4.46	119.98	112.30
49	C	1101	GTP	C2-N1-C6	-2.90	119.86	125.11
49	C	1101	GTP	N9-C8-N7	-2.84	108.14	113.40
49	C	1101	GTP	N9-C4-N3	2.60	131.15	125.95
49	C	1101	GTP	C8-N7-C5	2.41	108.56	104.26
49	C	1101	GTP	C5-C6-N1	2.35	119.22	113.25
49	C	1101	GTP	O6-C6-C5	-2.34	120.36	126.53
49	C	1101	GTP	O2A-PA-O3A	2.30	113.50	107.27

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
49	C	1101	GTP	C5'-O5'-PA-O3A
49	C	1101	GTP	C5'-O5'-PA-O2A
49	C	1101	GTP	O4'-C4'-C5'-O5'
49	C	1101	GTP	C3'-C4'-C5'-O5'
48	A	3000	IHP	C2-O12-P2-O22
49	C	1101	GTP	C5'-O5'-PA-O1A

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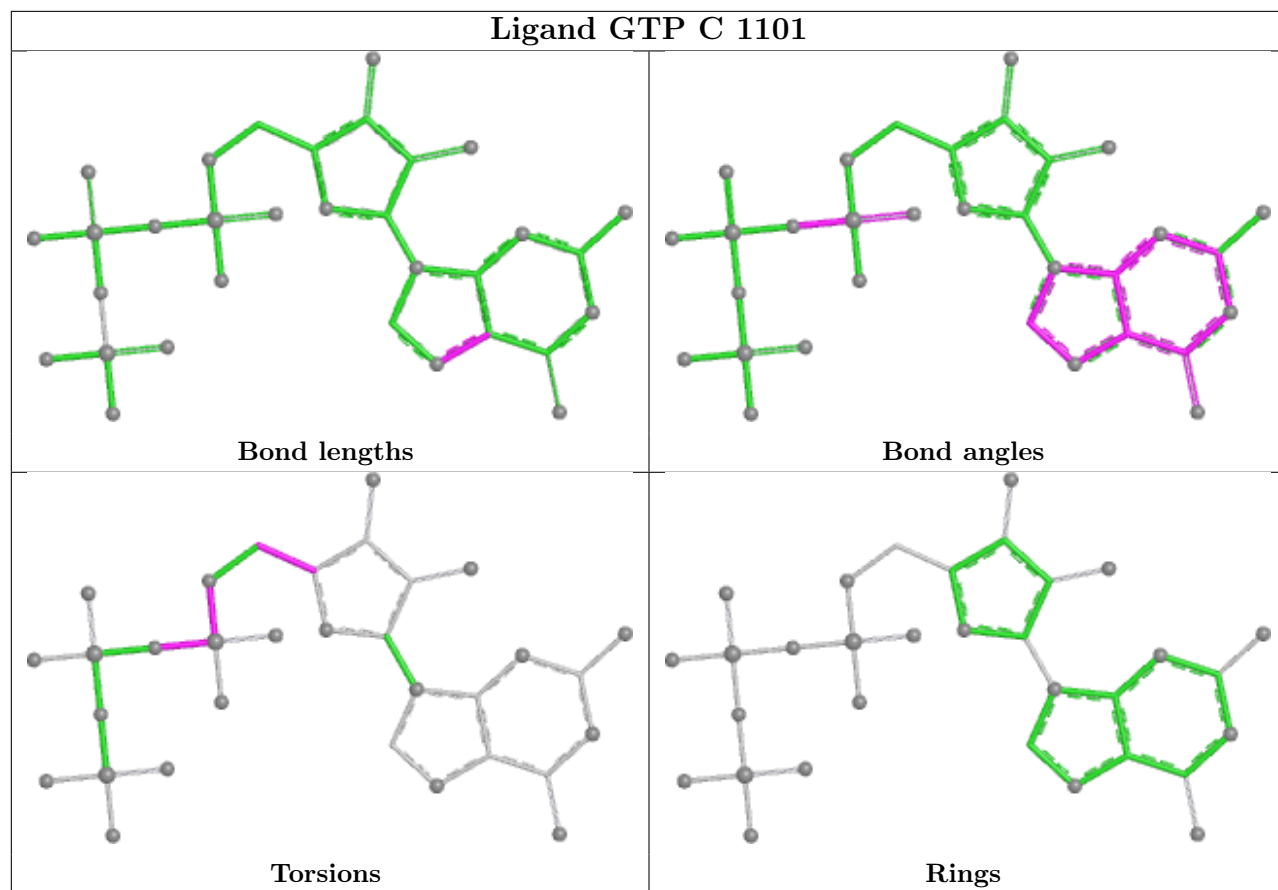
Mol	Chain	Res	Type	Atoms
49	C	1101	GTP	PB-O3A-PA-O2A
48	A	3000	IHP	C4-O14-P4-O44
48	A	3000	IHP	C4-O14-P4-O24
48	A	3000	IHP	C6-O16-P6-O26
49	C	1101	GTP	PB-O3A-PA-O1A

