



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 08:56 PM UTC

PDB ID : 6AH0 / pdb_00006ah0
EMDB ID : EMD-9621
Title : The Cryo-EM Structure of the Precursor of Human Pre-catalytic Spliceosome (pre-B complex)
Authors : Zhan, X.; Yan, C.; Zhang, X.; Shi, Y.
Deposited on : 2018-08-15
Resolution : 5.70 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

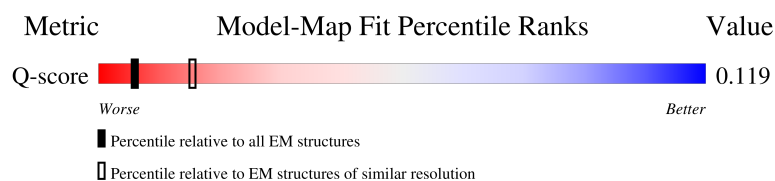
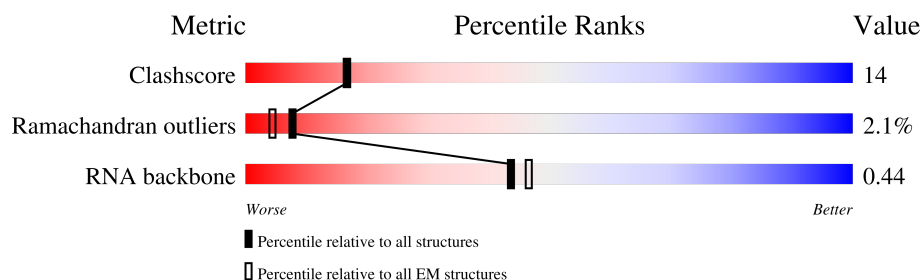
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.70 Å.

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



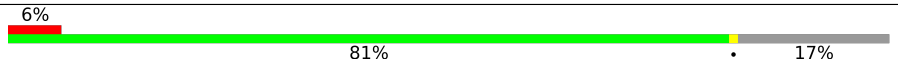
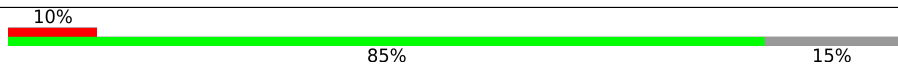
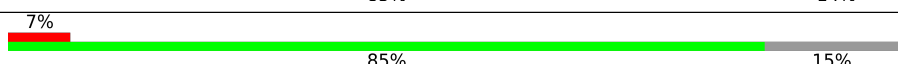
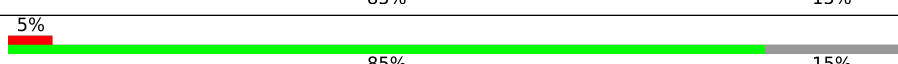
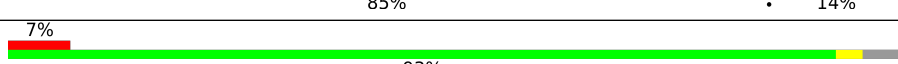
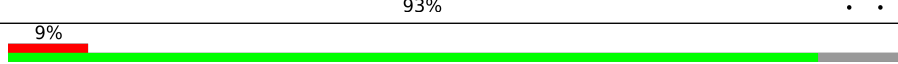
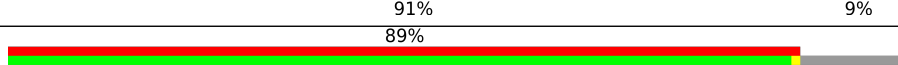
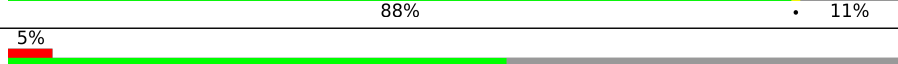
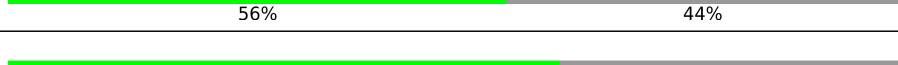
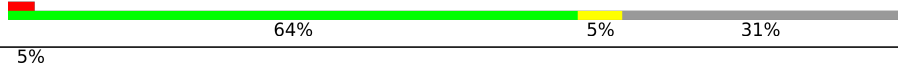
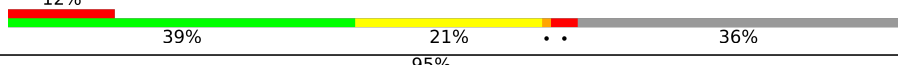
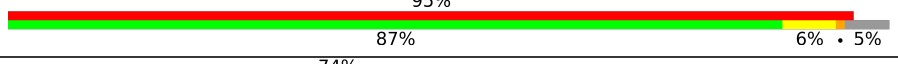
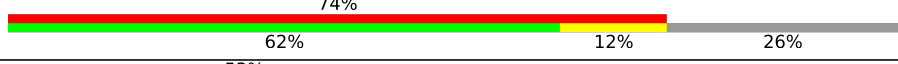
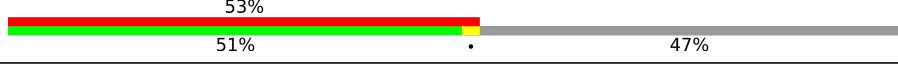
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
RNA backbone	8273	3508	-
Q-score	-	25397	503 (5.20 - 6.20)

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	B	117	
2	D	2136	
3	E	357	
4	P	118	

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Mol	Chain	Length	Quality of chain
4	a	118	
4	k	118	
5	Q	86	
5	b	86	
5	m	86	
6	R	92	
6	c	92	
6	l	92	
7	S	76	
7	d	76	
7	n	76	
8	T	126	
8	e	126	
8	h	126	
9	U	231	
9	f	231	
9	i	231	
10	V	119	
10	g	119	
10	j	119	
11	F	107	
12	q	95	
13	r	102	
14	s	139	
15	t	91	

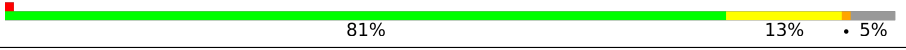
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Mol	Chain	Length	Quality of chain
16	x	80	
17	y	103	
18	z	96	
19	G	274	
20	H	188	
21	o	255	
22	p	225	
23	u	793	
24	v	464	
25	w	501	
26	1	1304	
27	2	895	
28	3	1217	
29	4	424	
30	5	125	
31	6	110	
32	7	86	
33	J	683	
34	K	522	
35	N	941	
36	L	499	
37	M	128	
38	O	142	
39	W	565	
40	I	144	

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Mol	Chain	Length	Quality of chain
41	X	820	
42	A	2335	
43	C	972	

2 Entry composition [i](#)

There are 46 unique types of molecules in this entry. The entry contains 63369 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called U5snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	115	Total	C	N	O	P	0	0
			2419	1084	402	818	115		

- Molecule 2 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	1874	Total	C	N	O	0	0
			7496	3748	1874	1874		

- Molecule 3 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	299	Total	C	N	O	0	0
			1196	598	299	299		

- Molecule 4 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	a	78	Total	C	N	O	0	0
			318	162	78	78		
4	k	85	Total	C	N	O	0	0
			340	170	85	85		
4	P	74	Total	C	N	O	0	0
			300	152	74	74		

- Molecule 5 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	b	73	Total	C	N	O	0	0
			300	154	73	73		
5	m	74	Total	C	N	O	0	0
			296	148	74	74		

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Mol	Chain	Residues	Atoms				AltConf	Trace
5	Q	71	Total	C	N	O	0	0
			292	150	71	71		

- Molecule 6 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	c	78	Total	C	N	O	0	0
			314	158	78	78		
6	l	79	Total	C	N	O	0	0
			316	158	79	79		
6	R	78	Total	C	N	O	0	0
			314	158	78	78		

- Molecule 7 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	d	69	Total	C	N	O	0	0
			282	144	69	69		
7	n	68	Total	C	N	O	0	0
			272	136	68	68		
7	S	73	Total	C	N	O	0	0
			298	152	73	73		

- Molecule 8 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	e	78	Total	C	N	O	0	0
			318	162	78	78		
8	h	80	Total	C	N	O	0	0
			320	160	80	80		
8	T	71	Total	C	N	O	0	0
			288	146	71	71		

- Molecule 9 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	f	64	Total	C	N	O	0	0
			260	132	64	64		
9	i	73	Total	C	N	O	0	0
			292	146	73	73		
9	U	64	Total	C	N	O	0	0
			256	128	64	64		

- Molecule 10 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	g	93	Total	C	N	O	0	0
			380	194	93	93		
10	j	82	Total	C	N	O	0	0
			328	164	82	82		
10	V	82	Total	C	N	O	0	0
			334	170	82	82		

- Molecule 11 is a RNA chain called U6snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	69	Total	C	N	O	P	0	0
			1470	656	259	486	69		

- Molecule 12 is a protein called U6 snRNA-associated Sm-like protein LSm2.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	q	90	Total	C	N	O	0	0
			360	180	90	90		

- Molecule 13 is a protein called U6 snRNA-associated Sm-like protein LSm3.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	r	75	Total	C	N	O	0	0
			300	150	75	75		

- Molecule 14 is a protein called U6 snRNA-associated Sm-like protein LSm4.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	s	74	Total	C	N	O	0	0
			296	148	74	74		

- Molecule 15 is a protein called U6 snRNA-associated Sm-like protein LSm5.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	t	75	Total	C	N	O	0	0
			300	150	75	75		

- Molecule 16 is a protein called U6 snRNA-associated Sm-like protein LSm6.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	x	70	Total	C	N	O	0	0
			280	140	70	70		

- Molecule 17 is a protein called U6 snRNA-associated Sm-like protein LSm7.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	y	65	Total	C	N	O	0	0
			260	130	65	65		

- Molecule 18 is a protein called U6 snRNA-associated Sm-like protein LSm8.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	z	61	Total	C	N	O	0	0
			244	122	61	61		

- Molecule 19 is a RNA chain called pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	G	42	Total	C	N	O	P	0	0
			862	387	122	311	42		

- Molecule 20 is a RNA chain called U2snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	H	109	Total	C	N	O	P	0	0
			2311	1032	396	774	109		

- Molecule 21 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	o	162	Total	C	N	O	0	0
			648	324	162	162		

- Molecule 22 is a protein called U2 small nuclear ribonucleoprotein B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	p	94	Total	C	N	O	0	0
			376	188	94	94		

- Molecule 23 is a protein called Splicing factor 3A subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	u	124	Total	C	N	O	0	0
			496	248	124	124		

- Molecule 24 is a protein called Splicing factor 3A subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	v	99	Total	C	N	O	0	0
			396	198	99	99		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
25	w	443	Total	C	N	O	0	0
			1773	887	443	443		

- Molecule 26 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	1	1030	Total	C	N	O	0	0
			4120	2060	1030	1030		

- Molecule 27 is a protein called Splicing factor 3B subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	2	186	Total	C	N	O	0	0
			744	372	186	186		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
28	3	1174	Total	C	N	O	0	0
			4696	2348	1174	1174		

- Molecule 29 is a protein called Splicing factor 3B subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	4	78	Total	C	N	O	0	0
			312	156	78	78		

- Molecule 30 is a protein called Splicing factor 3B subunit 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	5	108	Total	C	N	O	0	0
			432	216	108	108		

- Molecule 31 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	6	89	Total	C	N	O	0	0
			356	178	89	89		

- Molecule 32 is a protein called Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	7	66	Total	C	N	O	0	0
			264	132	66	66		

- Molecule 33 is a protein called U4/U6 small nuclear ribonucleoprotein Prp3.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	J	167	Total	C	N	O	0	0
			668	334	167	167		

- Molecule 34 is a protein called U4/U6 small nuclear ribonucleoprotein Prp4.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	K	343	Total	C	N	O	0	0
			1371	686	343	342		

- Molecule 35 is a protein called Pre-mRNA-processing factor 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	N	579	Total	C	N	O	0	0
			2316	1158	579	579		

- Molecule 36 is a protein called U4/U6 small nuclear ribonucleoprotein Prp31.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	L	226	Total	C	N	O	0	0
			904	452	226	226		

- Molecule 37 is a protein called NHP2-like protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	M	125	Total	C	N	O	0	0
			500	250	125	125		

- Molecule 38 is a protein called Thioredoxin-like protein 4A.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	O	139	Total	C	N	O	0	0
			556	278	139	139		

- Molecule 39 is a protein called U4/U6.U5 tri-snRNP-associated protein 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	W	463	Total	C	N	O	0	0
			1852	926	463	463		

- Molecule 40 is a RNA chain called U4snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	I	117	Total	C	N	O	P	0	0
			2491	1112	439	823	117		

- Molecule 41 is a protein called Probable ATP-dependent RNA helicase DDX23.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	X	414	Total	C	N	O	0	0
			1661	833	414	414		

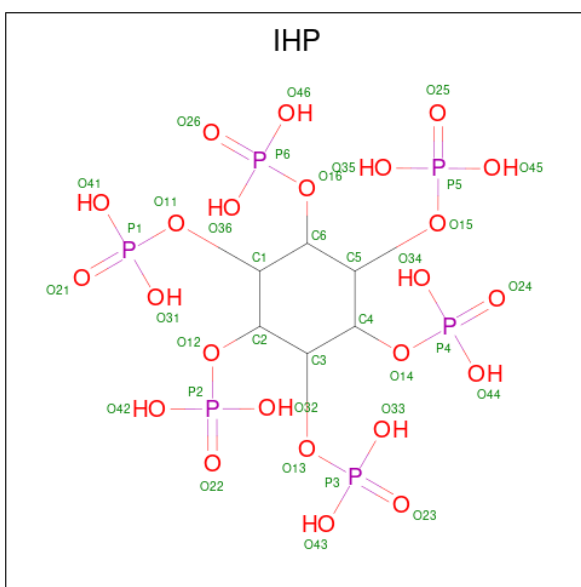
- Molecule 42 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	A	2221	Total	C	N	O	0	0
			8884	4442	2221	2221		

- Molecule 43 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

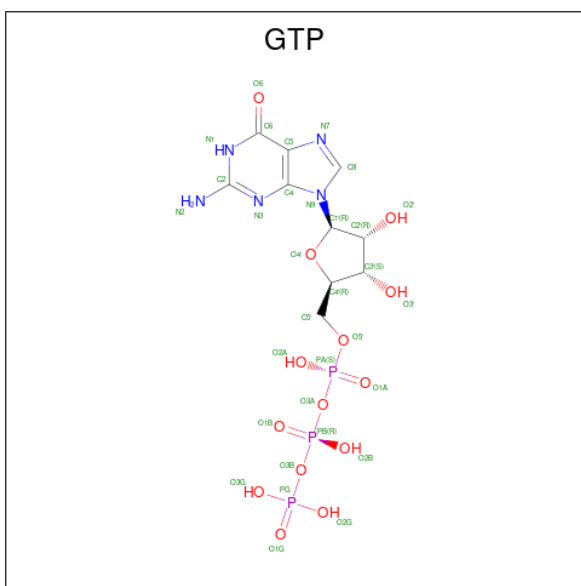
Mol	Chain	Residues	Atoms				AltConf	Trace
43	C	818	Total	C	N	O	0	0
			3272	1636	818	818		

- Molecule 44 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: C₆H₁₈O₂₄P₆).



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

- Molecule 45 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

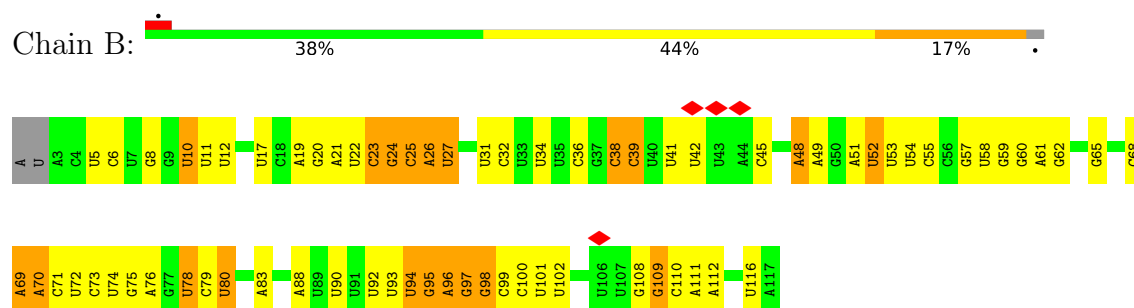
- Molecule 46 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
46	C	1	Total	Mg	0
			1	1	

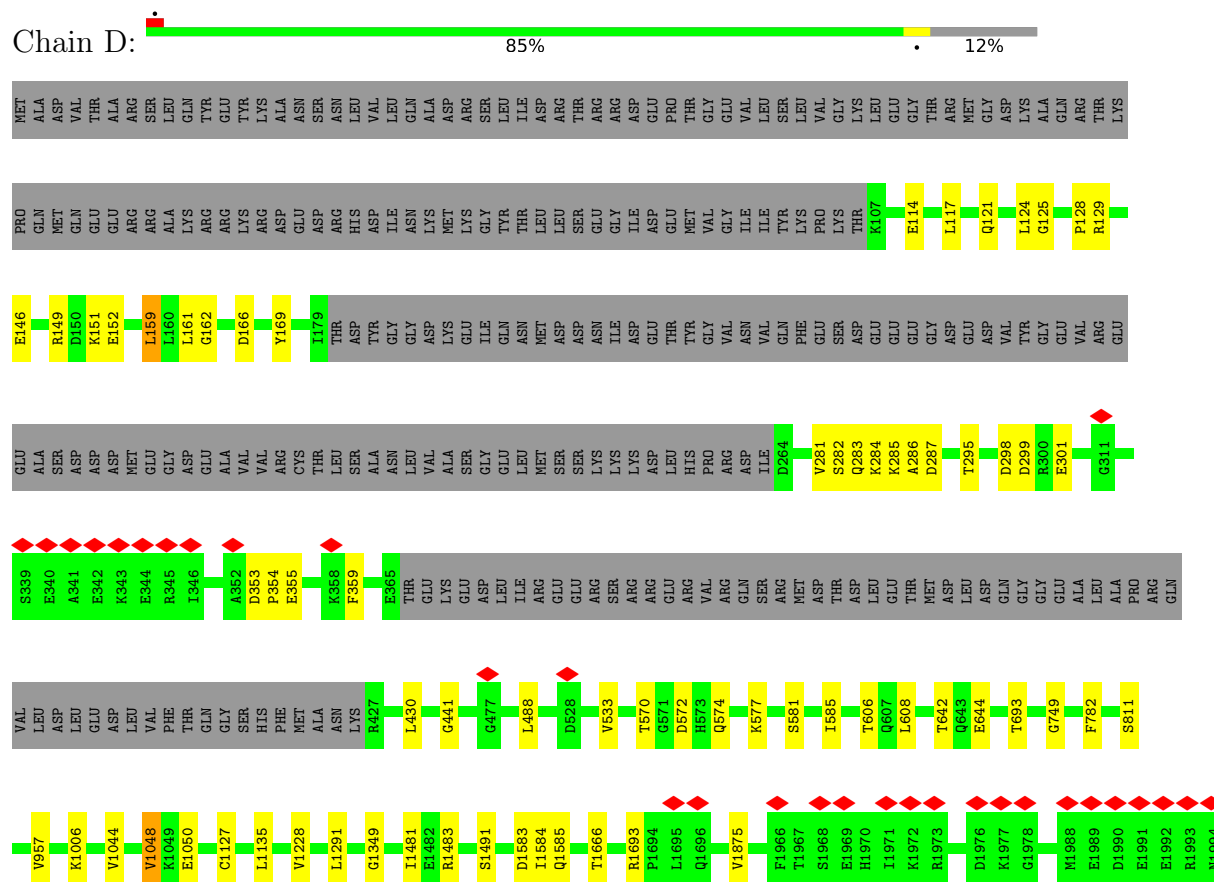
3 Residue-property plots

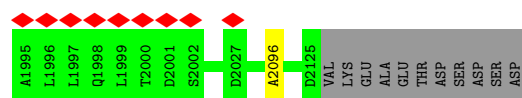
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: U5snRNA

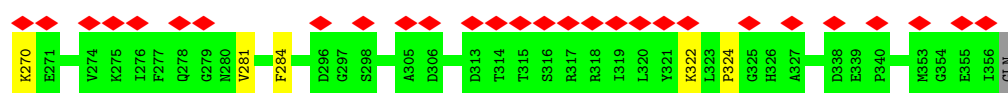
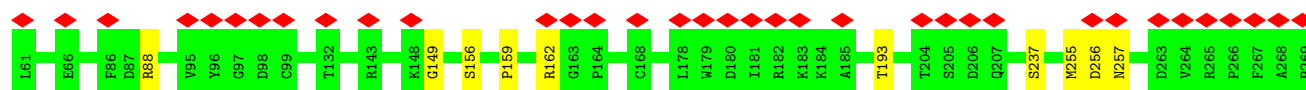
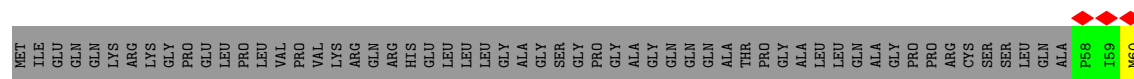
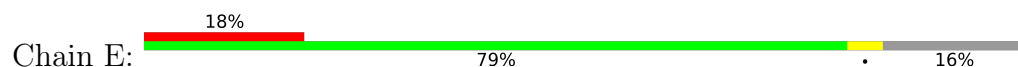


• Molecule 2: U5 small nuclear ribonucleoprotein 200 kDa helicase

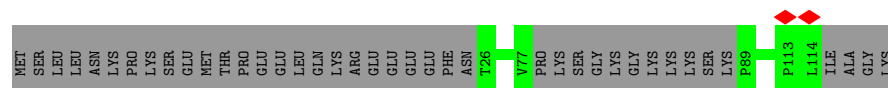




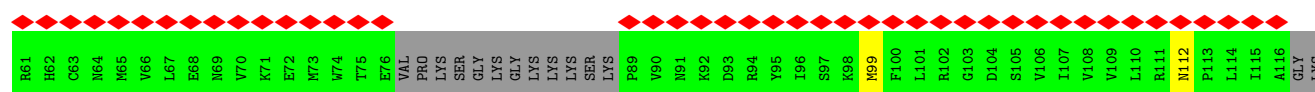
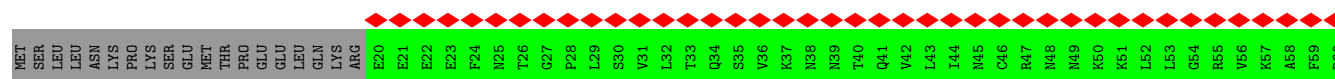
- Molecule 3: U5 small nuclear ribonucleoprotein 40 kDa protein



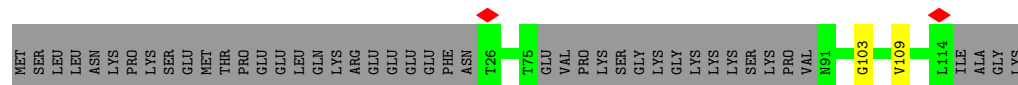
- Molecule 4: Small nuclear ribonucleoprotein Sm D2



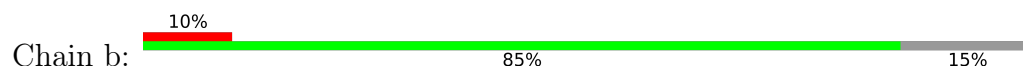
- Molecule 4: Small nuclear ribonucleoprotein Sm D2

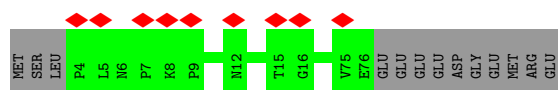


- Molecule 4: Small nuclear ribonucleoprotein Sm D2

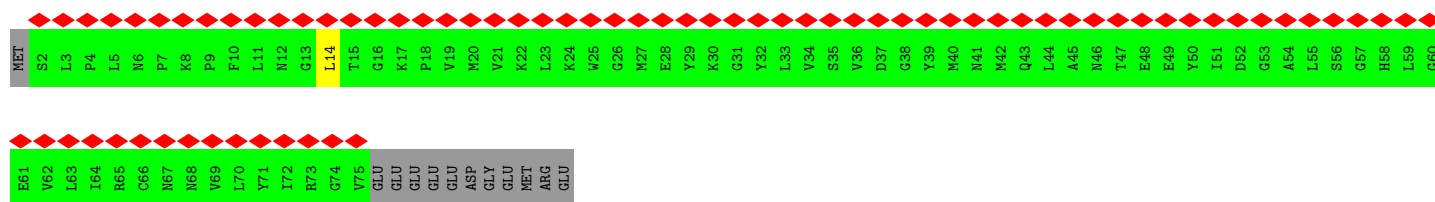
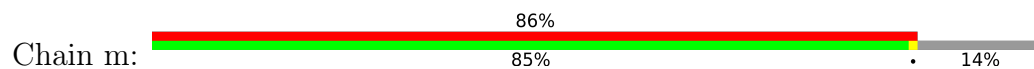


- Molecule 5: Small nuclear ribonucleoprotein F

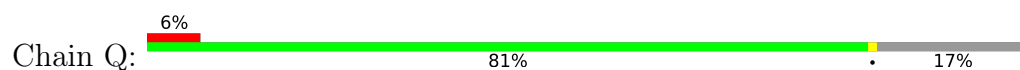




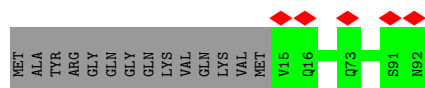
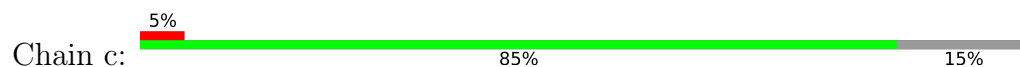
- Molecule 5: Small nuclear ribonucleoprotein F



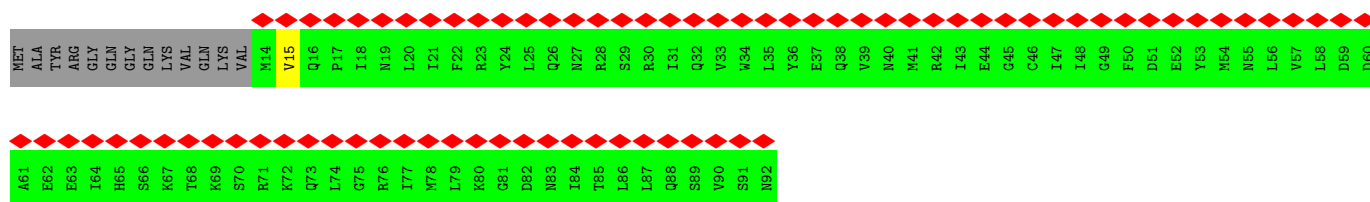
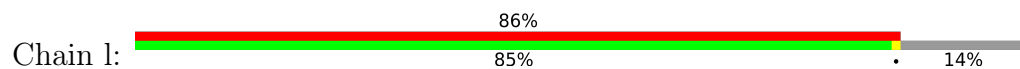
- Molecule 5: Small nuclear ribonucleoprotein F



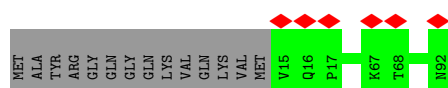
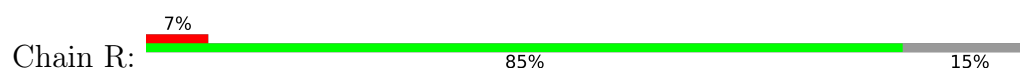
- Molecule 6: Small nuclear ribonucleoprotein E



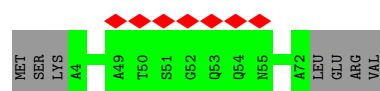
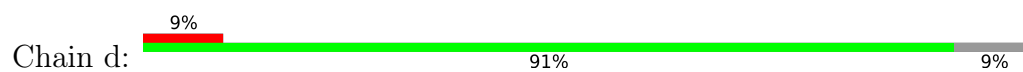
- Molecule 6: Small nuclear ribonucleoprotein E



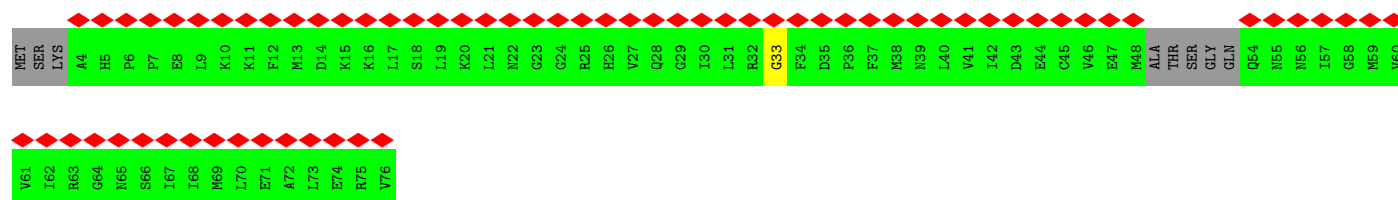
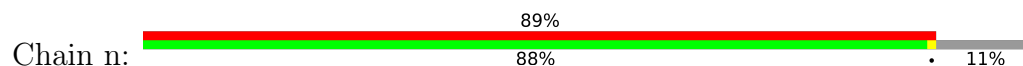
- Molecule 6: Small nuclear ribonucleoprotein E



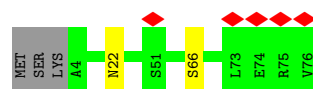
- Molecule 7: Small nuclear ribonucleoprotein G



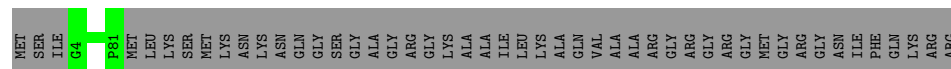
- Molecule 7: Small nuclear ribonucleoprotein G



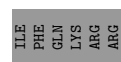
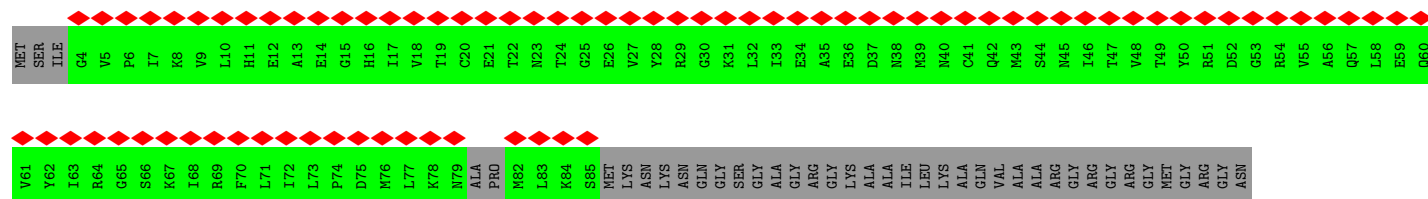
- Molecule 7: Small nuclear ribonucleoprotein G



- Molecule 8: Small nuclear ribonucleoprotein Sm D3



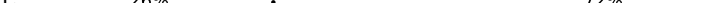
- Molecule 8: Small nuclear ribonucleoprotein Sm D3

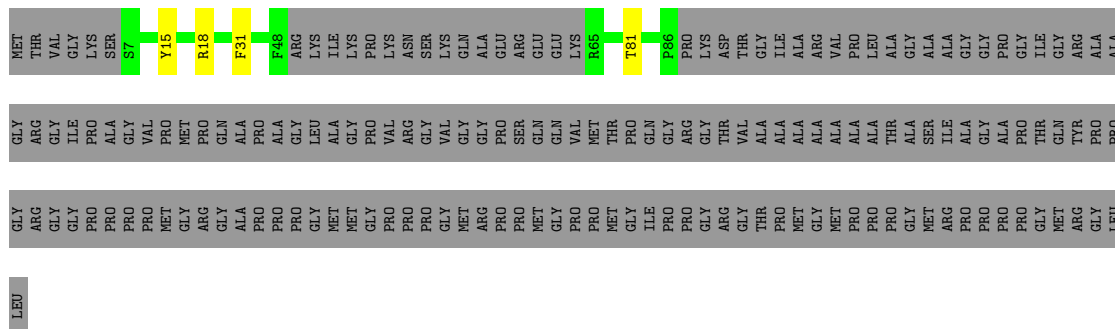


- Molecule 8: Small nuclear ribonucleoprotein Sm D3

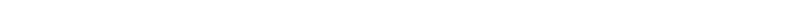


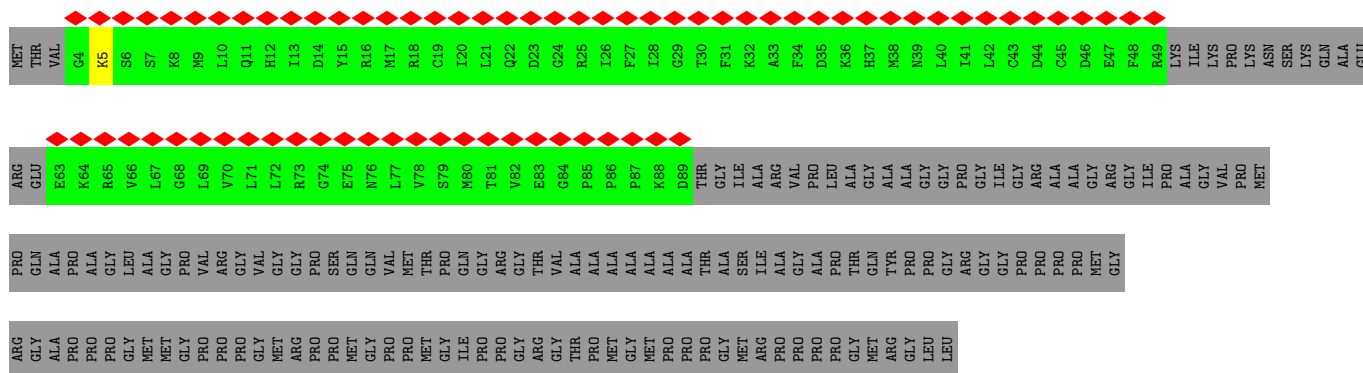
- Molecule 9: Small nuclear ribonucleoprotein-associated proteins B and B'

Chain f:  26% . 72%

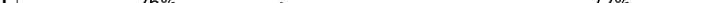


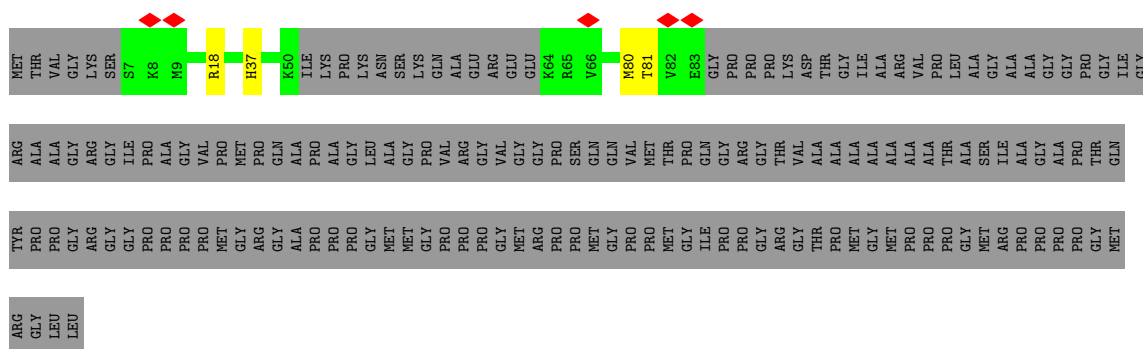
- Molecule 9: Small nuclear ribonucleoprotein-associated proteins B and B'

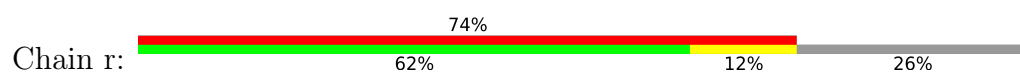
Chain i:  32% 31% 68%



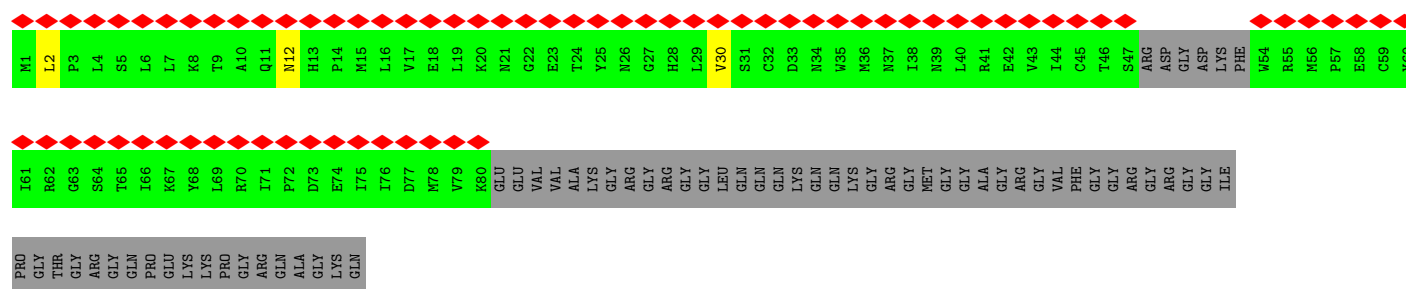
- Molecule 9: Small nuclear ribonucleoprotein-associated proteins B and B'

Chain U:  26% 72%

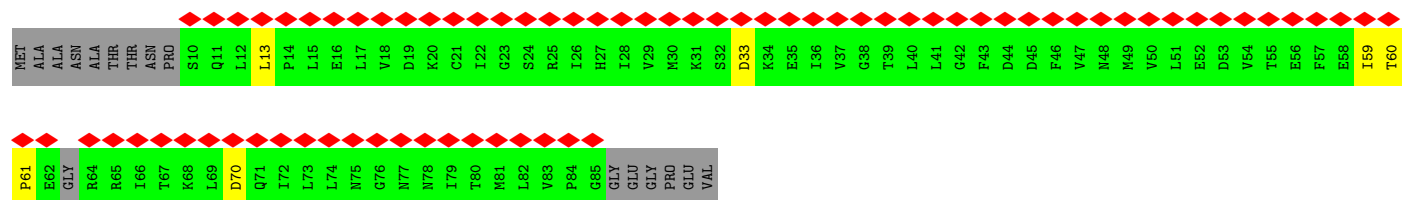
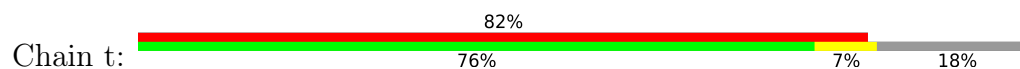




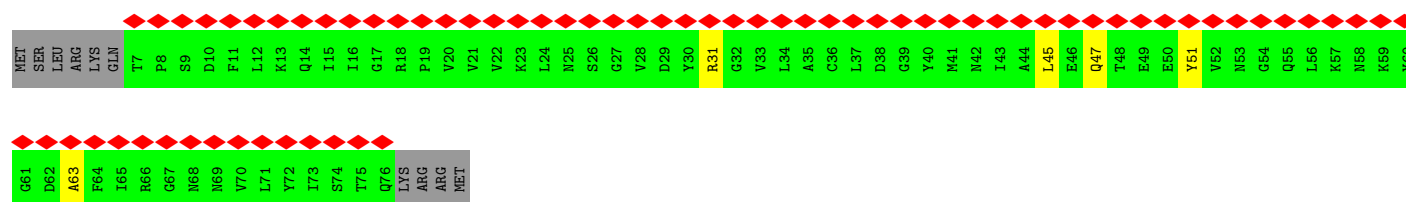
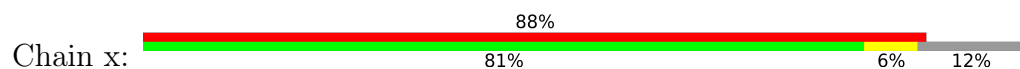
• Molecule 14: U6 snRNA-associated Sm-like protein LSm4



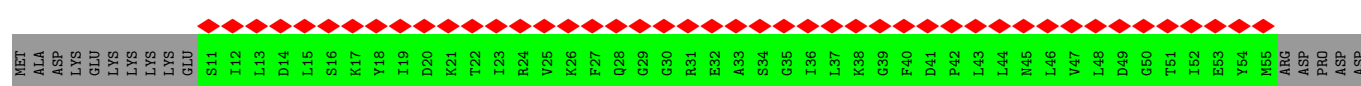
• Molecule 15: U6 snRNA-associated Sm-like protein LSm5



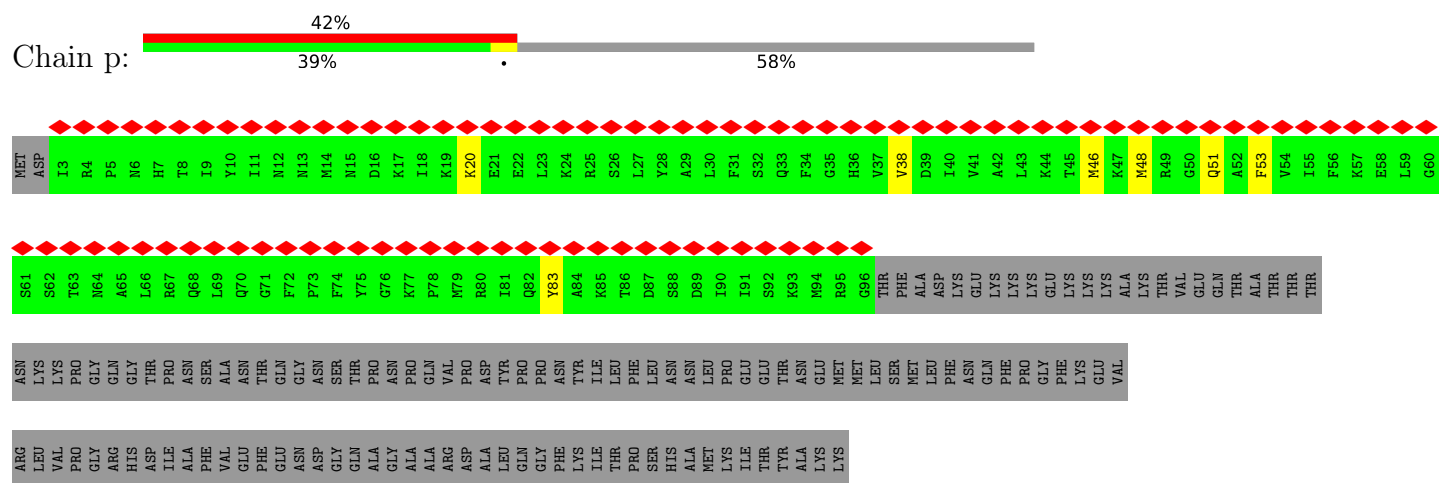
• Molecule 16: U6 snRNA-associated Sm-like protein LSm6