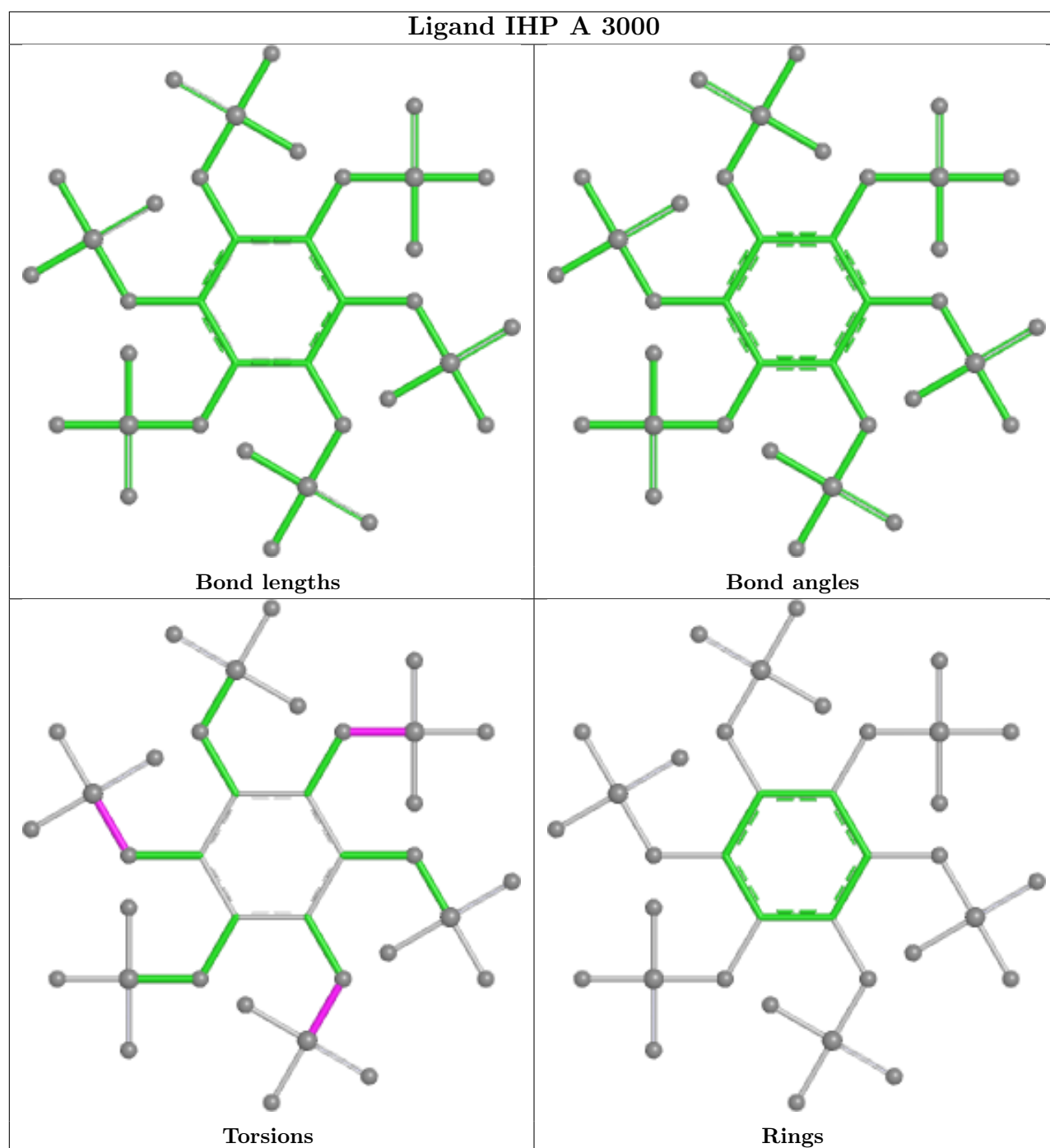
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	C	1101	GTP	2	0
48	A	3000	IHP	2	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

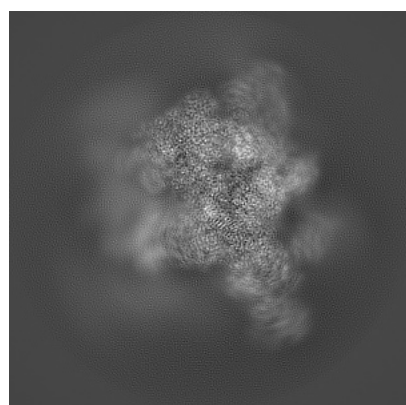
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30637. These allow visual inspection of the internal detail of the map and identification of artifacts.