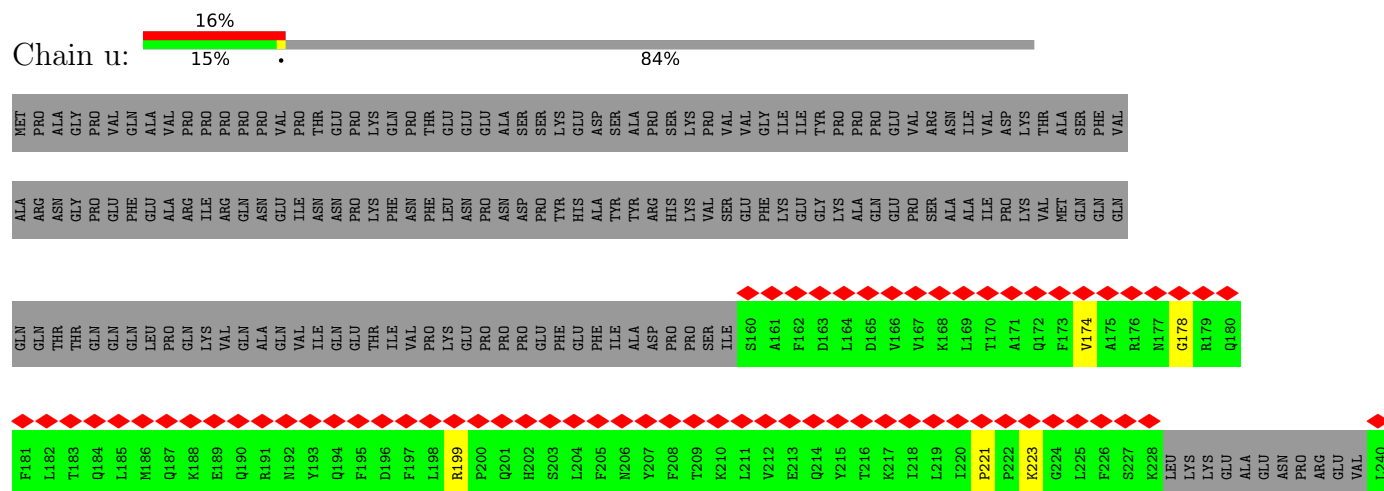
• Molecule 17: U6 snRNA-associated Sm-like protein LSm7

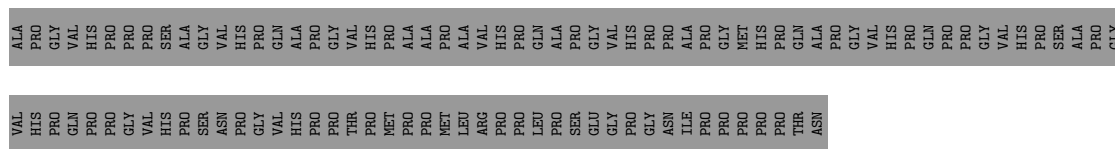


- Molecule 22: U2 small nuclear ribonucleoprotein B''

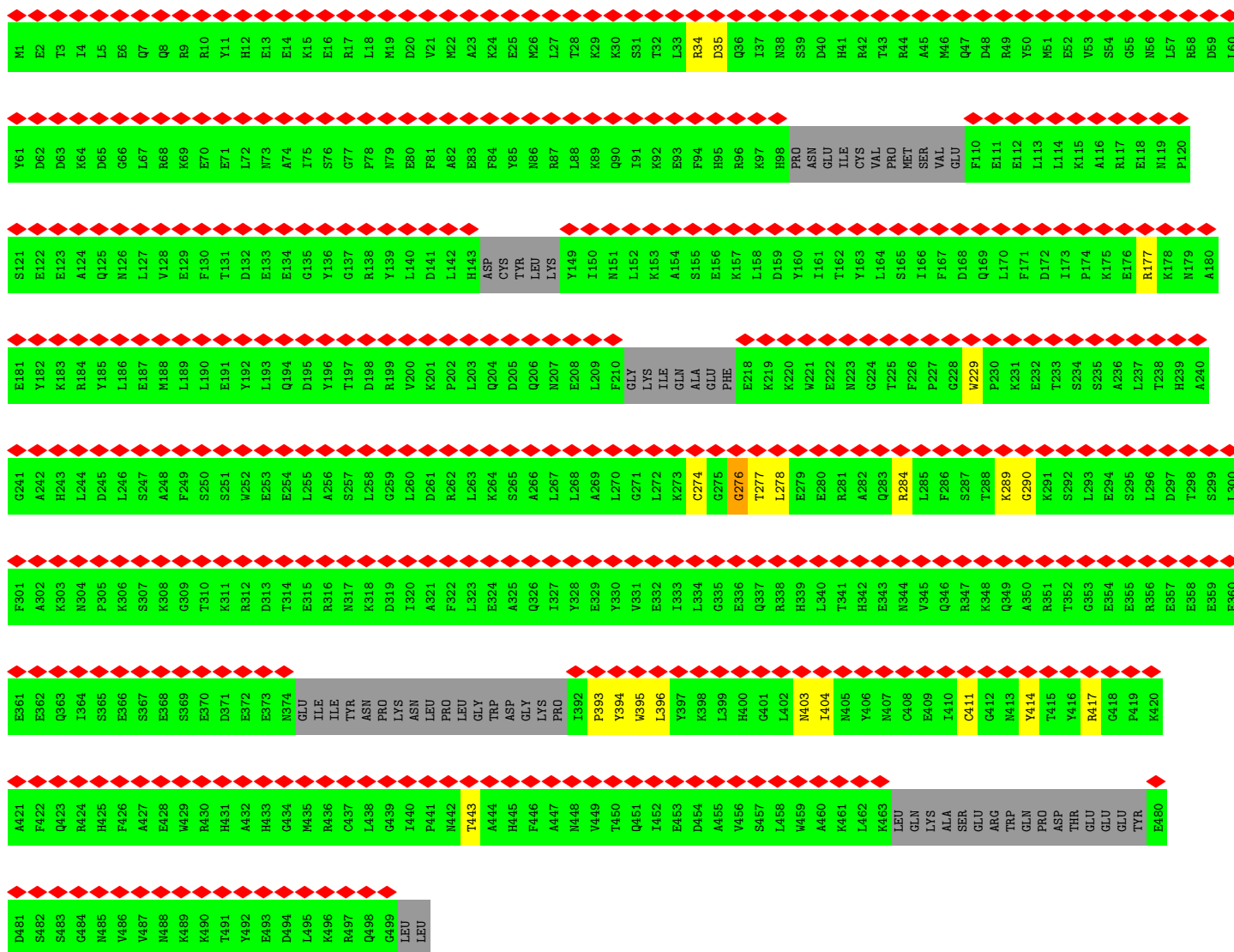
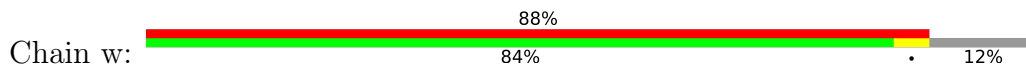


- Molecule 23: Splicing factor 3A subunit 1

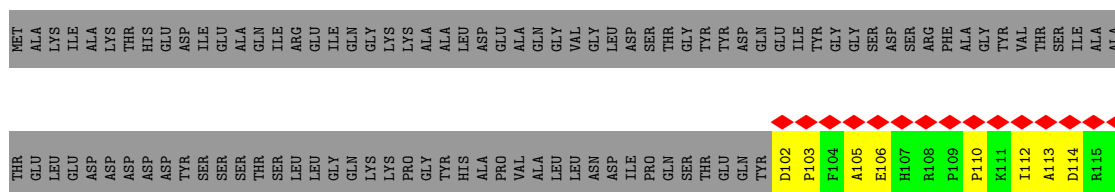
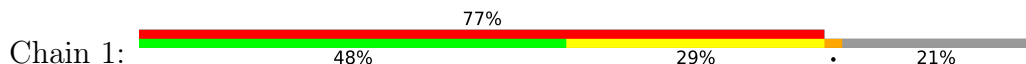




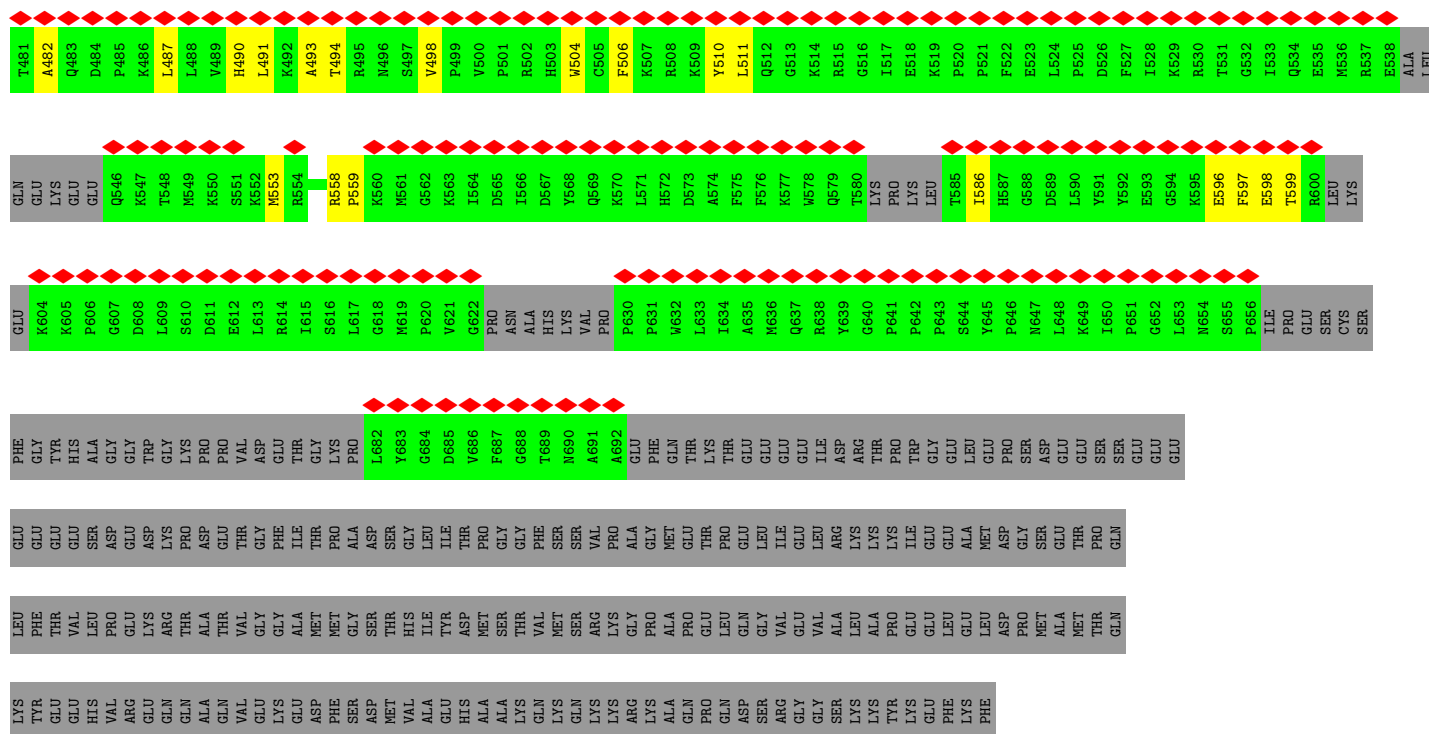
- Molecule 25: Splicing factor 3A subunit 3



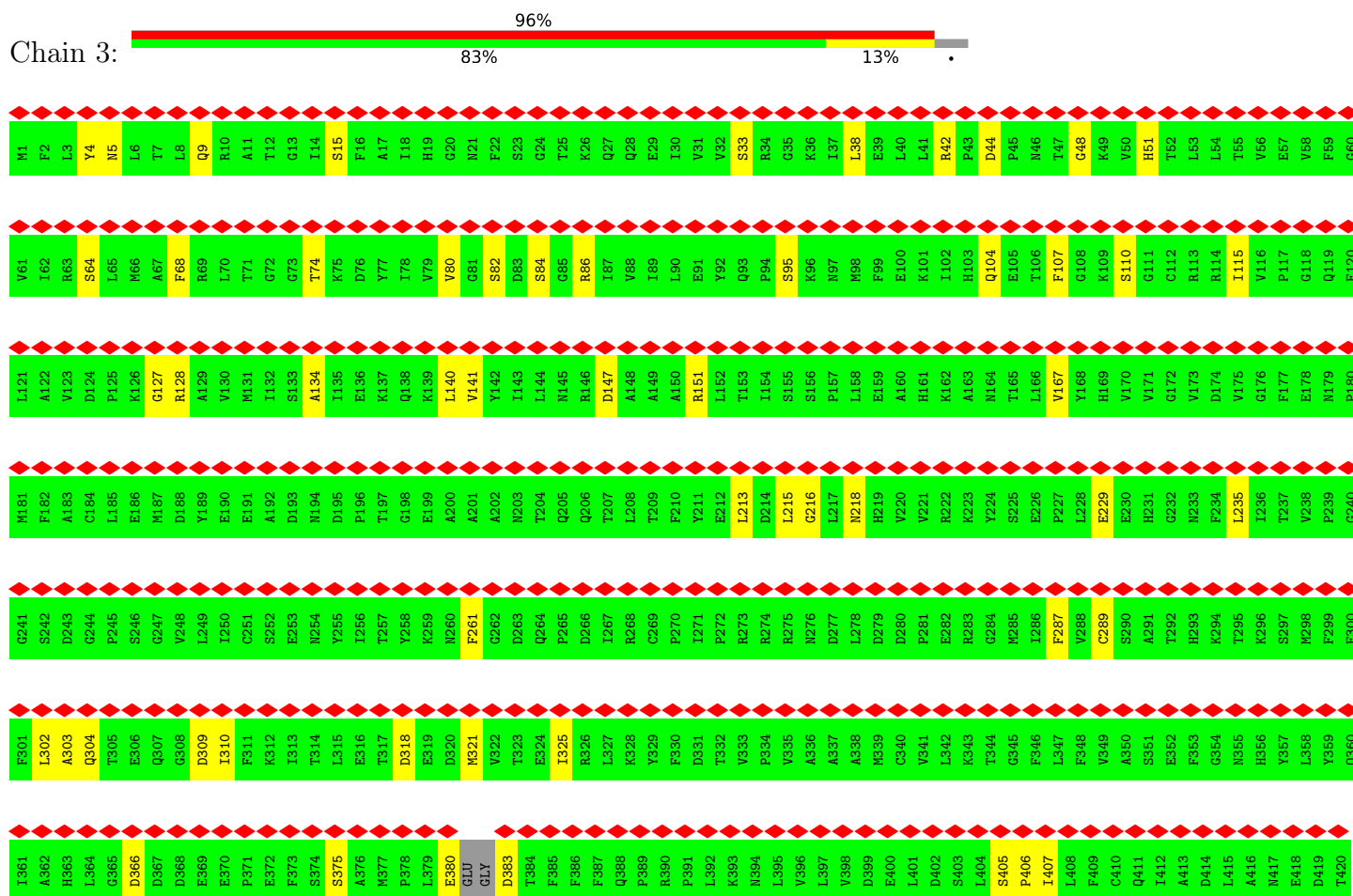
- Molecule 26: Splicing factor 3B subunit 1



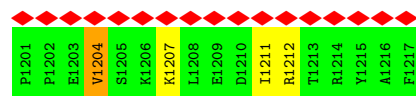
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Q903	K843	E783	S723	A603	T543	D483	P423	PRO	T303	E243	V183	R123
T904	V844	M784	S724	A604	L544	E484	I424	ALA	P304	T244	V184	R124
T905	G845	K785	D725	G605	E545	S485	R425	ASN	G305	P245	N185	M125
E906	A846	K786	S726	L606	D546	THR	T426	MET	H306	G246	G186	M126
D907	A847	I787	T727	A607	Q547	LEU	P427	ALA	G307	A247	A187	I127
S908	E848	V788	L728	T608	E548	PRO	A428	THR	S308	T248	A188	I128
V909	I849	L789	K729	M609	R549	PRO	R429	PRO	G309	P249	A189	S129
M910	T850	K790	P730	T610	H550	GLY	K430	GLY	W310	G250	S190	PRO
L911	S851	V791	L731	S611	L551	HIS	L431	HIS	A311	S251	GLN	ARG
N912	R852	T792	W732	T612	L552	ILE	T432	ILE	E312	K252	PRO	LEU
G913	I853	K793	K733	M613	V553	SER	A433	SER	T313	I253	PRO	ASP
F914	V854	Q794	G734	R614	K554	THR	T434	THR	P314	W254	PRO	PRO
G915	D855	C795	I735	P615	V555	THR	P435	THR	R315	D255	ARG	PHE
T916	D856	C796	R736	D616	I556	PRO	T436	PRO	T316	P256	ALA	ALA
V917	L857	G797	Q737	L617	D557	GLN	P437	GLN	R317	T257	ARG	ASP
V918	K858	T798	H738	D618	R558	LEU	L438	LEU	D318	P258	TRP	GLY
N919	D859	D799	R739	M619	I559	GLN	G439	GLN	G319	S259	ASP	LYS
A920	E860	G800	G740	M620	L560	ALA	G440	ALA	H320	THR	GLN	THR
L921	A861	V801	K741	D621	V561	TRP	M441	TRP	D321	THR	ALA	ASP
K922	E862	E802	G742	E622	K562	ARG	T442	ARG	S322	ALA	D205	PRO
K923	K863	A803	L743	G623	L563	GLU	G443	GLU	I323	GLY	Q206	LYS
R924	Y864	N804	A744	G624	D564	ARG	F444	ARG	G324	ALA	Q207	ASN
V925	R865	T805	A745	R625	D565	ILE	H445	ILE	A325	THR	P208	ALA
K926	K866	I806	F746	D626	D566	ASP	M446	ASP	T326	PRO	G209	ARG
P927	M867	K807	L747	N627	V567	THR	Q447	THR	P327	GLY	A210	THR
V928	V868	T808	K748	T628	R568	GLU	GLU	GLU	T328	ARG	P211	TYR
L929	M869	E809	A749	A629	P569	ASP	ASP	ASP	P329	GLY	T212	MET
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C933	E873	P813	Y752	F632	H572	MET	K454	MET	L399	GLY	K214	ARG
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V936	H876	K816	L756	A636	V576	LEU	M457	LEU	E402	ALA	S217	THR
L937	G877	H817	K757	S637	V577	LEU	Q459	LEU	E403	THR	W218	LEU
V938	N878	F818	D758	A638	I578	LEU	P460	LEU	TRP	GLY	D219	LYS
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C943	D883	K823	N763	S643	I582	ASN	L464	ASN	GLN	SER	T223	GLN
S944	I884	A824	T764	L644	L583	LEU	P465	LEU	GLY	ALA	H226	LEU
A945	D885	L825	T765	L645	D584	LEU	F466	LEU	GLY	ASN	T227	E174
K946	H886	D826	T766	P646	E585	LEU	L467	LEU	THR	THR	P228	K175
V947	K887	R827	R767	F647	S587	LEU	K468	LEU	PRO	ASP	S229	K177
R948	L888	R828	E768	L648	V588	LEU	D470	LEU	LEU	GLU	L230	A176
Q949	E889	W829	T769	K649	A589	LEU	P471	LEU	PRO	THR	R231	LEU
V950	E890	Y830	W770	A650	R590	LEU	D471	LEU	PRO	GLY	W232	PRO
A951	Q891	R831	L771	V651	V591	LEU	I472	LEU	LYS	THR	D233	GLY
A952	L892	Q832	L772	C652	E592	LEU	Q473	LEU	THR	THR	E234	E180
D953	I893	L833	L773	K653	G593	LEU	Y474	LEU	PRO	THR	T235	LEU
L954	V894	K834	I774	S654	R594	LEU	F475	LEU	THR	THR	G237	LEU
I955	C895	D835	R775	K655	E595	LEU	D476	LEU	THR	THR	R238	LEU
S956	I896	T836	E776	K656	I596	LEU	K477	LEU	THR	THR	A239	LEU
R957	L897	T837	F777	S657	I597	LEU	L478	LEU	THR	THR	K240	LEU
T958	V898	V838	Q778	P718	V598	LEU	L479	LEU	THR	THR		
A959	A899	E839	S779	Q659	N599	LEU	V480	LEU	THR	THR		
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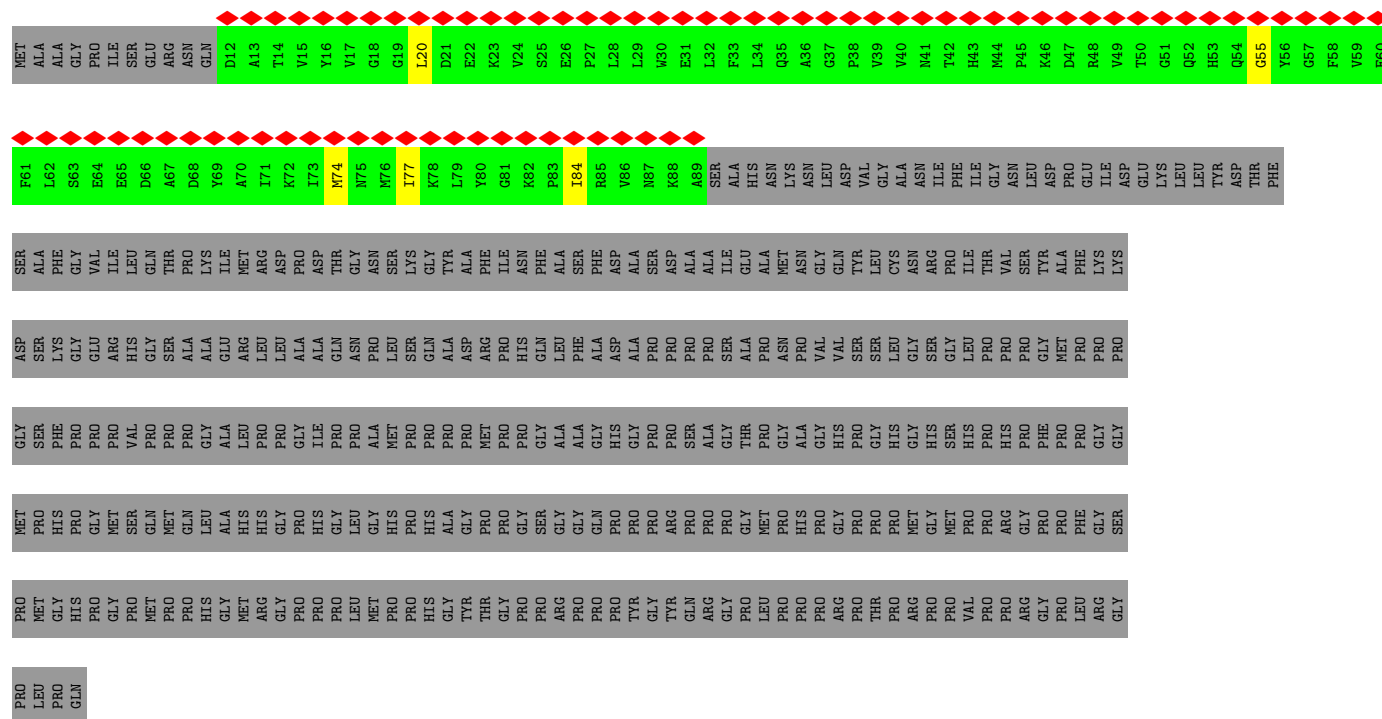
• Molecule 28: Splicing factor 3B subunit 3