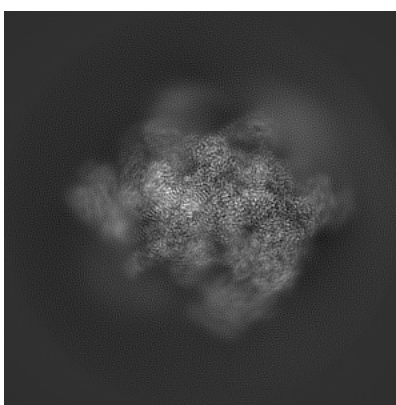
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

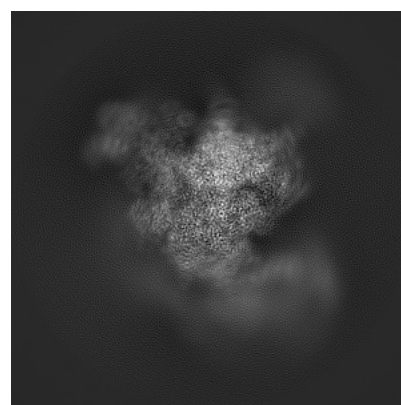
6.1.1 Primary map



X



Y

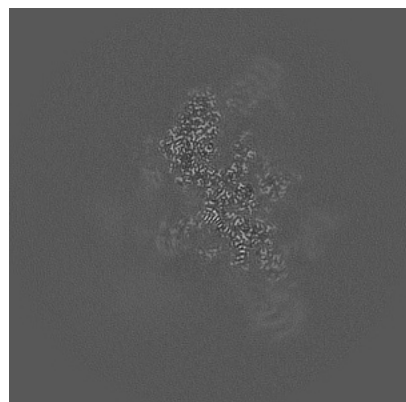


Z

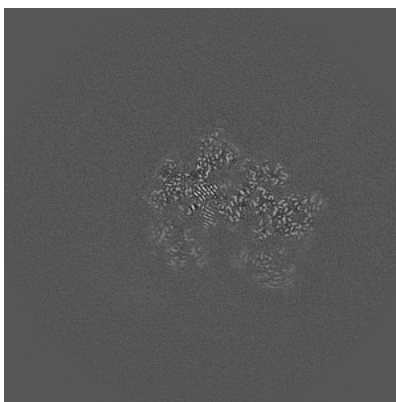
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

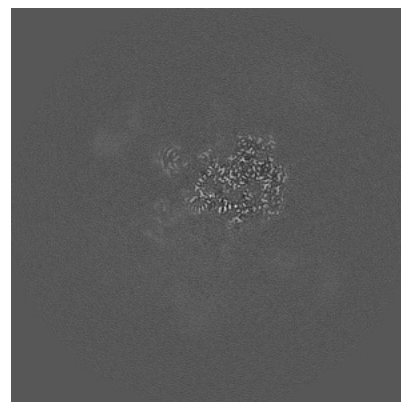
6.2.1 Primary map



X Index: 200



Y Index: 200

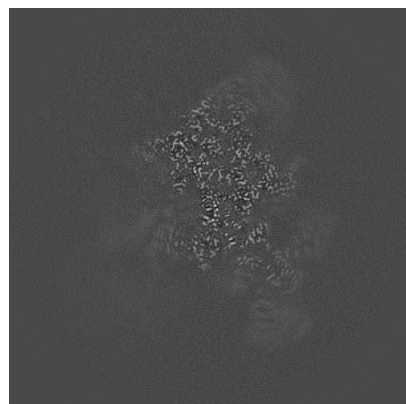


Z Index: 200

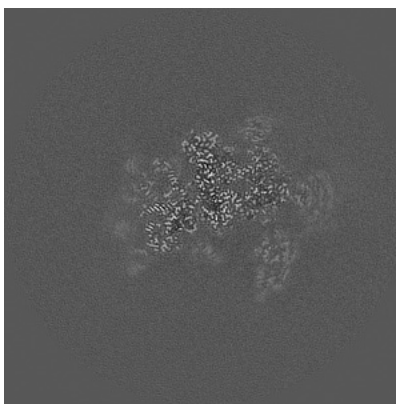
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