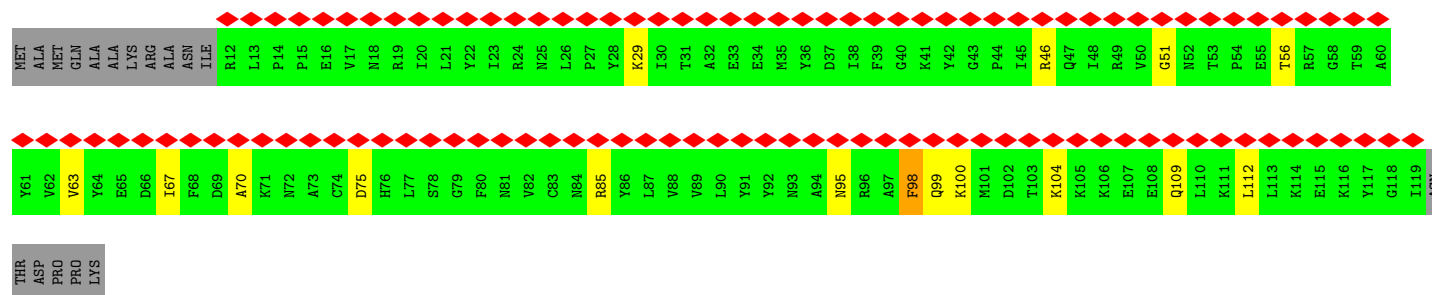
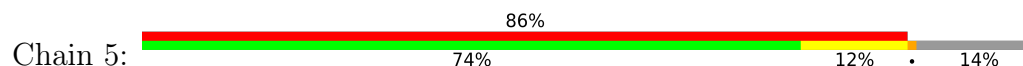
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H1143	I1023	A903	L843	T783	Y723	L663	R603	T543	L483	L423
V1144	F1024	Y904	N844	T784	S724	Y664	F604	I544	V484	Y424
E1145	K965	Y905	E845	P785	Y725	L665	L605	V485	L485	V425
M1146	A1026	L906	N846	P786	Q726	N666	A606	K546	S486	A426
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R1149	V969	Y909	E849	F789	F729	L669	L609	V489	R429	R429
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P1153	G973	L913	G853	E793	F733	V673	T613	Q553	E493	S433
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L1155	K975	L915	P855	M795	S735	L675	R615	V555	T495	L435
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G1098	L978	R918	G858	L798	T738	V678	S618	L558	G498	L438
E1099	R979	S919	N859	I799	L739	L679	L619	T559	F499	R439
T1100	K980	V920	G860	I800	E740	D680	D620	G560	L500	HIS
V1101	Y1041	A921	Q861	E801	F741	P681	P621	G561	G501	G441
L1102	E982	G922	V862	T802	A742	V682	S622	E562	T502	L442
S1103	N983	G923	A863	D803	S743	T683	D623	L563	T503	E443
R1164	V1044	F924	S864	H804	G744	G684	Q624	V564	P504	A444
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K1106	G1046	Y926	L866	A806	A746	L686	Q626	F566	L506	E446
T1107	A1047	T927	R867	Y807	S747	S687	P627	E567	S507	M447
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L1109	K1049	X929	N869	E809	Q749	T689	S629	D569	S509	V449
I1110	F1050	L930	N870	A810	G750	R690	M630	P570	L510	S450
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G1113	I1053	N933	Q873	A813	G753	G695	L633	Q573	D513	P453
S1114	C1054	G934	G874	Q814	I754	C695	P634	L574	D514	G454
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G1125	V1065	Y945	N885	E825	L765	M706	M645	A585	R525	H465
I1126	Q1066	E946	E886	A826	A766	Q707	GLY	D586	H526	I466
G1127	E1007	E947	A887	A827	L767	G708	GLY	V587	I527	E467
I1128	S1008	V948	A888	GLU	F767	T709	THR	V588	R528	D468
L1129	F1009	P949	F889	GLU	E768	Q709	GLU	C589	A529	E469
V1130	I1010	A950	S890	GLU	K769	E710	GLN	M590	D530	F470
P1131	W1011	A951	V891	ARG	G771	A711	ASP	S591	K531	D471
V1012	V1012	N952	A892	GLU	A772	V712	LEU	L592	R532	A472
R1013	R1013	A953	V893	L834	V773	L713	GLY	A593	V533	V473
Y1014	Y1014	P954	C894	A835	F774	A714	GLU	N594	N534	I474
K1015	K1015	F955	R895	A836	N775	M715	ARG	V595	E535	I475
R1016	R1016	Q956	F956	E837	Q776	S716	GLY	V596	W536	V476
N1017	N1017	G957	S897	M838	V777	S717	SER	P597	K537	S477
E1018	E1018	G958	N898	A839	A778	R718	ILE	P598	T538	F478
N1019	N1019	V959	T899	A840	F779	S719		E599	P539	V479
Q1200	Q1200	L960	G900		P780	W720		Q600	G540	N480



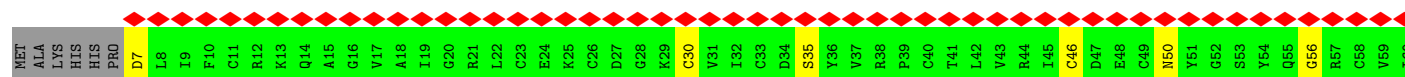
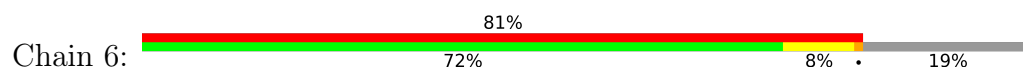
• Molecule 29: Splicing factor 3B subunit 4

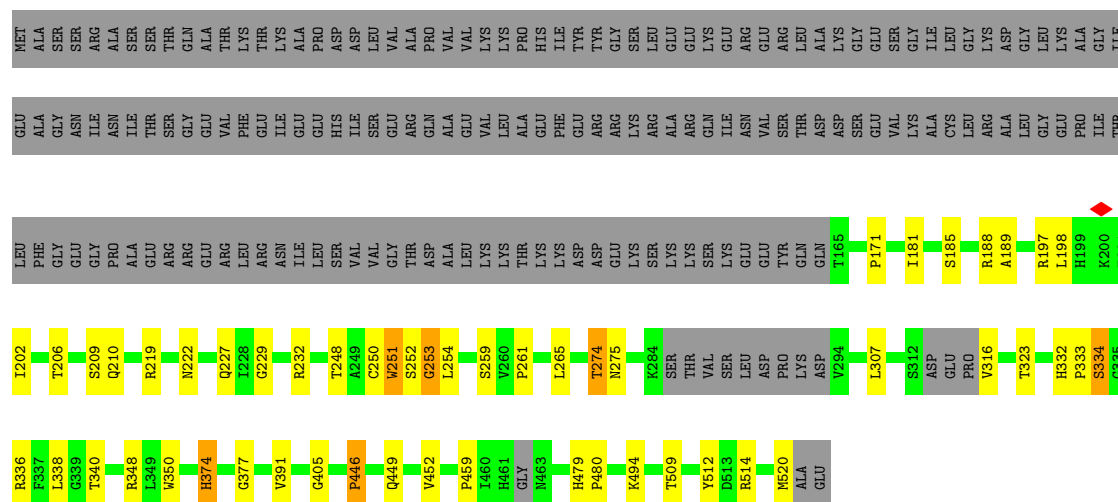


• Molecule 30: Splicing factor 3B subunit 6

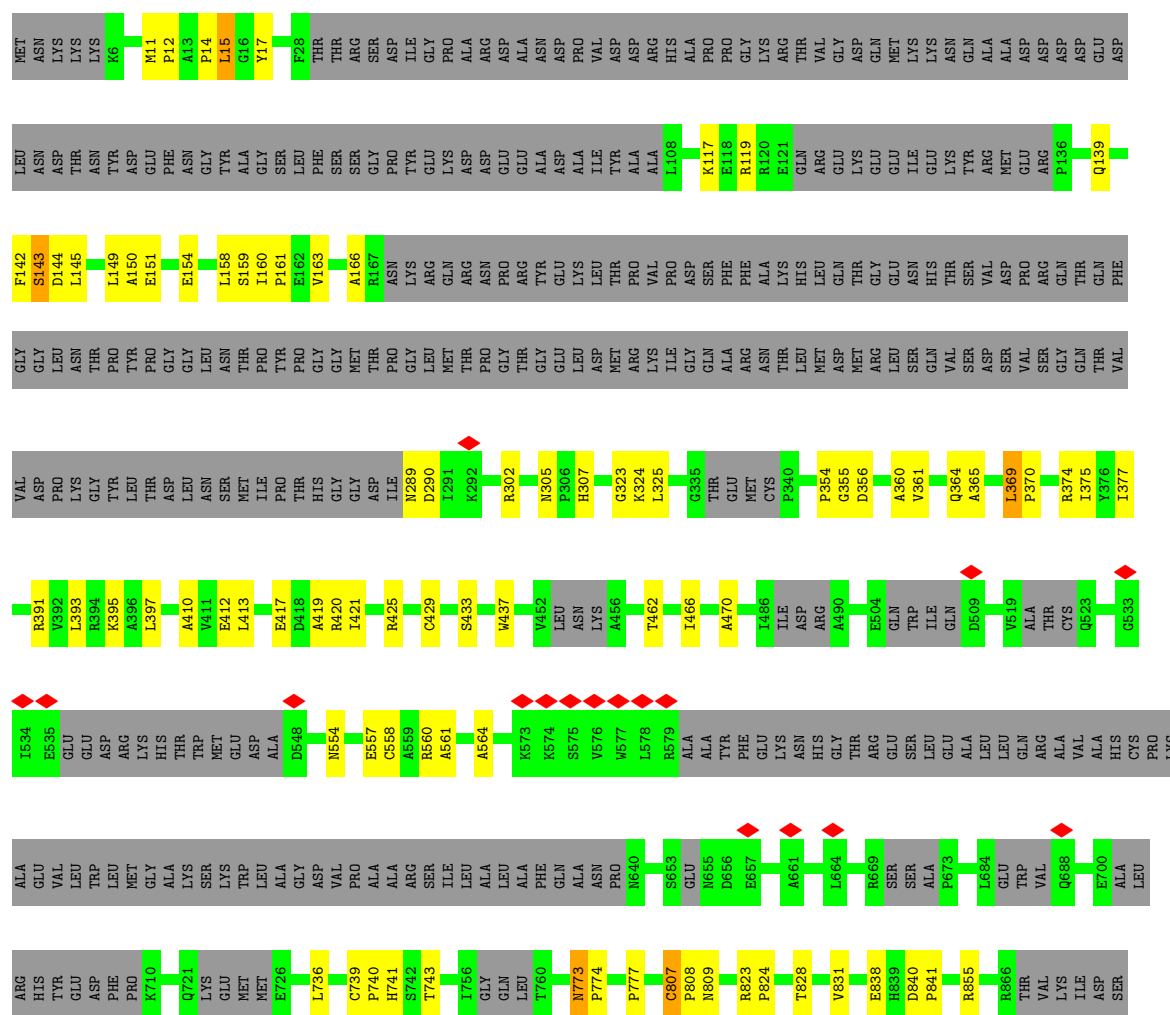


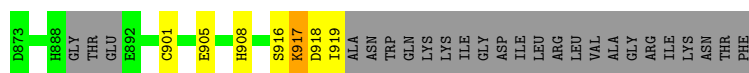
• Molecule 31: PHD finger-like domain-containing protein 5A



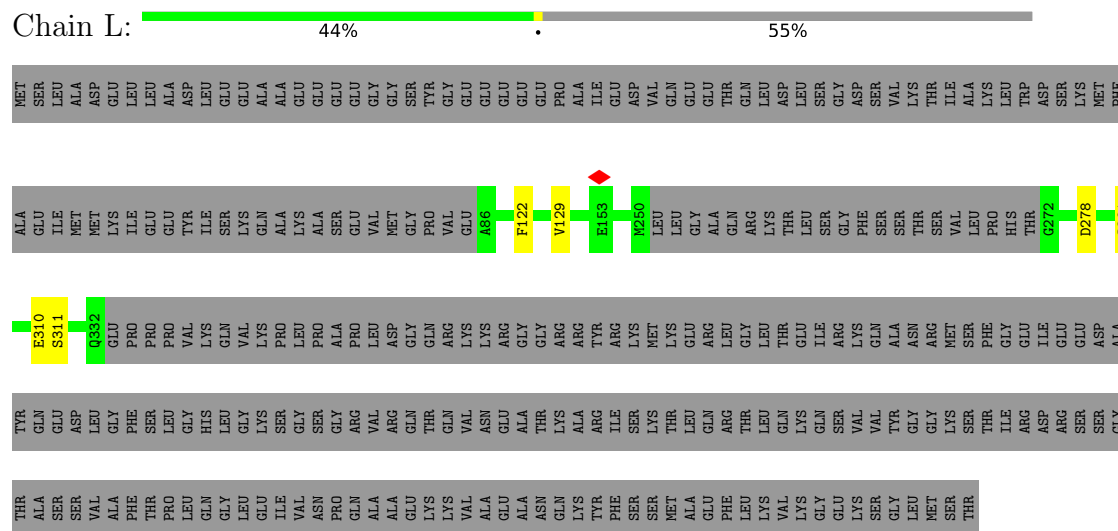


• Molecule 35: Pre-mRNA-processing factor 6

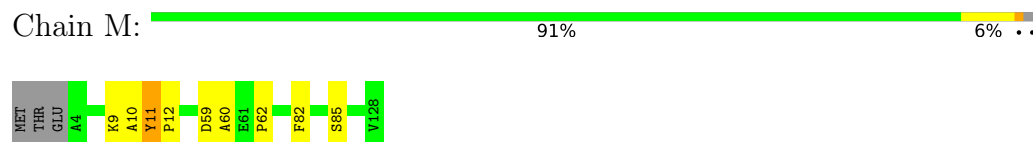




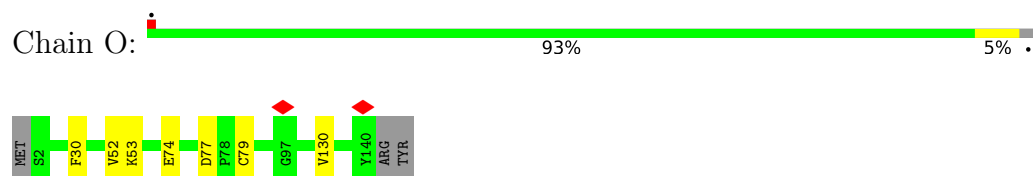
- Molecule 36: U4/U6 small nuclear ribonucleoprotein Prp31



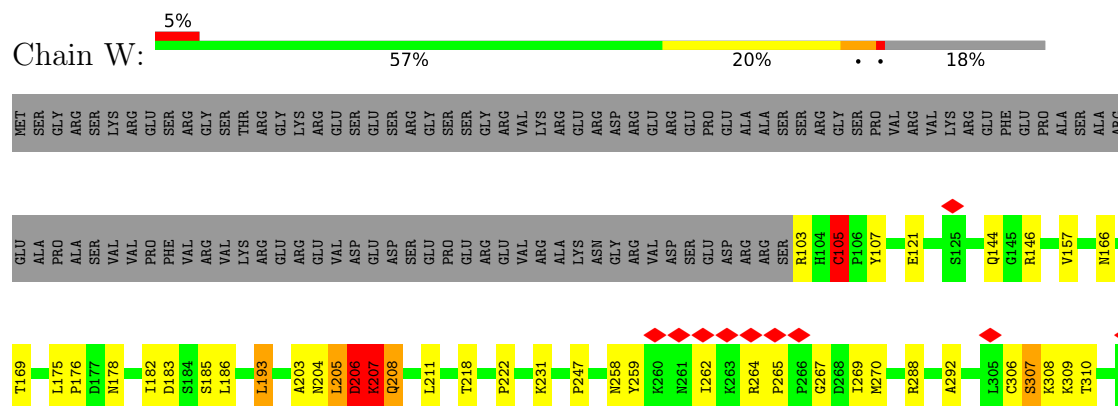
- Molecule 37: NHP2-like protein 1



- Molecule 38: Thioredoxin-like protein 4A



- Molecule 39: U4/U6.U5 tri-snRNP-associated protein 2





E156	I157	R158	LYS	ARG	TYR	ASP	GLN	ASP	ASP	LEU	CYS	TYR	THR	ASP	ILE	LEU	PHE	T173	R177	V225	V226	M236	L237	I257	L263	K268	S310	Q313	D333	Y336	K341	R342	L343	W344	R354	K355	A360	P361	Q366	R367	V385	G386	D387	V388
F427	T428	Q436	H437	I438	P439	S440	G444	A445	K448	I449	T452	V457	D458	G462	P470	G471	G472	P473	L474	M475	V496	I497	S498	G499	L516	E519	A535	R536	G547	D556	I559	E572	E573	F577	R578	P615	I651	D652	I653	D657				
T661	E664	T665	V666	V667	N680	K681	K682	N683	K684	G736	L750	K756	A757	E776	G777	P778	D781	E782	R785	V795	V796	A797	Q798	E799	A823	T824	P825	R826	L827	A838	H856	L868	I906	V907	F908	G909	R919	E922	F923	Q924	A930			
K936	I943	SER	GLU	ASP	VAL	SER	ILE	SER	LYS	PHE	PHE	ASP	ASP	PRO	MET	LEU	LEU	GLU	ALA	LYS	GLN	ASP	VAL	VAL	LEU	ASN	TYR	PRO	MET															