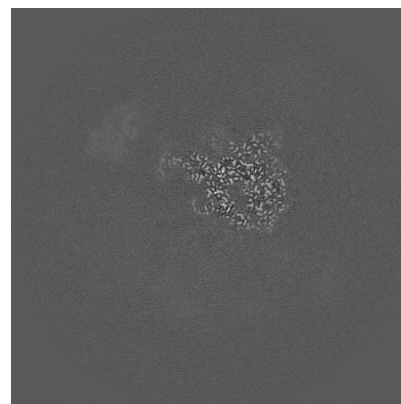
6.3.1 Primary map



X Index: 211



Y Index: 233

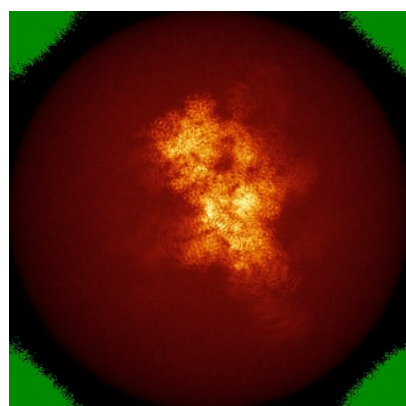


Z Index: 209

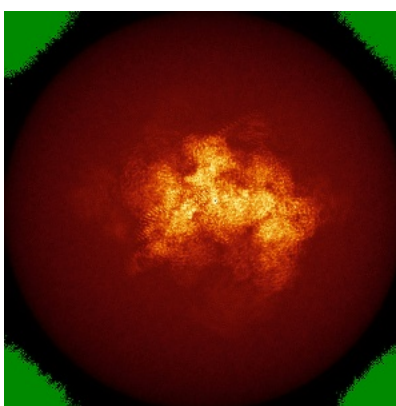
The images above show the largest variance slices of the map in three orthogonal directions.

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

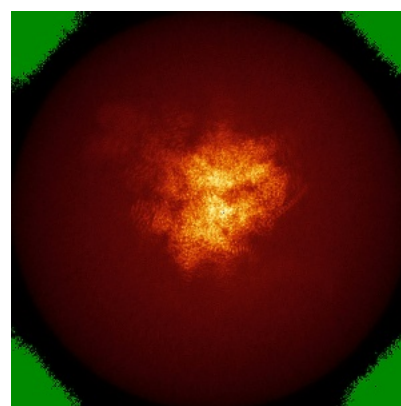
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

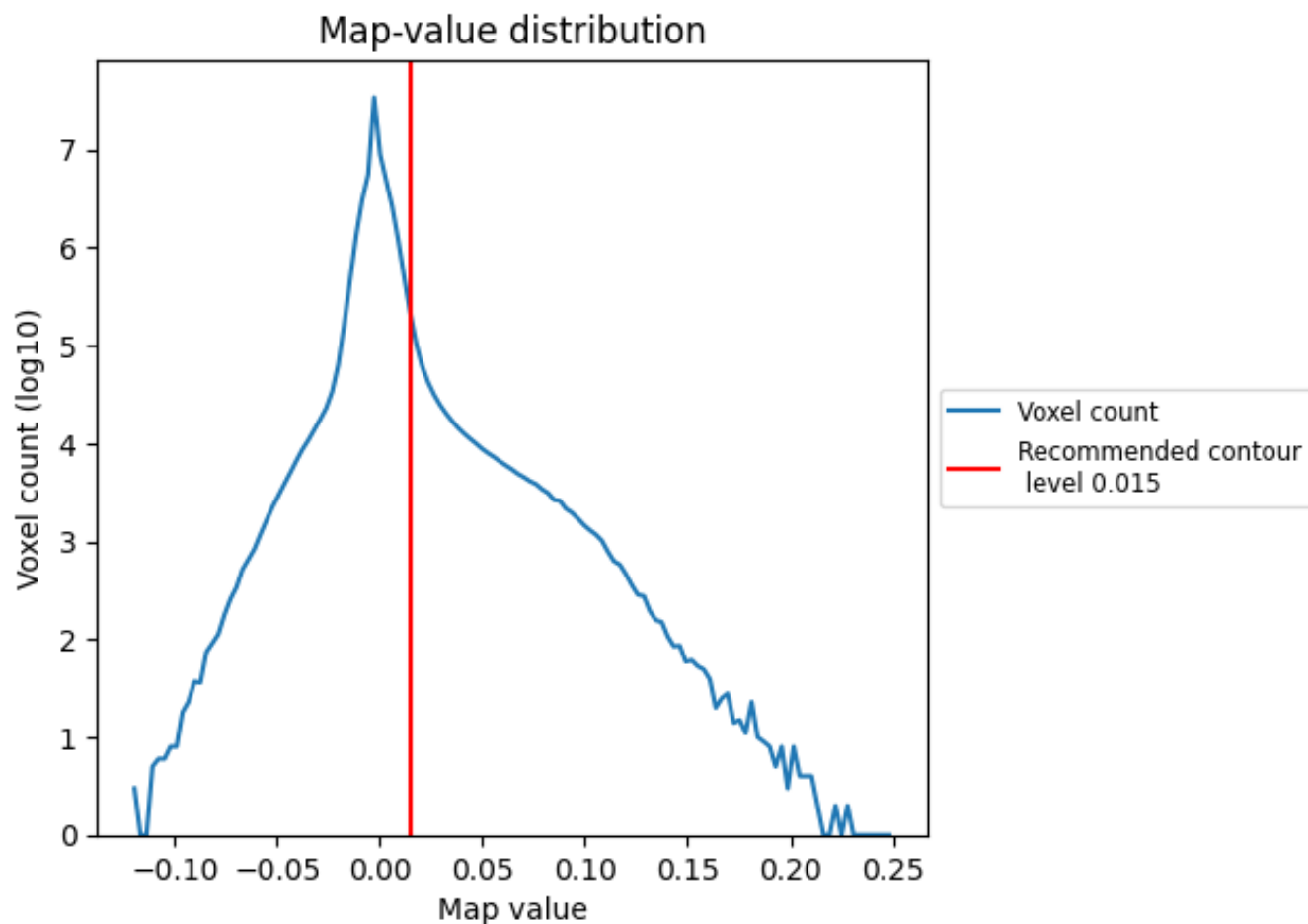
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

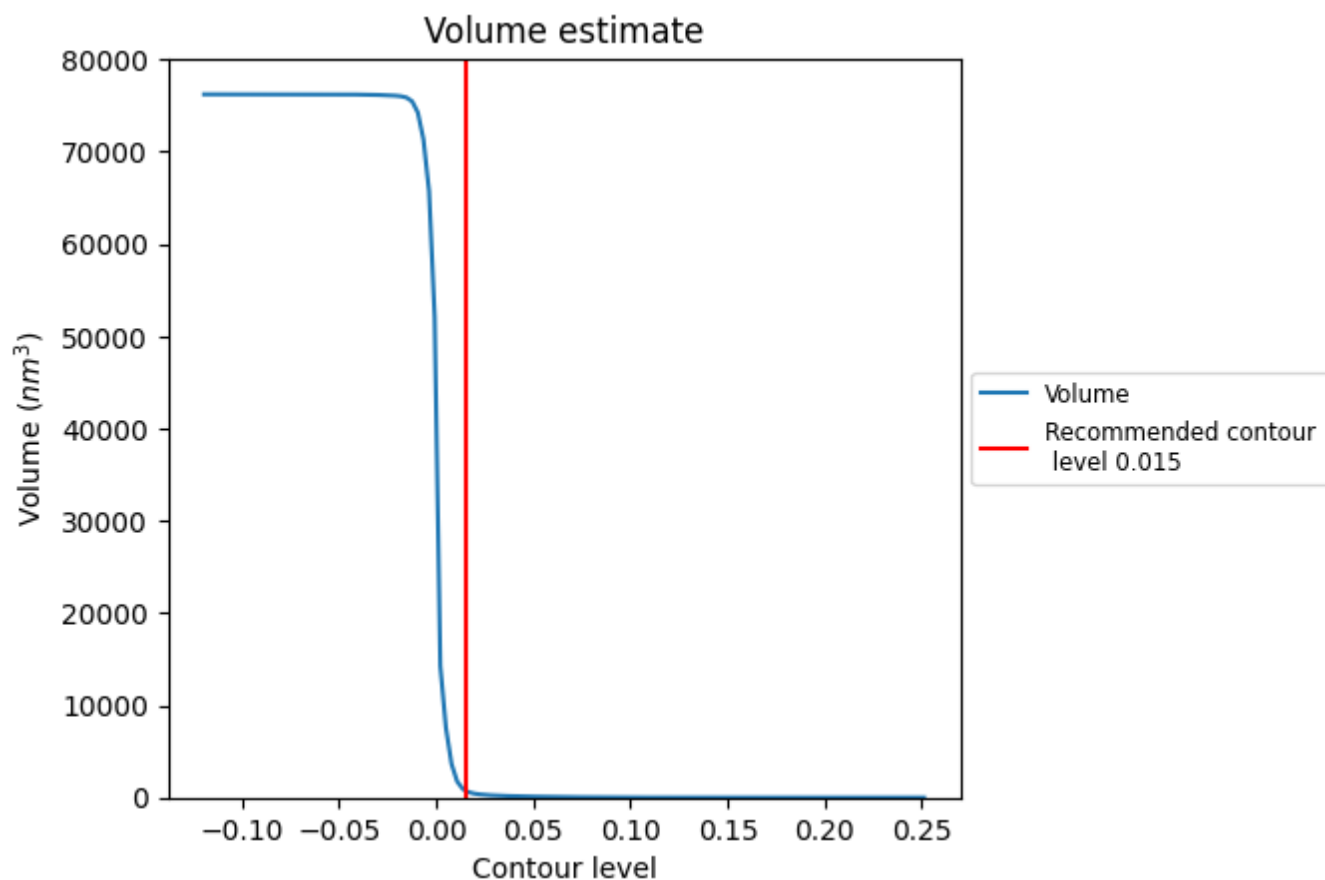
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