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	186162	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	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	0.116	Depositor
Minimum map value	-0.035	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.015	Depositor
Map size ($\text{\AA}$)	535.2, 535.2, 535.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.338, 1.338, 1.338	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	B	0.12	0/2697	0.23	0/4193
2	D	0.55	0/7493	1.20	34/9361 (0.4%)
3	E	1.08	0/1195	1.22	5/1492 (0.3%)
4	P	0.15	0/298	0.49	0/370
4	a	0.13	0/316	0.46	0/392
4	k	1.18	0/338	1.20	1/419 (0.2%)
5	Q	0.20	0/291	0.47	0/363
5	b	0.20	0/299	0.45	0/373
5	m	1.24	1/295 (0.3%)	1.26	0/367
6	R	0.16	0/313	0.46	0/390
6	c	0.15	0/313	0.45	0/390
6	l	1.02	0/315	1.26	0/392
7	S	0.22	0/297	0.59	0/371
7	d	0.21	0/281	0.58	0/351
7	n	0.86	0/270	1.05	0/334
8	T	0.13	0/287	0.35	0/358
8	e	0.13	0/317	0.61	0/396
8	h	0.81	0/318	1.01	0/394
9	U	0.12	0/254	0.39	0/314
9	f	0.13	0/258	0.41	0/320
9	i	0.77	0/290	1.10	1/359 (0.3%)
10	V	0.14	0/333	0.46	0/416
10	g	0.13	0/378	0.44	0/471
10	j	0.89	0/327	1.11	0/407
11	F	0.25	1/1639 (0.1%)	0.38	2/2545 (0.1%)
12	q	0.69	0/359	1.28	0/447
13	r	0.74	0/298	1.87	5/369 (1.4%)
14	s	0.58	0/294	1.32	3/364 (0.8%)
15	t	0.69	0/298	1.27	2/369 (0.5%)
16	x	0.68	0/279	1.29	0/347
17	y	0.59	0/258	1.14	0/319
18	z	0.69	0/242	1.22	1/299 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	G	0.60	4/954 (0.4%)	0.80	2/1477 (0.1%)
20	H	0.68	12/2576 (0.5%)	1.00	18/4003 (0.4%)
21	o	0.98	0/647	2.34	34/807 (4.2%)
22	p	0.97	0/375	1.97	7/467 (1.5%)
23	u	0.36	0/493	0.97	2/611 (0.3%)
24	v	0.40	0/392	1.38	6/483 (1.2%)
25	w	0.37	0/1767	0.90	4/2199 (0.2%)
26	1	1.71	38/4112 (0.9%)	1.37	21/5126 (0.4%)
27	2	1.15	0/738	1.22	3/912 (0.3%)
28	3	1.39	26/4689 (0.6%)	1.19	7/5849 (0.1%)
29	4	1.07	0/311	1.15	1/387 (0.3%)
30	5	1.23	2/431 (0.5%)	1.27	1/537 (0.2%)
31	6	1.17	0/355	1.13	0/442
32	7	1.59	1/263 (0.4%)	1.23	0/327
33	J	1.13	2/664 (0.3%)	1.25	5/823 (0.6%)
34	K	1.20	3/1367 (0.2%)	1.40	18/1702 (1.1%)
35	N	0.89	2/2297 (0.1%)	1.51	18/2838 (0.6%)
36	L	0.63	0/902	1.13	4/1124 (0.4%)
37	M	0.67	0/499	1.25	5/622 (0.8%)
38	O	1.23	1/555 (0.2%)	1.24	1/692 (0.1%)
39	W	0.88	1/1851 (0.1%)	1.96	56/2312 (2.4%)
40	I	0.23	1/2779 (0.0%)	0.37	0/4319
41	X	0.74	0/1655	1.28	6/2062 (0.3%)
42	A	1.03	12/8880 (0.1%)	1.58	156/11093 (1.4%)
43	C	1.05	2/3270 (0.1%)	1.50	44/4084 (1.1%)
All	All	0.93	109/64262 (0.2%)	1.23	473/83350 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	1
4	k	0	1
16	x	0	1
25	w	0	1
26	1	0	15
27	2	0	2
28	3	0	13
30	5	0	1
31	6	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
32	7	0	1
34	K	0	1
35	N	0	6
39	W	0	62
43	C	0	1
All	All	0	108

All (109) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	A	597	LYS	C-N	17.92	1.58	1.33
26	1	719	TYR	C-O	-13.59	1.11	1.24
42	A	877	ALA	C-N	12.10	1.50	1.33
26	1	718	PRO	CA-C	-11.67	1.41	1.52
26	1	1243	PRO	N-CA	-9.51	1.35	1.47
26	1	944	SER	N-CA	-8.37	1.34	1.46
43	C	661	THR	C-N	-8.13	1.22	1.33
28	3	84	SER	CA-C	-7.78	1.42	1.53
20	H	142	C	C1'-N1	7.51	1.59	1.48
26	1	718	PRO	C-O	-7.41	1.16	1.23
42	A	1862	ILE	C-O	-7.24	1.16	1.24
26	1	868	VAL	CA-C	-7.21	1.42	1.52
28	3	1101	VAL	CA-C	-7.14	1.44	1.52
20	H	182	U	C1'-N1	7.13	1.59	1.48
28	3	82	SER	CA-C	-7.10	1.44	1.52
28	3	110	SER	C-O	-7.09	1.15	1.23
28	3	1101	VAL	C-O	-7.04	1.16	1.24
20	H	150	U	C1'-N1	6.89	1.58	1.48
42	A	1863	VAL	CA-C	-6.86	1.44	1.52
38	O	130	VAL	N-CA	-6.79	1.37	1.46
20	H	151	C	C1'-N1	6.70	1.58	1.48
26	1	1273	TYR	CA-C	-6.70	1.43	1.52
20	H	97	G	C1'-N9	-6.68	1.38	1.48
28	3	141	VAL	C-O	-6.64	1.17	1.24
20	H	141	C	C1'-N1	6.63	1.58	1.48
20	H	148	C	C1'-N1	6.60	1.58	1.48
42	A	461	HIS	C-N	-6.59	1.23	1.33
28	3	289	CYS	C-O	-6.58	1.15	1.23
20	H	184	C	C1'-N1	6.58	1.58	1.48
30	5	98	PHE	N-CA	-6.56	1.37	1.46
26	1	939	ARG	CA-C	-6.53	1.44	1.52
33	J	469	MET	C-N	6.52	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	3	64	SER	N-CA	-6.50	1.38	1.46
42	A	1311	PHE	C-N	6.39	1.41	1.33
26	1	814	PHE	CA-C	-6.26	1.45	1.52
42	A	1772	PHE	C-O	-6.17	1.16	1.24
28	3	302	LEU	C-O	-6.10	1.16	1.24
28	3	213	LEU	CA-C	-6.09	1.45	1.52
26	1	678	ALA	N-CA	-6.06	1.38	1.46
26	1	571	VAL	CA-C	-5.99	1.45	1.52
28	3	167	VAL	CA-C	-5.99	1.46	1.52
26	1	893	ILE	N-CA	-5.99	1.39	1.46
19	G	122	U	C1'-N1	5.95	1.56	1.47
28	3	64	SER	C-O	-5.92	1.16	1.23
26	1	945	ALA	CA-C	-5.92	1.44	1.52
40	I	63	U	C1'-N1	5.88	1.57	1.48
28	3	140	LEU	CA-C	-5.87	1.45	1.52
20	H	48	A	C1'-N9	-5.86	1.39	1.48
43	C	333	ASP	N-CA	5.84	1.53	1.46
26	1	940	LEU	CA-C	-5.82	1.45	1.52
28	3	115	ILE	N-CA	-5.80	1.40	1.46
26	1	1167	TYR	CA-C	-5.77	1.45	1.52
26	1	482	VAL	C-O	-5.77	1.17	1.24
28	3	235	LEU	C-O	-5.75	1.16	1.23
28	3	104	GLN	CA-C	-5.74	1.46	1.52
42	A	1870	ASP	CA-C	5.74	1.59	1.52
28	3	1153	PRO	C-O	-5.72	1.18	1.24
42	A	1816	GLN	C-O	-5.72	1.16	1.23
26	1	989	VAL	CA-C	-5.68	1.45	1.52
19	G	131	U	C1'-N1	5.67	1.56	1.48
30	5	95	ASN	N-CA	-5.66	1.38	1.46
26	1	233	ASP	CA-C	-5.65	1.45	1.52
20	H	65	U	C1'-N1	5.65	1.56	1.48
26	1	838	VAL	N-CA	-5.63	1.40	1.46
26	1	1177	LEU	C-O	-5.60	1.17	1.24
26	1	235	THR	C-O	-5.59	1.19	1.24
34	K	509	THR	C-O	-5.59	1.17	1.24
33	J	584	VAL	CA-C	-5.57	1.45	1.52
28	3	1123	SER	CA-C	-5.55	1.45	1.52
28	3	80	VAL	C-O	-5.53	1.18	1.24
28	3	134	ALA	C-O	-5.50	1.18	1.23
20	H	110	A	C1'-N9	-5.46	1.39	1.48
26	1	562	LYS	CA-C	-5.42	1.48	1.53
19	G	125	C	C1'-N1	5.42	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	3	107	PHE	CA-C	-5.40	1.45	1.52
28	3	941	HIS	C-O	5.39	1.30	1.23
26	1	738	HIS	N-CA	-5.37	1.39	1.45
26	1	439	GLY	CA-C	5.35	1.56	1.52
26	1	627	THR	N-CA	-5.35	1.40	1.46
11	F	103	U	C1'-N1	5.34	1.55	1.47
34	K	449	GLN	CA-C	-5.33	1.46	1.52
19	G	161	U	C1'-N1	5.28	1.55	1.47
35	N	11	MET	N-CA	5.28	1.51	1.46
26	1	680	LEU	C-O	-5.25	1.19	1.24
28	3	38	LEU	CA-C	-5.25	1.46	1.52
26	1	672	ALA	CA-C	-5.24	1.46	1.52
39	W	360	LEU	CA-C	5.24	1.59	1.52
26	1	721	ILE	N-CA	-5.24	1.40	1.46
35	N	166	ALA	CA-C	-5.24	1.46	1.52
42	A	628	GLY	CA-C	-5.23	1.47	1.52
28	3	1034	THR	CA-C	-5.22	1.47	1.53
26	1	601	ALA	N-CA	-5.21	1.40	1.46
26	1	864	TYR	CA-C	-5.21	1.46	1.52
26	1	1281	ILE	CA-C	-5.20	1.46	1.52
32	7	44	MET	C-O	-5.17	1.18	1.24
26	1	776	GLU	CA-C	-5.17	1.45	1.52
26	1	898	TYR	C-N	-5.15	1.27	1.33
42	A	1806	ALA	CA-C	-5.15	1.46	1.52
26	1	415	LEU	C-N	5.10	1.39	1.33
26	1	1279	ALA	CA-C	-5.09	1.46	1.52
42	A	1890	GLN	CA-C	-5.09	1.46	1.52
28	3	68	PHE	N-CA	-5.07	1.40	1.46
26	1	739	ARG	N-CA	-5.06	1.40	1.46
26	1	944	SER	CA-C	5.04	1.59	1.53
5	m	14	LEU	CA-C	5.04	1.59	1.52
20	H	60	U	C1'-N1	5.03	1.55	1.48
34	K	391	VAL	CA-C	-5.02	1.47	1.52
26	1	899	ALA	N-CA	-5.01	1.40	1.46
28	3	86	ARG	N-CA	-5.01	1.40	1.46

All (473) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	N	369	LEU	CA-C-N	-25.14	88.41	119.84
35	N	369	LEU	C-N-CA	-25.14	88.41	119.84
13	r	82	ILE	CA-C-N	17.59	141.83	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	r	82	ILE	C-N-CA	17.59	141.83	119.84
42	A	1451	ASN	CA-C-N	16.74	140.77	119.84
42	A	1451	ASN	C-N-CA	16.74	140.77	119.84
41	X	584	ASP	CA-C-N	16.54	137.41	119.05
41	X	584	ASP	C-N-CA	16.54	137.41	119.05
39	W	427	GLU	N-CA-C	15.86	128.57	111.28
42	A	941	LYS	CA-C-N	14.73	135.40	119.05
42	A	941	LYS	C-N-CA	14.73	135.40	119.05
26	1	408	PHE	CA-C-N	-12.85	103.78	119.84
26	1	408	PHE	C-N-CA	-12.85	103.78	119.84
42	A	877	ALA	O-C-N	12.79	135.24	122.07
24	v	161	PRO	CA-C-N	11.93	134.75	119.84
24	v	161	PRO	C-N-CA	11.93	134.75	119.84
42	A	828	PRO	CA-C-N	11.84	131.92	120.31
42	A	828	PRO	C-N-CA	11.84	131.92	120.31
35	N	419	ALA	N-CA-C	-11.59	98.64	111.28
43	C	750	LEU	CA-C-N	11.10	131.37	119.05
43	C	750	LEU	C-N-CA	11.10	131.37	119.05
42	A	937	PRO	CA-C-N	10.84	130.61	119.56
42	A	937	PRO	C-N-CA	10.84	130.61	119.56
29	4	74	MET	N-CA-C	10.71	122.95	111.28
42	A	936	PHE	CA-C-N	10.51	131.20	120.38
42	A	936	PHE	C-N-CA	10.51	131.20	120.38
43	C	824	THR	CA-C-N	10.28	132.69	119.84
43	C	824	THR	C-N-CA	10.28	132.69	119.84
42	A	1468	ASN	N-CA-C	10.24	122.44	111.28
42	A	1760	GLU	CA-C-N	9.96	132.29	119.84
42	A	1760	GLU	C-N-CA	9.96	132.29	119.84
42	A	1879	PHE	CA-C-N	9.92	129.66	118.85
42	A	1879	PHE	C-N-CA	9.92	129.66	118.85
41	X	475	ALA	CA-C-N	9.51	129.61	119.05
41	X	475	ALA	C-N-CA	9.51	129.61	119.05
2	D	353	ASP	CA-C-N	9.51	131.72	119.84
2	D	353	ASP	C-N-CA	9.51	131.72	119.84
42	A	946	GLU	CA-C-N	9.41	130.07	120.38
42	A	946	GLU	C-N-CA	9.41	130.07	120.38
26	1	114	ASP	N-CA-C	9.36	121.25	111.14
42	A	439	GLN	CA-C-N	9.28	129.21	120.03
42	A	439	GLN	C-N-CA	9.28	129.21	120.03
42	A	801	ILE	N-CA-C	9.13	119.94	110.62
42	A	165	ARG	N-CA-C	9.07	123.67	109.07
42	A	1920	TYR	N-CA-C	9.01	122.27	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	C	428	THR	N-CA-C	8.84	120.99	111.36
42	A	1801	LYS	CA-C-N	-8.77	110.36	119.83
42	A	1801	LYS	C-N-CA	-8.77	110.36	119.83
39	W	354	ARG	O-C-N	8.73	133.19	123.33
20	H	149	A	O3'-P-O5'	-8.69	90.97	104.00
20	H	183	G	O3'-P-O5'	-8.63	91.05	104.00
20	H	182	U	O3'-P-O5'	-8.62	91.08	104.00
20	H	141	C	O3'-P-O5'	-8.61	91.09	104.00
20	H	148	C	O3'-P-O5'	-8.60	91.11	104.00
34	K	251	TRP	N-CA-C	-8.59	101.92	111.28
2	D	152	GLU	N-CA-C	-8.59	101.87	111.14
42	A	1053	LEU	N-CA-C	8.58	120.72	111.36
20	H	113	G	O3'-P-O5'	-8.55	91.18	104.00
20	H	181	G	O3'-P-O5'	-8.55	91.18	104.00
28	3	405	SER	CA-C-N	8.54	130.51	119.84
28	3	405	SER	C-N-CA	8.54	130.51	119.84
39	W	359	LYS	N-CA-C	-8.54	101.94	111.07
20	H	114	A	O3'-P-O5'	-8.53	91.20	104.00
20	H	150	U	O3'-P-O5'	-8.51	91.23	104.00
42	A	211	GLN	CA-C-N	8.43	130.38	119.84
42	A	211	GLN	C-N-CA	8.43	130.38	119.84
34	K	188	ARG	N-CA-C	8.42	120.46	111.28
43	C	448	LYS	N-CA-C	8.40	120.52	111.36
42	A	1052	VAL	N-CA-C	8.32	118.35	110.53
43	C	452	THR	N-CA-C	8.31	120.42	111.36
42	A	347	LEU	CA-C-N	-8.20	111.16	119.93
42	A	347	LEU	C-N-CA	-8.20	111.16	119.93
43	C	472	GLY	CA-C-N	8.07	128.16	119.28
43	C	472	GLY	C-N-CA	8.07	128.16	119.28
21	o	16	THR	CA-C-O	-8.01	111.79	120.36
21	o	99	SER	N-CA-C	7.97	122.78	112.26
42	A	186	GLU	CA-C-N	7.96	127.89	119.05
42	A	186	GLU	C-N-CA	7.96	127.89	119.05
43	C	436	GLN	N-CA-C	7.93	119.70	111.14
42	A	1994	LYS	N-CA-C	7.82	119.58	111.14
21	o	117	TYR	CA-C-O	7.80	128.59	120.40
42	A	1971	LEU	N-CA-C	7.78	121.21	108.99
42	A	1373	GLN	CA-C-N	7.75	127.79	119.89
42	A	1373	GLN	C-N-CA	7.75	127.79	119.89
42	A	713	LEU	N-CA-C	-7.66	102.93	111.28
33	J	558	PHE	N-CA-C	7.64	119.39	111.14
43	C	799	GLU	CA-C-N	7.52	127.39	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	C	799	GLU	C-N-CA	7.52	127.39	119.05
42	A	112	GLN	N-CA-C	-7.44	103.25	111.36
39	W	457	PHE	N-CA-C	7.42	126.61	110.80
42	A	1900	GLU	N-CA-C	7.41	119.00	111.07
39	W	457	PHE	CA-C-N	7.36	135.59	121.54
39	W	457	PHE	C-N-CA	7.36	135.59	121.54
33	J	469	MET	CA-C-N	-7.35	112.81	120.38
33	J	469	MET	C-N-CA	-7.35	112.81	120.38
43	C	661	THR	CA-C-N	-7.33	110.51	122.82
43	C	661	THR	C-N-CA	-7.33	110.51	122.82
42	A	873	ASN	CA-C-N	7.30	127.31	119.28
42	A	873	ASN	C-N-CA	7.30	127.31	119.28
2	D	1044	VAL	CA-C-N	7.28	126.78	118.85
2	D	1044	VAL	C-N-CA	7.28	126.78	118.85
42	A	1961	ILE	N-CA-C	7.28	118.97	107.98
42	A	1945	VAL	N-CA-C	7.25	117.34	110.53
21	o	71	VAL	CA-C-N	7.23	131.67	120.75
21	o	71	VAL	C-N-CA	7.23	131.67	120.75
26	1	613	MET	N-CA-C	7.19	121.77	112.92
2	D	1666	THR	N-CA-C	7.18	121.48	112.87
42	A	1866	LYS	N-CA-C	7.17	119.09	111.28
42	A	204	LEU	N-CA-C	7.15	119.08	111.28
42	A	1539	SER	CA-C-N	-7.14	111.42	119.28
42	A	1539	SER	C-N-CA	-7.14	111.42	119.28
34	K	197	ARG	N-CA-C	7.08	120.05	108.08
42	A	1825	SER	N-CA-C	7.08	118.99	111.28
20	H	170	C	C3'-C2'-O2'	-7.06	104.01	114.60
2	D	533	VAL	N-CA-C	7.03	118.89	112.29
42	A	60	ASP	N-CA-C	7.02	120.40	110.50
42	A	136	ILE	N-CA-C	-6.97	100.58	109.30
42	A	276	GLY	CA-C-N	6.97	127.53	120.14
42	A	276	GLY	C-N-CA	6.97	127.53	120.14
23	u	199	ARG	CA-C-N	6.96	127.91	120.47
23	u	199	ARG	C-N-CA	6.96	127.91	120.47
42	A	1213	VAL	N-CA-C	6.95	117.91	108.17
43	C	141	GLY	N-CA-C	6.92	125.19	115.43
21	o	121	LEU	CA-C-O	6.88	128.87	121.44
25	w	290	GLY	N-CA-C	6.87	120.98	112.73
21	o	4	LEU	N-CA-C	-6.86	98.03	108.67
34	K	274	THR	N-CA-C	6.86	121.74	113.23
39	W	364	ASP	N-CA-C	6.85	125.40	110.80
43	C	919	ARG	CA-C-N	6.85	126.45	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	C	919	ARG	C-N-CA	6.85	126.45	119.19
42	A	1467	LEU	N-CA-C	6.84	118.81	111.36
42	A	462	ARG	CA-C-N	-6.83	113.34	120.38
42	A	462	ARG	C-N-CA	-6.83	113.34	120.38
22	p	53	PHE	CA-C-O	-6.83	112.81	120.32
36	L	129	VAL	CA-C-N	6.79	126.26	118.85
36	L	129	VAL	C-N-CA	6.79	126.26	118.85
35	N	15	LEU	N-CA-C	-6.79	102.05	110.41
39	W	247	PRO	N-CA-C	6.74	118.92	110.70
39	W	342	LYS	N-CA-C	-6.73	105.07	113.55
42	A	182	ILE	N-CA-C	6.72	117.47	110.62
43	C	113	VAL	N-CA-C	6.70	117.46	110.62
42	A	74	GLY	N-CA-C	6.70	120.77	112.73
42	A	1083	HIS	CA-C-N	6.69	126.48	119.05
42	A	1083	HIS	C-N-CA	6.69	126.48	119.05
43	C	922	GLU	CA-C-N	6.67	127.07	119.93
43	C	922	GLU	C-N-CA	6.67	127.07	119.93
42	A	319	LEU	N-CA-C	-6.67	104.06	112.93
42	A	1201	ARG	N-CA-C	-6.66	104.02	111.28
26	1	1120	ALA	CA-C-N	-6.64	111.42	120.44
26	1	1120	ALA	C-N-CA	-6.64	111.42	120.44
42	A	877	ALA	CA-C-N	-6.63	110.88	120.29
42	A	877	ALA	C-N-CA	-6.63	110.88	120.29
39	W	427	GLU	CA-C-N	-6.58	108.98	121.54
39	W	427	GLU	C-N-CA	-6.58	108.98	121.54
42	A	948	PRO	N-CA-C	6.58	118.72	110.70
43	C	438	ILE	CA-C-N	6.57	126.34	119.05
43	C	438	ILE	C-N-CA	6.57	126.34	119.05
42	A	1311	PHE	CA-C-N	-6.55	113.63	120.38
42	A	1311	PHE	C-N-CA	-6.55	113.63	120.38
42	A	166	PHE	CA-C-N	6.54	127.12	120.38
42	A	166	PHE	C-N-CA	6.54	127.12	120.38
33	J	450	ARG	N-CA-C	6.54	118.20	111.14
42	A	1495	PHE	CA-C-N	6.52	126.28	119.05
42	A	1495	PHE	C-N-CA	6.52	126.28	119.05
42	A	113	ILE	N-CA-C	6.51	116.99	107.75
39	W	157	VAL	N-CA-C	6.50	118.47	111.58
21	o	87	LEU	CA-C-N	6.48	126.24	119.05
21	o	87	LEU	C-N-CA	6.48	126.24	119.05
42	A	489	TRP	N-CA-C	6.45	118.98	108.08
42	A	157	ASP	N-CA-C	6.42	118.28	111.28
26	1	719	TYR	N-CA-C	6.42	116.33	107.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	W	354	ARG	CA-C-N	6.41	133.50	121.97
39	W	354	ARG	C-N-CA	6.41	133.50	121.97
42	A	1908	LYS	N-CA-C	6.40	118.34	111.36
34	K	232	ARG	N-CA-C	-6.38	99.88	108.11
42	A	696	MET	N-CA-C	6.38	118.23	111.28
39	W	204	ASN	N-CA-C	6.38	118.76	111.11
21	o	40	THR	CA-C-N	6.36	131.62	122.40
21	o	40	THR	C-N-CA	6.36	131.62	122.40
34	K	253	GLY	N-CA-C	6.32	120.38	110.96
35	N	908	HIS	N-CA-C	6.29	119.07	107.99
42	A	1474	MET	N-CA-C	-6.26	104.45	111.28
39	W	519	LEU	CA-C-N	6.26	132.96	122.76
39	W	519	LEU	C-N-CA	6.26	132.96	122.76
20	H	169	C	P-O3'-C3'	6.26	129.58	120.20
35	N	808	PRO	N-CA-C	6.24	122.07	113.65
43	C	657	ASP	CA-C-N	6.24	126.56	119.83
43	C	657	ASP	C-N-CA	6.24	126.56	119.83
43	C	519	GLU	N-CA-C	6.21	118.85	111.71
42	A	1312	PRO	N-CA-C	6.21	118.28	110.70
39	W	508	LYS	CA-C-N	6.20	127.59	119.84
39	W	508	LYS	C-N-CA	6.20	127.59	119.84
42	A	1676	ILE	N-CA-C	6.20	116.94	110.62
42	A	1055	LEU	N-CA-C	6.19	118.10	111.36
42	A	798	GLY	N-CA-C	6.18	124.95	112.34
43	C	756	LYS	N-CA-C	6.17	118.09	111.36
42	A	1926	THR	N-CA-C	6.17	118.08	111.36
42	A	1737	ASN	CA-C-N	6.15	125.88	119.05
42	A	1737	ASN	C-N-CA	6.15	125.88	119.05
43	C	776	GLU	N-CA-C	6.15	118.07	111.36
42	A	82	ARG	N-CA-C	6.14	118.05	111.36
21	o	73	ASN	N-CA-C	6.13	119.82	111.17
35	N	412	GLU	N-CA-C	-6.13	104.59	111.28
26	1	1180	ARG	N-CA-C	-6.11	103.34	111.96
26	1	1275	GLY	N-CA-C	-6.11	104.90	111.93
30	5	85	ARG	N-CA-C	6.10	118.78	110.55
43	C	336	TYR	N-CA-C	6.09	118.00	111.36
39	W	185	SER	CA-C-O	6.09	126.80	119.61
42	A	1063	GLY	CA-C-N	6.08	124.04	119.66
42	A	1063	GLY	C-N-CA	6.08	124.04	119.66
42	A	1309	SER	N-CA-C	6.07	117.97	111.36
27	2	559	PRO	N-CA-C	6.07	120.01	111.33
42	A	585	VAL	N-CA-C	6.03	116.77	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	W	448	PRO	N-CA-C	6.03	121.68	113.84
42	A	1871	PRO	N-CA-C	6.01	121.77	113.65
22	p	46	MET	N-CA-C	-6.01	104.64	111.07
2	D	284	LYS	N-CA-C	-5.99	104.75	111.28
42	A	106	MET	CA-C-N	5.98	126.09	119.87
42	A	106	MET	C-N-CA	5.98	126.09	119.87
21	o	79	ILE	CA-C-N	5.98	125.78	120.10
21	o	79	ILE	C-N-CA	5.98	125.78	120.10
2	D	1006	LYS	CA-C-N	5.97	126.13	119.32
2	D	1006	LYS	C-N-CA	5.97	126.13	119.32
42	A	173	GLU	CA-C-N	5.97	123.96	119.66
42	A	173	GLU	C-N-CA	5.97	123.96	119.66
26	1	415	LEU	O-C-N	-5.96	114.46	121.32
42	A	273	ILE	CA-C-N	5.96	127.29	119.84
42	A	273	ILE	C-N-CA	5.96	127.29	119.84
39	W	388	PHE	N-CA-C	5.95	117.85	107.49
43	C	536	ARG	N-CA-C	-5.95	100.61	109.83
42	A	353	ASP	CA-C-N	5.93	125.63	119.05
42	A	353	ASP	C-N-CA	5.93	125.63	119.05
42	A	1603	ALA	CA-C-N	-5.93	110.22	121.54
42	A	1603	ALA	C-N-CA	-5.93	110.22	121.54
39	W	288	ARG	CA-C-N	5.93	129.18	120.82
39	W	288	ARG	C-N-CA	5.93	129.18	120.82
35	N	917	LYS	CA-C-N	5.92	132.85	121.54
35	N	917	LYS	C-N-CA	5.92	132.85	121.54
42	A	1488	THR	N-CA-C	5.91	117.68	110.41
39	W	182	ILE	CA-C-N	5.90	132.81	121.54
39	W	182	ILE	C-N-CA	5.90	132.81	121.54
43	C	343	LEU	N-CA-C	5.89	117.79	111.36
14	s	2	LEU	CA-C-N	5.88	127.19	119.84
14	s	2	LEU	C-N-CA	5.88	127.19	119.84
21	o	50	SER	CA-C-O	5.88	127.79	121.55
43	C	449	ILE	N-CA-C	5.87	116.61	110.62
39	W	307	SER	CA-C-N	5.87	128.72	120.28
39	W	307	SER	C-N-CA	5.87	128.72	120.28
42	A	1789	THR	N-CA-C	5.87	119.03	109.59
42	A	1702	LEU	N-CA-C	5.86	118.46	108.90
34	K	323	THR	N-CA-C	5.84	117.45	111.14
15	t	13	LEU	CA-C-N	5.83	125.96	119.32
15	t	13	LEU	C-N-CA	5.83	125.96	119.32
35	N	807	CYS	CA-C-N	5.82	125.68	119.28
35	N	807	CYS	C-N-CA	5.82	125.68	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	A	1312	PRO	CA-C-N	5.82	126.22	119.47
42	A	1312	PRO	C-N-CA	5.82	126.22	119.47
21	o	113	LYS	N-CA-C	5.81	118.36	111.33
11	F	52	U	C2'-C3'-O3'	-5.81	104.98	113.70
39	W	389	MET	N-CA-C	5.81	119.47	112.38
42	A	490	VAL	N-CA-C	5.79	116.53	110.62
42	A	563	GLN	N-CA-C	-5.79	104.97	111.28
39	W	329	ALA	N-CA-C	5.79	117.26	111.07
26	1	1106	ARG	N-CA-C	-5.77	104.34	111.33
37	M	10	ALA	N-CA-C	-5.77	100.22	109.39
28	3	679	LEU	N-CA-C	5.76	119.48	110.32
39	W	529	LEU	CA-C-N	5.76	129.84	121.26
39	W	529	LEU	C-N-CA	5.76	129.84	121.26
26	1	1101	LEU	N-CA-C	5.76	118.44	109.52
42	A	1813	ARG	N-CA-C	5.76	117.23	111.07
2	D	159	LEU	N-CA-C	-5.75	105.01	111.28
43	C	680	ASN	N-CA-C	-5.75	99.87	109.24
42	A	570	ASP	N-CA-C	5.74	118.26	108.90
43	C	445	ALA	N-CA-C	5.74	117.53	111.28
39	W	105	CYS	CA-C-N	5.72	125.84	119.32
39	W	105	CYS	C-N-CA	5.72	125.84	119.32
21	o	27	ARG	CA-C-N	5.70	128.71	120.11
21	o	27	ARG	C-N-CA	5.70	128.71	120.11
34	K	189	ALA	N-CA-C	5.70	117.49	111.28
34	K	336	ARG	N-CA-C	5.68	117.47	111.28
42	A	1566	ILE	CA-C-N	-5.68	112.74	119.84
42	A	1566	ILE	C-N-CA	-5.68	112.74	119.84
42	A	2153	THR	N-CA-C	-5.68	101.77	109.95
43	C	344	TRP	N-CA-C	5.67	118.15	108.90
2	D	1291	LEU	CA-C-N	5.66	125.98	119.92
2	D	1291	LEU	C-N-CA	5.66	125.98	119.92
21	o	71	VAL	O-C-N	-5.66	115.50	122.57
42	A	1657	THR	N-CA-C	5.66	116.02	108.38
2	D	1135	LEU	CA-C-N	5.66	125.59	119.76
2	D	1135	LEU	C-N-CA	5.66	125.59	119.76
26	1	942	ASN	CA-C-N	-5.65	114.76	124.82
26	1	942	ASN	C-N-CA	-5.65	114.76	124.82
2	D	782	PHE	N-CA-C	5.65	118.00	109.41
42	A	1056	HIS	N-CA-C	5.62	117.41	111.28
20	H	160	A	P-O5'-C5'	-5.62	112.47	120.90
24	v	160	GLU	CA-C-N	5.61	126.16	120.38
24	v	160	GLU	C-N-CA	5.61	126.16	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	295	THR	CA-C-N	-5.61	114.86	123.04
2	D	295	THR	C-N-CA	-5.61	114.86	123.04
42	A	1318	THR	CA-C-N	5.60	125.55	119.78
42	A	1318	THR	C-N-CA	5.60	125.55	119.78
39	W	292	ALA	N-CA-C	5.60	118.15	111.71
26	1	942	ASN	N-CA-C	-5.58	98.91	110.80
2	D	1048	VAL	N-CA-C	-5.57	106.37	113.22
34	K	202	ILE	CA-C-N	5.57	125.67	119.32
34	K	202	ILE	C-N-CA	5.57	125.67	119.32
39	W	414	PRO	N-CA-C	5.57	123.94	112.47
21	o	34	ILE	CA-C-O	-5.56	114.18	120.74
26	1	466	PHE	N-CA-C	5.56	118.79	109.95
39	W	259	TYR	N-CA-C	5.56	117.03	110.97
21	o	32	PRO	CA-C-N	5.55	130.70	122.99
21	o	32	PRO	C-N-CA	5.55	130.70	122.99
42	A	2225	LEU	N-CA-C	5.54	117.81	109.23
42	A	946	GLU	N-CA-C	5.54	118.26	109.40
39	W	537	ILE	N-CA-C	5.52	116.07	108.12
42	A	2241	ASN	N-CA-C	5.51	118.31	110.10
42	A	1247	ILE	N-CA-C	-5.51	105.00	110.62
3	E	322	LYS	N-CA-C	-5.51	98.22	108.02
3	E	284	PHE	N-CA-C	5.50	119.50	112.34
41	X	399	PRO	O-C-N	5.50	123.84	121.31
21	o	16	THR	O-C-N	5.50	129.49	123.22
39	W	325	TRP	CA-C-N	5.50	127.59	120.44
39	W	325	TRP	C-N-CA	5.50	127.59	120.44
2	D	124	LEU	N-CA-C	5.50	117.35	111.36
37	M	11	TYR	CA-C-N	-5.50	113.65	120.79
37	M	11	TYR	C-N-CA	-5.50	113.65	120.79
42	A	1578	ARG	N-CA-C	5.49	118.53	109.85
42	A	2203	ASN	N-CA-C	5.49	120.81	109.11
27	2	511	LEU	N-CA-C	5.49	117.61	108.99
37	M	62	PRO	N-CA-C	-5.49	101.16	112.47
33	J	538	SER	N-CA-C	5.49	117.26	111.28
42	A	429	ASN	N-CA-C	-5.47	105.31	111.28
3	E	281	VAL	N-CA-C	5.47	116.18	108.36
43	C	838	ALA	N-CA-C	5.47	115.16	108.11
21	o	159	GLU	N-CA-C	-5.46	104.98	111.69
26	1	1128	VAL	N-CA-C	5.46	117.91	111.09
3	E	237	SER	N-CA-C	5.45	117.93	110.24
13	r	49	HIS	N-CA-C	-5.45	106.71	113.19
42	A	1541	THR	N-CA-C	-5.45	105.42	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	H	157	G	P-O5'-C5'	-5.43	112.75	120.90
42	A	624	GLY	CA-C-N	-5.43	113.13	119.32
42	A	624	GLY	C-N-CA	-5.43	113.13	119.32
19	G	143	U	C4'-C3'-O3'	-5.43	104.86	113.00
34	K	209	SER	N-CA-C	5.43	117.00	111.14
21	o	40	THR	N-CA-C	-5.42	106.17	112.89
28	3	488	GLY	N-CA-C	-5.42	106.37	115.80
19	G	143	U	C2'-C3'-O3'	-5.40	105.60	113.70
24	v	163	ASP	N-CA-C	5.40	117.29	108.76
3	E	156	SER	N-CA-C	5.39	116.73	108.42
21	o	125	VAL	CA-C-N	5.39	128.05	120.28
21	o	125	VAL	C-N-CA	5.39	128.05	120.28
43	C	924	GLN	CA-C-N	5.39	125.33	119.78
43	C	924	GLN	C-N-CA	5.39	125.33	119.78
39	W	349	PHE	CA-C-N	5.38	131.82	121.54
39	W	349	PHE	C-N-CA	5.38	131.82	121.54
35	N	807	CYS	N-CA-C	5.37	121.68	109.81
42	A	1134	TRP	CA-C-N	5.37	125.31	119.78
42	A	1134	TRP	C-N-CA	5.37	125.31	119.78
24	v	199	TRP	N-CA-C	5.36	117.38	107.73
42	A	852	VAL	N-CA-C	5.35	117.55	111.88
43	C	653	ILE	N-CA-C	5.35	115.60	108.11
35	N	823	ARG	N-CA-C	-5.34	100.23	109.15
9	i	5	LYS	N-CA-C	5.34	118.01	111.82
41	X	461	ARG	N-CA-C	-5.34	106.72	113.18
42	A	2100	THR	N-CA-C	-5.34	106.77	113.28
42	A	1329	SER	N-CA-C	5.32	118.10	109.06
2	D	1228	VAL	N-CA-C	5.31	116.68	110.62
14	s	30	VAL	N-CA-C	5.31	116.20	111.90
42	A	1615	HIS	CA-C-N	5.31	125.63	119.47
42	A	1615	HIS	C-N-CA	5.31	125.63	119.47
43	C	651	ILE	N-CA-C	5.31	117.28	109.63
42	A	435	CYS	CA-C-N	-5.31	113.16	119.05
42	A	435	CYS	C-N-CA	-5.31	113.16	119.05
13	r	92	VAL	N-CA-C	5.30	115.92	109.30
34	K	446	PRO	N-CA-C	-5.30	101.56	112.47
26	1	718	PRO	CA-C-O	-5.29	114.28	120.85
42	A	132	ILE	CA-C-N	5.29	126.46	119.84
42	A	132	ILE	C-N-CA	5.29	126.46	119.84
43	C	535	ALA	N-CA-C	5.29	120.10	111.37
2	D	1127	CYS	CA-C-N	5.27	125.59	119.47
2	D	1127	CYS	C-N-CA	5.27	125.59	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	K	219	ARG	N-CA-C	5.27	120.72	113.97
2	D	811	SER	N-CA-C	5.27	115.09	108.45
2	D	2096	ALA	CA-C-N	5.27	125.47	120.31
2	D	2096	ALA	C-N-CA	5.27	125.47	120.31
28	3	4	TYR	N-CA-C	-5.26	102.49	110.28
38	O	130	VAL	N-CA-C	-5.26	101.02	108.65
39	W	307	SER	N-CA-C	5.26	122.00	110.80
39	W	394	ASP	CA-C-N	5.26	134.63	121.80
39	W	394	ASP	C-N-CA	5.26	134.63	121.80
42	A	1719	PHE	CA-C-N	-5.26	114.15	119.83
42	A	1719	PHE	C-N-CA	-5.26	114.15	119.83
39	W	193	LEU	CA-C-N	5.25	127.26	122.37
39	W	193	LEU	C-N-CA	5.25	127.26	122.37
43	C	559	ILE	N-CA-C	5.25	116.54	108.71
25	w	289	LYS	N-CA-C	5.25	121.97	110.80
22	p	20	LYS	N-CA-C	5.24	117.39	111.11
42	A	831	SER	N-CA-C	5.24	117.47	109.62
2	D	749	GLY	N-CA-C	-5.23	108.46	114.69
39	W	550	GLN	CA-C-N	-5.23	116.34	122.93
39	W	550	GLN	C-N-CA	-5.23	116.34	122.93
42	A	1852	LEU	CA-C-N	5.22	125.20	120.03
42	A	1852	LEU	C-N-CA	5.22	125.20	120.03
42	A	1365	ILE	CA-C-N	5.22	125.14	119.76
42	A	1365	ILE	C-N-CA	5.22	125.14	119.76
2	D	1693	ARG	CA-C-N	5.22	125.02	119.28
2	D	1693	ARG	C-N-CA	5.22	125.02	119.28
39	W	366	PRO	N-CA-C	5.21	119.38	111.19
21	o	146	ASP	CA-C-N	5.21	129.96	122.40
21	o	146	ASP	C-N-CA	5.21	129.96	122.40
2	D	488	LEU	N-CA-C	5.21	119.73	113.17
20	H	171	U	C2'-C3'-O3'	-5.19	105.92	113.70
34	K	449	GLN	N-CA-C	-5.18	101.32	109.50
18	z	69	VAL	N-CA-C	5.18	115.36	108.27
22	p	51	GLN	N-CA-C	5.18	117.54	109.52
13	r	44	HIS	N-CA-C	-5.17	107.03	113.55
2	D	1875	VAL	CA-C-N	5.17	124.62	119.24
2	D	1875	VAL	C-N-CA	5.17	124.62	119.24
34	K	452	VAL	N-CA-C	-5.17	101.53	108.35
20	H	170	C	O4'-C1'-C2'	-5.16	100.64	105.80
42	A	1963	GLU	CA-C-N	5.16	124.78	119.05
42	A	1963	GLU	C-N-CA	5.16	124.78	119.05
39	W	477	ASN	N-CA-C	5.16	120.71	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	C	556	ASP	N-CA-C	5.16	116.59	111.07
2	D	572	ASP	N-CA-C	-5.15	103.35	110.35
26	1	415	LEU	CA-C-N	5.15	125.68	120.38
26	1	415	LEU	C-N-CA	5.15	125.68	120.38
4	k	99	MET	N-CA-C	5.15	116.89	108.76
42	A	928	TYR	N-CA-C	-5.14	105.67	111.28
20	H	155	C	P-O3'-C3'	5.14	127.91	120.20
22	p	83	TYR	CA-C-O	-5.14	115.19	121.05
43	C	823	ALA	N-CA-C	5.14	117.56	109.39
37	M	85	SER	N-CA-C	5.13	116.78	108.41
43	C	667	VAL	N-CA-C	5.13	115.85	110.62
42	A	619	GLY	CA-C-N	5.12	124.74	119.05
42	A	619	GLY	C-N-CA	5.12	124.74	119.05
42	A	1451	ASN	N-CA-C	5.12	117.59	109.40
22	p	48	MET	N-CA-C	5.11	119.51	113.28
42	A	480	LYS	N-CA-C	5.10	118.97	112.34
39	W	306	CYS	CA-C-N	5.10	131.28	121.54
39	W	306	CYS	C-N-CA	5.10	131.28	121.54
42	A	316	PHE	CA-C-N	5.10	125.55	120.04
42	A	316	PHE	C-N-CA	5.10	125.55	120.04
34	K	332	HIS	CA-C-N	-5.09	113.40	119.05
34	K	332	HIS	C-N-CA	-5.09	113.40	119.05
27	2	498	VAL	N-CA-C	5.08	113.43	107.89
21	o	90	LEU	CA-C-O	-5.07	113.25	120.51
21	o	83	LEU	N-CA-C	5.07	117.47	111.33
21	o	90	LEU	O-C-N	5.07	129.33	122.59
28	3	445	SER	N-CA-C	-5.07	103.99	110.53
20	H	160	A	N9-C1'-C2'	5.06	119.59	112.00
36	L	122	PHE	CA-C-N	5.06	124.85	119.28
36	L	122	PHE	C-N-CA	5.06	124.85	119.28
39	W	430	TYR	N-CA-C	5.05	117.70	110.68
35	N	773	ASN	CA-C-N	5.04	126.14	119.84
35	N	773	ASN	C-N-CA	5.04	126.14	119.84
35	N	916	SER	N-CA-C	5.04	116.78	111.28
28	3	9	GLN	N-CA-C	-5.04	101.54	109.25
11	F	51	U	C2'-C3'-O3'	-5.04	106.14	113.70
35	N	417	GLU	CA-C-N	5.04	128.66	120.60
35	N	417	GLU	C-N-CA	5.04	128.66	120.60
21	o	81	GLU	N-CA-C	5.04	118.58	112.23
39	W	264	ARG	CA-C-N	5.03	125.56	120.38
39	W	264	ARG	C-N-CA	5.03	125.56	120.38
25	w	276	GLY	N-CA-C	-5.02	108.33	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	574	GLN	N-CA-C	5.02	117.86	111.69
21	o	28	GLY	N-CA-C	5.01	120.79	113.48
20	H	156	U	C4'-C3'-C2'	5.01	107.61	102.60
26	1	718	PRO	N-CA-C	5.01	118.42	110.21
25	w	274	CYS	N-CA-C	5.00	116.54	111.14
42	A	1307	MET	CA-C-N	-5.00	113.59	119.84
42	A	1307	MET	C-N-CA	-5.00	113.59	119.84
22	p	38	VAL	O-C-N	5.00	126.98	121.83

There are no chirality outliers.