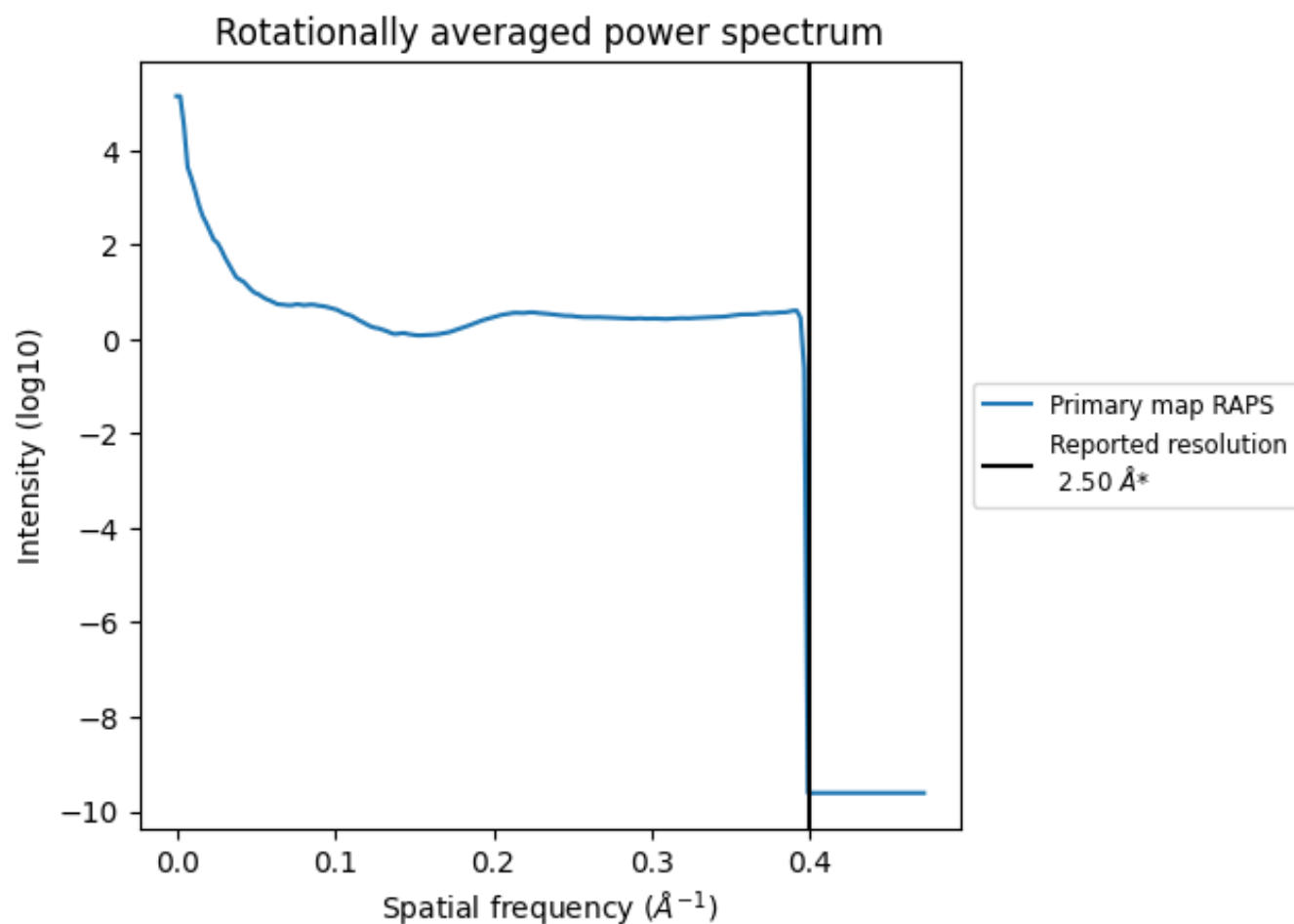
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 787 nm³; this corresponds to an approximate mass of 711 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 0.400 Å⁻¹

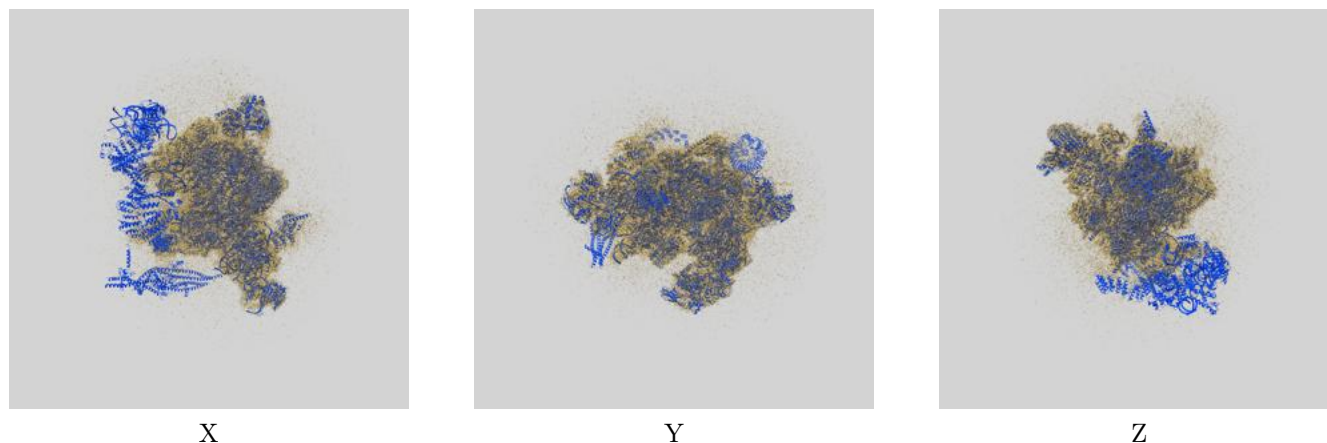
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