All (108) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	1	1025	LYS	Peptide
26	1	110	PRO	Peptide
26	1	1122	THR	Peptide
26	1	1127	THR	Peptide
26	1	1179	ASP	Peptide
26	1	1199	VAL	Peptide
26	1	220	GLN	Peptide
26	1	257	THR	Peptide
26	1	415	LEU	Peptide,Mainchain
26	1	545	GLU	Peptide
26	1	689	ILE	Peptide
26	1	717	THR	Peptide
26	1	941	ASN	Peptide
26	1	944	SER	Peptide
27	2	553	MET	Peptide
27	2	558	ARG	Peptide
28	3	261	PHE	Peptide
28	3	366	ASP	Peptide
28	3	468	ASP	Peptide
28	3	530	ASP	Peptide
28	3	534	ASN	Peptide
28	3	552	ARG	Peptide
28	3	670	GLN	Peptide
28	3	678	VAL	Peptide
28	3	74	THR	Peptide
28	3	885	ASN	Peptide
28	3	916	ASN	Peptide
28	3	980	LYS	Peptide
28	3	986	ILE	Peptide

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Mol	Chain	Res	Type	Group
30	5	29	LYS	Peptide
31	6	89	VAL	Peptide
31	6	91	LEU	Peptide
32	7	74	GLN	Peptide
43	C	736	GLY	Peptide
2	D	430	LEU	Peptide
34	K	374	HIS	Peptide
35	N	14	PRO	Peptide
35	N	773	ASN	Peptide,Mainchain
35	N	807	CYS	Peptide,Mainchain
35	N	838	GLU	Peptide
39	W	103	ARG	Peptide,Mainchain
39	W	105	CYS	Peptide
39	W	121	GLU	Peptide
39	W	144	GLN	Peptide
39	W	175	LEU	Peptide
39	W	193	LEU	Peptide
39	W	203	ALA	Peptide
39	W	205	LEU	Peptide
39	W	206	ASP	Peptide
39	W	207	LYS	Peptide
39	W	218	THR	Peptide
39	W	258	ASN	Peptide
39	W	267	GLY	Peptide
39	W	269	ILE	Peptide
39	W	270	MET	Peptide
39	W	308	LYS	Peptide
39	W	309	LYS	Peptide
39	W	310	THR	Peptide
39	W	315	LYS	Peptide
39	W	333	ALA	Peptide
39	W	346	THR	Peptide
39	W	356	PHE	Peptide
39	W	357	THR	Peptide
39	W	360	LEU	Peptide
39	W	362	HIS	Peptide
39	W	363	PRO	Peptide
39	W	364	ASP	Peptide
39	W	381	GLU	Peptide
39	W	384	VAL	Peptide
39	W	396	PRO	Peptide
39	W	403	ASP	Peptide

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Mol	Chain	Res	Type	Group
39	W	404	GLU	Peptide
39	W	405	LYS	Peptide
39	W	409	ILE	Peptide
39	W	412	GLN	Peptide
39	W	413	VAL	Peptide
39	W	414	PRO	Peptide
39	W	417	ASN	Peptide
39	W	419	LEU	Peptide
39	W	445	LYS	Peptide
39	W	446	LEU	Peptide
39	W	448	PRO	Peptide
39	W	456	ARG	Peptide
39	W	462	PHE	Peptide
39	W	464	VAL	Peptide
39	W	476	THR	Peptide
39	W	478	VAL	Peptide
39	W	479	ASP	Peptide
39	W	481	ARG	Peptide
39	W	482	GLU	Peptide
39	W	483	TYR	Peptide
39	W	486	GLU	Peptide
39	W	494	ASN	Peptide
39	W	511	GLU	Peptide
39	W	512	GLY	Peptide
39	W	528	GLU	Peptide
39	W	554	ARG	Peptide
39	W	556	ASP	Peptide
39	W	558	ASP	Peptide
39	W	559	GLU	Peptide
39	W	561	ASN	Peptide
4	k	112	ASN	Peptide
25	w	443	THR	Peptide
16	x	51	TYR	Peptide

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	B	2419	0	1224	61	0
2	D	7496	0	1961	22	0
3	E	1196	0	337	2	0
4	P	300	0	80	10	0
4	a	318	0	86	0	0
4	k	340	0	87	0	0
5	Q	292	0	93	1	0
5	b	300	0	95	0	0
5	m	296	0	87	0	0
6	R	314	0	86	0	0
6	c	314	0	86	0	0
6	l	316	0	85	1	0
7	S	298	0	89	1	0
7	d	282	0	85	0	0
7	n	272	0	75	1	0
8	T	288	0	84	0	0
8	e	318	0	92	0	0
8	h	320	0	88	0	0
9	U	256	0	70	3	0
9	f	260	0	74	2	0
9	i	292	0	80	0	0
10	V	334	0	92	16	0
10	g	380	0	103	0	0
10	j	328	0	89	0	0
11	F	1470	0	745	49	0
12	q	360	0	95	3	0
13	r	300	0	77	6	0
14	s	296	0	77	0	0
15	t	300	0	80	1	0
16	x	280	0	81	3	0
17	y	260	0	75	0	0
18	z	244	0	71	1	0
19	G	862	0	441	140	0
20	H	2311	0	1170	154	0
21	o	648	0	167	1	0
22	p	376	0	102	0	0
23	u	496	0	118	1	0
24	v	396	0	91	0	0
25	w	1773	0	477	27	0
26	1	4120	0	1091	239	0
27	2	744	0	189	6	0
28	3	4696	0	1266	69	0
29	4	312	0	87	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	5	432	0	114	7	0
31	6	356	0	105	5	0
32	7	264	0	70	11	0
33	J	668	0	179	8	0
34	K	1371	0	384	17	0
35	N	2316	0	581	46	0
36	L	904	0	235	2	0
37	M	500	0	128	4	0
38	O	556	0	147	2	0
39	W	1852	0	477	34	0
40	I	2491	0	1262	118	0
41	X	1661	0	440	0	0
42	A	8884	0	2284	159	0
43	C	3272	0	874	51	0
44	A	36	0	6	0	0
45	C	32	0	12	4	0
46	C	1	0	0	0	0
All	All	63369	0	19126	1151	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 14.