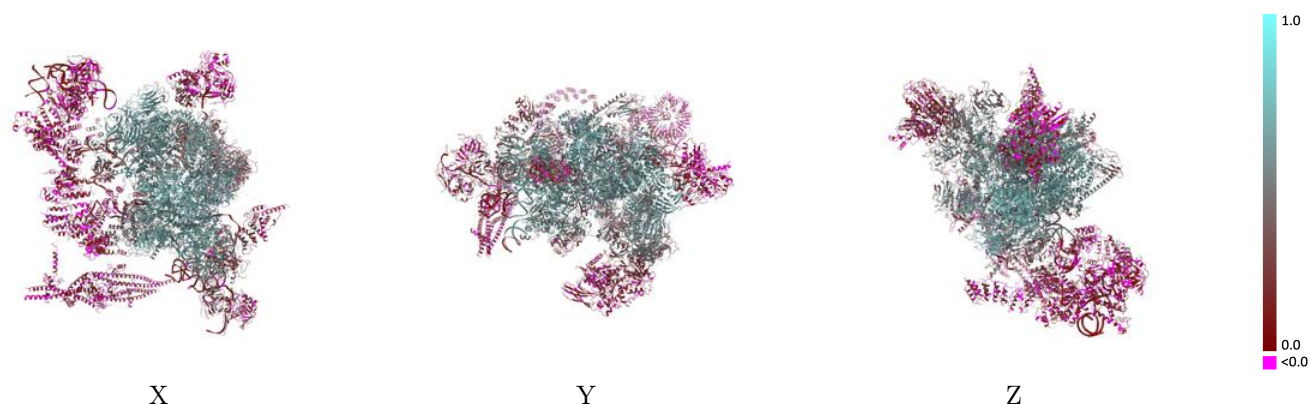
This section contains information regarding the fit between EMDB map EMD-30637 and PDB model 7DCO. Per-residue inclusion information can be found in section [3](#) on page [17](#).

9.1 Map-model overlay [i](#)



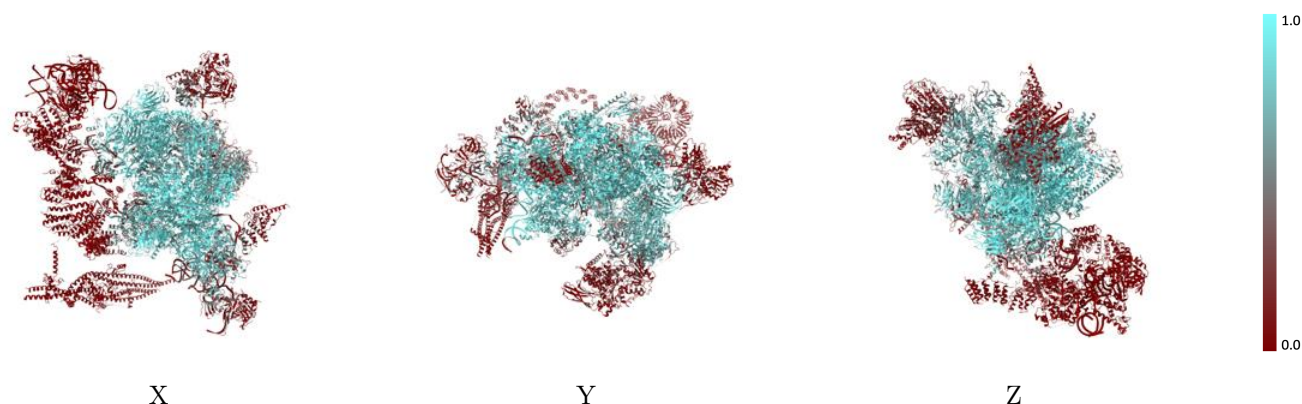
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



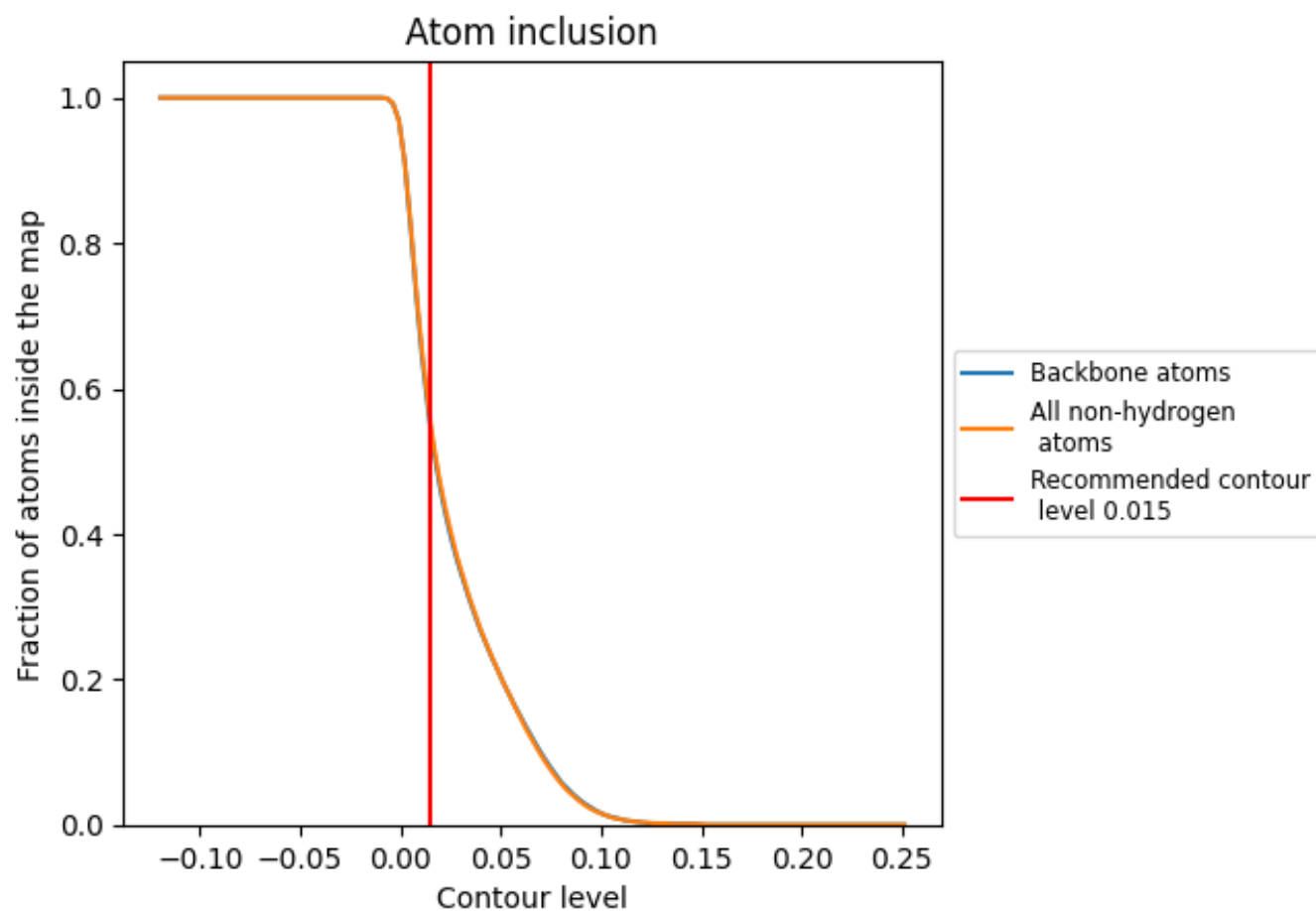
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.015).

9.4 Atom inclusion ⓘ



At the recommended contour level, 55% of all backbone atoms, 55% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5530	 0.4080
1	 0.9220	 0.6380
2	 0.7810	 0.5440
3	 0.8940	 0.6140
4	 0.3420	 0.2650
5	 0.9540	 0.6630
6	 0.9480	 0.6510
A	 0.8840	 0.6170
B	 0.5340	 0.3560
C	 0.7090	 0.4860
D	 0.4180	 0.3250
F	 0.8190	 0.5270
G	 0.5350	 0.3840
H	 0.2790	 0.2360
I	 0.0170	 0.1150
J	 0.2970	 0.2660
K	 0.0020	 0.0860
L	 0.3340	 0.3050
M	 0.6130	 0.4670
N	 0.8920	 0.5960
P	 0.7290	 0.5100
Q	 0.5000	 0.3620
R	 0.7500	 0.5030
S	 0.5910	 0.4930
T	 0.9080	 0.6170
U	 0.8660	 0.6060
V	 0.4750	 0.3730
W	 0.7890	 0.4970
X	 0.8940	 0.6040
Y	 0.6090	 0.4020
Z	 0.7450	 0.5220
a	 0.3660	 0.2980
b	 0.2730	 0.2640
c	 0.1780	 0.2200
d	 0.3990	 0.2990



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Chain	Atom inclusion	Q-score
e	 0.1290	 0.2060
f	 0.1210	 0.1970
g	 0.1110	 0.1900
h	 0.0020	 0.1030
i	 0.0040	 0.0620
j	 0.0020	 0.1110
k	 0.0020	 0.0870
l	 0.0050	 0.1030
m	 0.0020	 0.0930
n	 0.0040	 0.0790
o	 0.0040	 0.1290
p	 0.0110	 0.1330
q	 0.0040	 0.1050
r	 0.0020	 0.1400
s	 0.0050	 0.1100
t	 0.0020	 0.1190
u	 0.1370	 0.1700
v	 0.4320	 0.3700
w	 0.0030	 0.0800
x	 0.1680	 0.0830
y	 0.2280	 0.1810
z	 0.6640	 0.4540