All (1151) 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)
19:G:145:U:C2'	19:G:146:C:H5''	1.54	1.37
33:J:536:ASP:CA	33:J:587:GLY:CA	2.11	1.28
43:C:470:PRO:CA	43:C:499:GLY:HA2	1.64	1.27
40:I:63:U:H2'	40:I:64:G:C8	1.69	1.26
33:J:536:ASP:CA	33:J:587:GLY:HA3	1.64	1.25
39:W:341:LYS:CA	39:W:359:LYS:H	1.51	1.24
20:H:46:U:C6	25:w:395:TRP:CA	2.21	1.23
19:G:135:G:N2	20:H:42:G:C4	2.07	1.21
19:G:153:C:H4'	19:G:154:U:OP1	1.42	1.18
19:G:145:U:C4	19:G:146:C:C5	2.32	1.18
19:G:137:C:O2'	19:G:138:A:H5'	1.45	1.15
19:G:149:G:C8	19:G:150:U:C5	2.34	1.15
33:J:536:ASP:CA	33:J:587:GLY:N	2.10	1.15
19:G:145:U:H2'	19:G:146:C:C5'	1.78	1.14
40:I:51:A:O2'	40:I:56:U:H5''	1.46	1.14
20:H:46:U:C5	25:w:395:TRP:CA	2.31	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:H:46:U:C2	25:w:395:TRP:CA	2.31	1.14
42:A:398:THR:CA	43:C:386:GLY:HA2	1.79	1.11
42:A:1458:GLN:O	42:A:1462:GLY:CA	1.99	1.11
20:H:156:U:H6	20:H:156:U:H5''	1.10	1.09
43:C:665:THR:O	43:C:826:ARG:CA	2.00	1.08
39:W:344:ILE:C	39:W:360:LEU:CA	2.26	1.07
42:A:1833:LEU:O	42:A:1837:ALA:N	1.86	1.07
19:G:145:U:C3'	19:G:146:C:H5''	1.84	1.07
40:I:119:A:N3	4:P:103:GLY:O	1.87	1.06
19:G:145:U:O4	19:G:146:C:C4	2.09	1.06
34:K:250:CYS:N	34:K:253:GLY:O	1.88	1.06
42:A:1458:GLN:O	42:A:1462:GLY:N	1.88	1.05
20:H:46:U:C4	25:w:395:TRP:CA	2.40	1.05
40:I:119:A:N3	4:P:103:GLY:C	2.14	1.05
20:H:46:U:N1	25:w:395:TRP:CA	2.21	1.04
40:I:126:A:N1	10:V:65:ILE:O	1.91	1.04
11:F:59:G:H1'	40:I:21:U:H4'	1.41	1.03
19:G:155:U:H4'	19:G:156:U:H5'	1.38	1.03
19:G:149:G:C8	19:G:150:U:C4	2.47	1.02
11:F:59:G:H5'	40:I:22:C:H5''	1.36	1.02
19:G:145:U:H2'	19:G:146:C:H5''	1.03	1.01
19:G:135:G:N2	20:H:42:G:N3	2.06	1.01
20:H:46:U:C6	25:w:395:TRP:N	2.29	1.01
33:J:536:ASP:CA	33:J:587:GLY:H	1.72	1.01
20:H:46:U:N1	25:w:395:TRP:N	2.09	1.00
26:1:102:ASP:O	26:1:105:ALA:N	1.94	1.00
19:G:145:U:C3'	19:G:146:C:C5'	2.39	0.99
40:I:60:A:H2'	40:I:61:A:H1'	1.40	0.99
35:N:901:CYS:O	35:N:905:GLU:CA	2.09	0.99
43:C:776:GLU:O	43:C:781:ASP:C	2.06	0.99
40:I:127:C:H1'	10:V:21:ASN:CA	1.91	0.99
40:I:58:C:O2'	40:I:59:U:C5'	2.10	0.99
40:I:91:A:H2	40:I:110:G:N2	1.61	0.99
35:N:560:ARG:O	35:N:564:ALA:C	2.06	0.98
19:G:146:C:C2	20:H:33:G:N1	2.32	0.97
19:G:135:G:N3	20:H:42:G:C2	2.33	0.97
42:A:1519:THR:O	42:A:1521:ALA:N	1.96	0.97
26:1:501:LEU:O	26:1:504:ILE:N	1.98	0.97
40:I:58:C:H2'	40:I:59:U:O5'	1.65	0.96
19:G:143:U:H6	19:G:143:U:H5'	1.30	0.96
42:A:1458:GLN:O	42:A:1462:GLY:HA2	1.64	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:G:146:C:C2	20:H:33:G:C6	2.53	0.96
34:K:251:TRP:O	34:K:275:ASN:CA	2.14	0.95
19:G:145:U:C2'	19:G:146:C:C5'	2.38	0.95
42:A:378:PHE:O	43:C:355:LYS:CA	2.14	0.95
39:W:345:VAL:N	39:W:360:LEU:N	2.15	0.95
35:N:901:CYS:O	35:N:905:GLU:N	2.01	0.94
11:F:71:G:H1	40:I:4:U:H3	0.98	0.94
34:K:494:LYS:O	34:K:512:TYR:N	2.01	0.94
20:H:156:U:H5''	20:H:156:U:C6	2.02	0.94
19:G:146:C:O2	20:H:33:G:C6	2.20	0.94
42:A:1784:ASN:C	42:A:1806:ALA:O	2.12	0.93
11:F:52:U:H5''	11:F:52:U:H6	1.34	0.93
19:G:135:G:C2	20:H:42:G:C2	2.57	0.93
35:N:354:PRO:O	35:N:356:ASP:N	2.02	0.92
20:H:46:U:N3	25:w:395:TRP:CA	2.32	0.92
16:x:45:LEU:O	16:x:63:ALA:CA	2.18	0.92
1:B:94:U:H1'	1:B:95:G:OP1	1.70	0.92
40:I:63:U:H2'	40:I:64:G:H8	1.13	0.91
1:B:12:U:H3	1:B:65:G:H1	1.12	0.91
42:A:1785:VAL:CA	42:A:1806:ALA:O	2.18	0.91
42:A:1676:ILE:O	42:A:1679:TYR:N	2.03	0.91
35:N:560:ARG:O	35:N:564:ALA:N	2.04	0.91
35:N:375:ILE:O	35:N:377:ILE:N	2.03	0.91
40:I:58:C:C2'	40:I:59:U:O5'	2.15	0.90
19:G:143:U:H5'	19:G:143:U:C6	2.06	0.90
39:W:341:LYS:CA	39:W:359:LYS:N	2.34	0.90
40:I:119:A:N3	4:P:103:GLY:CA	2.35	0.90
42:A:398:THR:CA	43:C:386:GLY:CA	2.49	0.89
19:G:149:G:N7	19:G:150:U:C4	2.40	0.89
26:1:793:LYS:O	26:1:797:GLY:HA3	1.72	0.89
42:A:711:GLN:O	42:A:715:GLU:N	2.05	0.89
19:G:155:U:O2'	19:G:156:U:OP2	1.89	0.89
42:A:379:GLU:O	43:C:355:LYS:N	2.07	0.88
42:A:109:PRO:O	42:A:191:ILE:N	2.06	0.88
19:G:145:U:H3'	19:G:146:C:C5'	2.04	0.88
42:A:733:THR:C	42:A:735:ILE:H	1.78	0.88
42:A:941:LYS:N	42:A:1090:ARG:O	2.07	0.88
35:N:560:ARG:O	35:N:564:ALA:CA	2.23	0.86
40:I:58:C:O2'	40:I:59:U:H5'	1.73	0.86
20:H:154:C:O2	20:H:176:G:N2	2.07	0.86
11:F:59:G:H5'	40:I:22:C:C5'	2.05	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:A:1520:ASN:O	42:A:1523:ARG:N	2.08	0.86
35:N:160:ILE:CA	42:A:730:GLY:O	2.24	0.86
19:G:153:C:OP1	19:G:154:U:P	2.34	0.86
20:H:40:C:H5''	20:H:40:C:H6	1.39	0.86
40:I:63:U:C2'	40:I:64:G:H8	1.89	0.85
40:I:21:U:O2'	40:I:22:C:H5'	1.75	0.85
39:W:334:LEU:C	39:W:340:LYS:CA	2.50	0.85
42:A:197:PRO:O	42:A:201:ALA:CA	2.24	0.85
20:H:156:U:H6	20:H:156:U:C5'	1.88	0.85
34:K:494:LYS:O	34:K:512:TYR:CA	2.25	0.85
20:H:46:U:H1'	25:w:394:TYR:C	2.02	0.85
26:1:728:LEU:O	26:1:731:LEU:N	2.10	0.84
40:I:59:U:O2'	40:I:60:A:O5'	1.95	0.84
42:A:973:CYS:N	42:A:1101:PHE:O	2.11	0.83
19:G:151:C:H1'	19:G:152:C:OP1	1.78	0.83
40:I:58:C:C2'	40:I:59:U:C5'	2.57	0.83
19:G:151:C:H4'	19:G:152:C:H5	1.44	0.83
42:A:1785:VAL:N	42:A:1806:ALA:O	2.11	0.82
40:I:62:U:H2'	40:I:63:U:H6	1.44	0.82
20:H:152:G:N2	20:H:153:A:N7	2.27	0.82
19:G:145:U:C5	19:G:146:C:C5	2.66	0.82
19:G:146:C:O2	20:H:33:G:N1	2.13	0.82
26:1:406:ALA:O	30:5:98:PHE:CA	2.28	0.82
20:H:152:G:H5''	20:H:153:A:OP2	1.80	0.82
19:G:135:G:C2	20:H:42:G:C4	2.68	0.81
26:1:648:LEU:O	26:1:651:VAL:N	2.13	0.81
43:C:470:PRO:CA	43:C:499:GLY:CA	2.54	0.81
19:G:145:U:C4	19:G:146:C:C4	2.63	0.81
20:H:46:U:O2'	25:w:394:TYR:N	2.12	0.81
40:I:108:C:O2'	40:I:109:G:H5'	1.81	0.81
29:4:77:ILE:O	29:4:84:ILE:N	2.14	0.81
35:N:142:PHE:O	35:N:145:LEU:N	2.14	0.81
42:A:1125:ILE:O	42:A:1126:VAL:C	2.24	0.81
31:6:56:GLY:O	31:6:65:GLY:N	2.12	0.81
42:A:929:GLU:O	42:A:933:ARG:N	2.13	0.81
19:G:149:G:C2	19:G:150:U:H2'	2.16	0.80
20:H:165:A:O2'	20:H:166:G:H5'	1.81	0.80
19:G:149:G:N9	19:G:150:U:C5	2.49	0.80
43:C:827:LEU:O	43:C:906:ILE:CA	2.30	0.80
42:A:712:HIS:O	42:A:716:ALA:N	2.13	0.80
40:I:119:A:C2	4:P:103:GLY:O	2.34	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:570:THR:CA	42:A:2335:ALA:O	2.29	0.80
28:3:523:GLY:HA3	28:3:536:TRP:O	1.83	0.79
39:W:345:VAL:N	39:W:360:LEU:H	1.81	0.79
42:A:973:CYS:O	42:A:1101:PHE:N	2.13	0.79
1:B:17:U:H3	1:B:60:G:H1	0.83	0.79
11:F:52:U:H5''	11:F:52:U:C6	2.17	0.79
19:G:147:C:O2	20:H:31:G:N1	2.11	0.79
20:H:177:A:H5''	20:H:178:A:OP1	1.84	0.78
42:A:80:LYS:C	42:A:82:ARG:H	1.92	0.78
26:1:669:GLN:O	26:1:672:ALA:N	2.16	0.78
11:F:59:G:H4'	40:I:22:C:OP1	1.84	0.78
19:G:149:G:H2'	19:G:150:U:C6	2.19	0.77
26:1:428:ALA:O	26:1:432:THR:N	2.17	0.77
40:I:126:A:H2	10:V:64:ASN:C	1.93	0.77
19:G:146:C:H1'	20:H:33:G:N2	1.99	0.77
20:H:101:U:H5''	20:H:102:U:H5'	1.64	0.77
19:G:151:C:H4'	19:G:152:C:C5	2.18	0.77
11:F:59:G:C1'	40:I:21:U:H4'	2.14	0.77
28:3:839:ALA:O	28:3:843:LEU:N	2.13	0.77
19:G:146:C:O2	20:H:33:G:C2	2.37	0.77
40:I:127:C:H1'	10:V:21:ASN:C	2.08	0.77
20:H:46:U:C1'	25:w:395:TRP:N	2.48	0.77
19:G:145:U:H3	20:H:33:G:H1	1.33	0.77
19:G:155:U:H4'	19:G:156:U:C5'	2.13	0.77
42:A:908:VAL:CA	42:A:1445:TYR:O	2.33	0.77
19:G:146:C:H1'	20:H:33:G:C2	2.20	0.76
19:G:135:G:C2	20:H:42:G:N3	2.52	0.76
39:W:344:ILE:C	39:W:360:LEU:N	2.40	0.76
40:I:58:C:H2'	40:I:59:U:C5'	2.14	0.76
11:F:52:U:H6	11:F:52:U:C5'	1.97	0.76
26:1:102:ASP:O	26:1:105:ALA:CA	2.34	0.76
19:G:132:G:H1	20:H:44:U:H3	1.33	0.76
20:H:143:A:H3'	20:H:143:A:N3	2.01	0.76
20:H:153:A:H2'	20:H:154:C:H5'	1.65	0.76
40:I:62:U:H2'	40:I:63:U:C6	2.21	0.76
11:F:102:A:H2'	11:F:103:U:H5'	1.68	0.76
43:C:683:ASN:CA	43:C:795:VAL:O	2.34	0.76
42:A:630:TRP:O	42:A:632:ALA:N	2.18	0.76
19:G:149:G:H3'	19:G:150:U:H5''	1.67	0.76
25:w:276:GLY:C	25:w:278:LEU:H	1.92	0.76
26:1:1016:LEU:O	26:1:1019:ARG:N	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:W:340:LYS:O	39:W:358:LYS:CA	2.34	0.75
42:A:708:THR:O	42:A:711:GLN:N	2.19	0.75
11:F:59:G:C5'	40:I:22:C:H5''	2.15	0.75
2:D:282:SER:O	2:D:286:ALA:N	2.18	0.75
40:I:91:A:H2	40:I:110:G:H22	0.83	0.75
42:A:1702:LEU:O	42:A:1714:ALA:CA	2.34	0.75
19:G:149:G:H2'	19:G:150:U:H6	1.52	0.75
40:I:126:A:H2	10:V:64:ASN:O	1.70	0.75
26:1:1246:MET:O	26:1:1249:TYR:N	2.18	0.74
12:q:72:LEU:O	13:r:83:PRO:CA	2.36	0.74
42:A:1833:LEU:O	42:A:1837:ALA:CA	2.36	0.74
26:1:874:LYS:O	26:1:877:GLY:N	2.20	0.74
1:B:48:A:P	42:A:280:GLU:H	2.11	0.74
1:B:95:G:H5'	1:B:96:A:OP2	1.87	0.74
19:G:153:C:OP1	19:G:154:U:OP1	2.05	0.74
20:H:153:A:C2'	20:H:154:C:H5'	2.17	0.74
42:A:84:ASP:O	42:A:88:TYR:N	2.20	0.74
42:A:317:PRO:O	42:A:321:ASN:O	2.05	0.74
28:3:442:LEU:O	28:3:735:SER:N	2.19	0.74
40:I:51:A:HO2'	40:I:56:U:H5''	1.52	0.74
40:I:119:A:C4	4:P:103:GLY:HA3	2.22	0.74
43:C:143:THR:CA	45:C:1500:GTP:O1B	2.36	0.74
1:B:26:A:C5	42:A:423:ASP:CA	2.71	0.74
1:B:26:A:H5''	1:B:26:A:N3	2.02	0.74
25:w:276:GLY:O	25:w:278:LEU:N	2.20	0.73
28:3:304:GLN:CA	28:3:309:ASP:O	2.36	0.73
28:3:753:GLY:HA3	28:3:765:LEU:O	1.88	0.73
42:A:1500:GLY:O	42:A:1756:SER:CA	2.37	0.73
26:1:1270:ASN:O	26:1:1273:TYR:N	2.21	0.73
42:A:441:VAL:O	42:A:444:ARG:N	2.21	0.73
20:H:153:A:H2'	20:H:154:C:C5'	2.19	0.73
19:G:136:U:H1'	19:G:137:C:OP1	1.89	0.72
19:G:146:C:O2	20:H:33:G:C5	2.41	0.72
26:1:994:LEU:O	26:1:997:LEU:N	2.22	0.72
42:A:733:THR:O	42:A:735:ILE:N	2.21	0.72
26:1:660:ALA:O	26:1:663:THR:N	2.22	0.72
28:3:380:GLU:O	28:3:383:ASP:N	2.22	0.72
40:I:127:C:O2	10:V:21:ASN:O	2.08	0.72
40:I:58:C:C2'	40:I:59:U:H5'	2.20	0.72
26:1:531:LEU:O	26:1:534:GLN:N	2.18	0.72
42:A:186:GLU:O	42:A:565:ARG:O	2.08	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:G:145:U:C4	19:G:146:C:C6	2.77	0.72
20:H:46:U:H1'	25:w:394:TYR:CA	2.20	0.72
26:1:1055:TRP:O	26:1:1058:ILE:N	2.22	0.71
42:A:1519:THR:O	42:A:1520:ASN:C	2.31	0.71
26:1:535:ILE:O	26:1:538:LEU:N	2.23	0.71
42:A:470:ARG:O	42:A:472:LEU:N	2.23	0.71
26:1:122:HIS:O	26:1:125:THR:N	2.22	0.71
1:B:26:A:N3	1:B:26:A:H3'	2.05	0.71
42:A:471:TYR:O	42:A:474:ARG:N	2.24	0.71
26:1:700:LYS:O	26:1:703:THR:N	2.24	0.71
19:G:153:C:OP1	19:G:154:U:OP2	2.09	0.70
26:1:791:VAL:O	26:1:794:GLN:N	2.23	0.70
42:A:733:THR:C	42:A:735:ILE:N	2.49	0.70
11:F:102:A:C2'	11:F:103:U:H5'	2.21	0.70
42:A:1520:ASN:O	42:A:1522:GLN:N	2.24	0.70
40:I:59:U:HO2'	40:I:60:A:P	2.13	0.70
19:G:134:U:H3	20:H:42:G:H1	1.37	0.70
20:H:154:C:H2'	20:H:155:C:C6	2.27	0.70
42:A:114:ARG:O	42:A:489:TRP:N	2.25	0.70
43:C:909:GLY:HA3	43:C:930:ALA:H	1.56	0.70
40:I:21:U:H2'	40:I:22:C:H6	1.57	0.70
42:A:939:TRP:O	42:A:1090:ARG:N	2.17	0.70
20:H:153:A:N6	20:H:177:A:C2	2.60	0.69
20:H:168:A:C8	20:H:168:A:H5''	2.27	0.69
16:x:45:LEU:O	16:x:63:ALA:N	2.24	0.69
42:A:441:VAL:O	42:A:442:LYS:C	2.36	0.69
11:F:86:U:H3	20:H:12:G:H1	1.39	0.69
20:H:30:A:N3	20:H:30:A:H2'	2.06	0.69
42:A:331:TRP:O	43:C:177:ARG:O	2.10	0.69
42:A:930:ALA:O	42:A:934:ARG:O	2.10	0.69
27:2:479:ASP:O	27:2:482:ALA:N	2.25	0.69
42:A:930:ALA:O	42:A:934:ARG:N	2.25	0.69
2:D:159:LEU:O	2:D:162:GLY:N	2.24	0.69
20:H:150:U:H3	20:H:181:G:H1	1.41	0.69
28:3:545:VAL:N	28:3:557:ALA:O	2.25	0.69
35:N:361:VAL:O	35:N:365:ALA:N	2.26	0.69
42:A:61:MET:N	42:A:484:SER:O	2.26	0.69
42:A:1676:ILE:O	42:A:1677:GLU:C	2.33	0.69
20:H:40:C:H6	20:H:40:C:C5'	2.05	0.69
20:H:180:G:H2'	20:H:181:G:H8	1.57	0.69
40:I:119:A:C2	4:P:103:GLY:CA	2.76	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:C:776:GLU:O	43:C:781:ASP:CA	2.40	0.68
35:N:154:GLU:O	42:A:700:GLY:HA3	1.94	0.68
39:W:166:ASN:O	39:W:169:THR:O	2.11	0.68
40:I:63:U:C2'	40:I:64:G:C8	2.61	0.68
42:A:1125:ILE:O	42:A:1128:TYR:N	2.21	0.68
19:G:137:C:HO2'	19:G:138:A:H5'	1.54	0.68
39:W:335:GLY:N	39:W:340:LYS:CA	2.56	0.68
42:A:80:LYS:O	42:A:82:ARG:N	2.25	0.68
11:F:49:G:H1	40:I:63:U:H3	1.41	0.68
42:A:397:ASN:C	43:C:386:GLY:O	2.37	0.68
28:3:558:LEU:O	28:3:561:GLY:N	2.24	0.68
40:I:127:C:H1'	10:V:21:ASN:O	1.93	0.68
11:F:73:A:N1	40:I:2:G:O6	2.27	0.68
20:H:143:A:H2'	20:H:144:C:H6	1.59	0.68
20:H:152:G:O3'	20:H:153:A:O4'	2.11	0.68
42:A:570:ASP:O	42:A:572:PHE:N	2.26	0.67
19:G:146:C:H6	19:G:146:C:H5'	1.58	0.67
19:G:151:C:C4'	19:G:152:C:H5	2.07	0.67
40:I:24:U:H3	40:I:48:G:H1	1.42	0.67
40:I:21:U:H2'	40:I:22:C:C6	2.29	0.67
40:I:60:A:H2'	40:I:61:A:C1'	2.20	0.67
40:I:55:U:H5'	40:I:56:U:OP2	1.93	0.67
43:C:474:LEU:CA	43:C:498:SER:O	2.42	0.67
20:H:106:G:H21	20:H:107:A:N6	1.92	0.67
27:2:487:LEU:O	27:2:490:HIS:N	2.28	0.67
40:I:126:A:N1	10:V:65:ILE:C	2.53	0.67
20:H:151:C:H2'	20:H:152:G:H8	1.60	0.67
42:A:1519:THR:C	42:A:1521:ALA:N	2.53	0.66
20:H:151:C:O2	20:H:152:G:C8	2.48	0.66
42:A:471:TYR:O	42:A:472:LEU:C	2.38	0.66
2:D:166:ASP:O	2:D:169:TYR:N	2.26	0.66
40:I:20:A:H2'	40:I:21:U:C6	2.31	0.66
19:G:147:C:OP2	19:G:147:C:H3'	1.96	0.66
40:I:119:A:N3	4:P:103:GLY:HA3	2.09	0.66
20:H:151:C:C2	20:H:152:G:C8	2.83	0.66
20:H:153:A:C3'	20:H:154:C:H5'	2.25	0.66
28:3:753:GLY:CA	28:3:765:LEU:O	2.44	0.66
42:A:1539:SER:O	42:A:1543:ASN:N	2.17	0.66
34:K:251:TRP:O	34:K:274:THR:O	2.13	0.66
19:G:128:U:H6	19:G:128:U:O5'	1.78	0.65
11:F:59:G:H4'	40:I:22:C:P	2.37	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:G:127:U:O2'	19:G:128:U:O4'	2.13	0.65
26:1:1243:PRO:O	26:1:1246:MET:N	2.29	0.65
27:2:491:LEU:O	27:2:494:THR:N	2.30	0.65
40:I:6:U:H2'	40:I:7:G:H8	1.62	0.65
42:A:1110:ILE:O	42:A:1114:LEU:N	2.29	0.65
35:N:161:PRO:N	42:A:730:GLY:O	2.29	0.65
1:B:58:U:H2'	1:B:59:G:H8	1.62	0.65
1:B:78:U:O2'	1:B:80:U:OP1	2.13	0.65
39:W:344:ILE:C	39:W:360:LEU:H	2.03	0.65
19:G:137:C:H6	19:G:137:C:O5'	1.78	0.65
26:1:886:HIS:O	26:1:889:GLU:N	2.30	0.65
40:I:111:C:H6	40:I:111:C:O5'	1.78	0.65
19:G:151:C:H1'	19:G:152:C:P	2.36	0.65
42:A:543:ALA:O	42:A:547:CYS:N	2.17	0.65
19:G:151:C:C4'	19:G:152:C:C5	2.79	0.65
20:H:153:A:H3'	20:H:154:C:H5'	1.79	0.65
28:3:1148:LEU:O	28:3:1152:HIS:N	2.27	0.65
42:A:441:VAL:O	42:A:443:VAL:N	2.30	0.65
39:W:344:ILE:O	39:W:360:LEU:CA	2.44	0.64
1:B:97:G:H1	1:B:116:U:H3	1.44	0.64
39:W:341:LYS:C	39:W:359:LYS:H	2.04	0.64
40:I:117:C:H6	40:I:117:C:O5'	1.80	0.64
26:1:758:ASP:O	26:1:762:ALA:N	2.28	0.64
28:3:868:VAL:O	28:3:877:LEU:N	2.30	0.64
39:W:338:LYS:O	39:W:339:LYS:C	2.37	0.64
19:G:146:C:N3	20:H:33:G:C6	2.66	0.64
26:1:1280:LEU:O	26:1:1283:HIS:N	2.22	0.64
19:G:153:C:C4'	19:G:154:U:OP1	2.35	0.64
26:1:749:ALA:O	26:1:752:TYR:N	2.31	0.64
40:I:51:A:O2'	40:I:56:U:C5'	2.35	0.64
26:1:1018:PRO:O	26:1:1021:THR:N	2.30	0.64
42:A:1438:VAL:O	42:A:1442:PHE:N	2.31	0.64
26:1:658:TRP:O	26:1:661:ARG:N	2.30	0.63
32:7:40:TYR:O	32:7:43:TYR:N	2.31	0.63
19:G:145:U:O4	19:G:146:C:N4	2.31	0.63
19:G:150:U:OP1	31:6:63:GLY:HA3	1.98	0.63
33:J:658:ARG:O	33:J:662:LYS:N	2.31	0.63
34:K:248:THR:O	34:K:254:LEU:CA	2.46	0.63
34:K:338:LEU:O	34:K:350:TRP:N	2.29	0.63
42:A:1784:ASN:O	42:A:1806:ALA:N	2.30	0.63
20:H:152:G:C2	20:H:153:A:C5	2.87	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:3:931:VAL:O	28:3:936:LYS:N	2.31	0.63
20:H:147:G:H2'	20:H:148:C:H6	1.63	0.63
26:1:1264:VAL:O	26:1:1267:LYS:N	2.32	0.63
42:A:80:LYS:C	42:A:82:ARG:N	2.54	0.63
19:G:135:G:H5'	19:G:136:U:OP2	1.99	0.63
20:H:114:A:H61	20:H:142:C:H42	1.44	0.63
28:3:325:ILE:O	28:3:375:SER:N	2.30	0.63
40:I:89:U:C2'	40:I:90:G:H5'	2.29	0.63
40:I:126:A:C2	10:V:20:LYS:CA	2.82	0.63
42:A:1784:ASN:O	42:A:1806:ALA:O	2.16	0.63
19:G:137:C:C2'	19:G:138:A:H5'	2.28	0.63
40:I:89:U:O2'	40:I:90:G:H5'	1.99	0.63
42:A:1125:ILE:O	42:A:1127:GLY:N	2.31	0.62
20:H:106:G:H4'	20:H:107:A:O4'	1.99	0.62
1:B:98:G:H2'	1:B:99:C:C6	2.34	0.62
19:G:127:U:OP2	19:G:127:U:H2'	1.99	0.62
19:G:146:C:C2	19:G:147:C:C5	2.87	0.62
26:1:914:PHE:O	26:1:917:VAL:N	2.32	0.62
40:I:91:A:O5'	40:I:91:A:H8	1.82	0.62
26:1:179:GLY:O	26:1:182:LYS:N	2.33	0.62
35:N:410:ALA:O	35:N:413:LEU:N	2.33	0.62
42:A:542:ASN:O	42:A:546:LEU:N	2.30	0.62
20:H:154:C:H2'	20:H:155:C:H6	1.63	0.62
35:N:828:THR:O	35:N:831:VAL:N	2.31	0.62
42:A:371:LEU:CA	43:C:341:LYS:O	2.47	0.62
20:H:157:G:H8	20:H:157:G:H5''	1.65	0.62
28:3:973:GLY:HA3	28:3:976:LYS:O	2.00	0.62
19:G:146:C:O2'	19:G:147:C:H5'	2.00	0.62
28:3:1191:LYS:O	28:3:1194:SER:N	2.32	0.62
1:B:98:G:H2'	1:B:99:C:H6	1.65	0.62
20:H:46:U:H1'	25:w:395:TRP:N	2.14	0.62
42:A:379:GLU:C	43:C:355:LYS:CA	2.73	0.62
11:F:49:G:H2'	11:F:50:A:H8	1.64	0.61
19:G:150:U:H4'	19:G:151:C:OP2	1.98	0.61
40:I:119:A:C2	4:P:103:GLY:HA2	2.35	0.61
19:G:146:C:C2'	19:G:147:C:H5'	2.30	0.61
20:H:143:A:H2'	20:H:144:C:C6	2.35	0.61
40:I:108:C:H2'	40:I:109:G:H8	1.63	0.61
19:G:155:U:H5''	19:G:156:U:H5''	1.83	0.61
26:1:895:GLY:O	26:1:898:TYR:N	2.34	0.61
19:G:146:C:H2'	19:G:147:C:C6	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:H:112:G:H2'	20:H:113:G:H8	1.65	0.61
28:3:586:ASP:O	28:3:610:VAL:N	2.32	0.61
40:I:127:C:C1'	10:V:21:ASN:CA	2.74	0.61
42:A:630:TRP:O	42:A:631:ALA:C	2.43	0.61
26:1:551:LEU:O	26:1:554:LYS:N	2.34	0.61
26:1:862:GLU:O	26:1:865:ARG:N	2.33	0.61
1:B:12:U:O4	1:B:65:G:O6	2.19	0.61
20:H:153:A:N6	20:H:177:A:H2	1.98	0.61
20:H:156:U:C6	20:H:156:U:C5'	2.72	0.61
34:K:252:SER:CA	34:K:274:THR:O	2.49	0.61
20:H:142:C:C2'	20:H:143:A:H5'	2.30	0.61
26:1:953:ASP:O	26:1:956:SER:N	2.34	0.61
19:G:136:U:H1'	19:G:137:C:P	2.41	0.60
28:3:638:GLU:N	28:3:668:GLY:O	2.32	0.60
42:A:768:ASP:O	42:A:772:CYS:N	2.34	0.60
26:1:491:GLU:O	26:1:494:GLU:N	2.32	0.60
39:W:345:VAL:N	39:W:360:LEU:CA	2.62	0.60
26:1:897:LEU:O	26:1:900:PHE:N	2.34	0.60
40:I:33:A:H62	40:I:43:G:H21	1.49	0.60
42:A:371:LEU:CA	43:C:341:LYS:C	2.74	0.60
42:A:1489:LEU:N	42:A:1537:TRP:O	2.33	0.60
28:3:563:LEU:N	28:3:581:LYS:O	2.27	0.60
43:C:143:THR:N	45:C:1500:GTP:O1B	2.34	0.60
40:I:126:A:C2	10:V:64:ASN:C	2.79	0.60
26:1:784:MET:O	26:1:787:ILE:N	2.34	0.60
26:1:929:LEU:O	26:1:932:ILE:N	2.34	0.60
26:1:1094:LEU:O	26:1:1098:LEU:N	2.32	0.60
40:I:59:U:C2	40:I:60:A:C8	2.90	0.60
19:G:146:C:H2'	19:G:147:C:H6	1.65	0.60
26:1:173:ALA:C	26:1:176:ALA:H	2.09	0.60
40:I:125:G:H1'	10:V:63:ASN:C	2.27	0.60
26:1:610:ILE:O	26:1:613:MET:N	2.34	0.60
43:C:313:GLN:N	45:C:1500:GTP:O6	2.24	0.60
37:M:12:PRO:O	37:M:82:PHE:CA	2.50	0.59
1:B:94:U:C1'	1:B:95:G:OP1	2.47	0.59
2:D:128:PRO:O	2:D:129:ARG:C	2.45	0.59
19:G:130:A:C2	25:w:396:LEU:CA	2.85	0.59
26:1:1182:LEU:O	26:1:1185:ARG:N	2.35	0.59
2:D:281:VAL:O	2:D:285:LYS:N	2.30	0.59
28:3:550:ASN:N	28:3:553:GLN:O	2.27	0.59
34:K:181:ILE:O	34:K:185:SER:N	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:N:917:LYS:O	35:N:919:ILE:N	2.36	0.59
42:A:300:ASN:O	43:C:936:LYS:CA	2.50	0.59
42:A:1676:ILE:O	42:A:1678:ARG:N	2.35	0.59
42:A:1779:PHE:N	42:A:1810:PHE:O	2.29	0.59
42:A:359:ILE:O	42:A:360:SER:C	2.44	0.59
28:3:664:TYR:CA	28:3:677:THR:O	2.50	0.59
33:J:536:ASP:N	33:J:587:GLY:HA3	2.17	0.59
39:W:344:ILE:CA	39:W:360:LEU:H	2.16	0.59
26:1:1125:PRO:O	26:1:1128:VAL:N	2.35	0.59
35:N:466:ILE:O	35:N:470:ALA:N	2.35	0.59
39:W:427:GLU:N	39:W:441:PHE:H	2.01	0.59
19:G:145:U:H3'	19:G:146:C:H5'	1.82	0.59
26:1:308:SER:O	26:1:311:ALA:N	2.35	0.59
28:3:645:MET:N	28:3:662:PHE:O	2.28	0.59
35:N:142:PHE:O	35:N:143:SER:C	2.45	0.59
40:I:62:U:C2	40:I:63:U:C5	2.91	0.59
30:5:67:ILE:O	30:5:70:ALA:N	2.36	0.59
42:A:770:THR:O	42:A:773:LYS:N	2.32	0.58
11:F:59:G:H4'	40:I:21:U:O3'	2.04	0.58
19:G:135:G:N3	20:H:42:G:N2	2.50	0.58
19:G:146:C:O2	20:H:33:G:C4	2.55	0.58
37:M:12:PRO:O	37:M:82:PHE:N	2.36	0.58
1:B:96:A:H3'	1:B:96:A:OP1	2.03	0.58
42:A:2010:ILE:O	42:A:2013:GLY:O	2.21	0.58
43:C:496:VAL:O	43:C:547:GLY:N	2.30	0.58
26:1:745:ALA:O	26:1:748:LYS:N	2.36	0.58
26:1:1149:LYS:O	26:1:1152:SER:N	2.36	0.58
26:1:811:LEU:O	26:1:814:PHE:N	2.36	0.58
20:H:154:C:O2'	20:H:155:C:H5'	2.04	0.58
1:B:96:A:H3'	1:B:96:A:P	2.43	0.58
19:G:145:U:N3	19:G:146:C:C6	2.71	0.58
40:I:59:U:C2	40:I:60:A:N7	2.71	0.58
42:A:1506:ALA:O	42:A:1510:GLU:N	2.34	0.58
42:A:689:VAL:O	42:A:693:ILE:N	2.32	0.58
35:N:361:VAL:O	35:N:365:ALA:CA	2.52	0.58
1:B:95:G:H3'	1:B:95:G:N3	2.19	0.58
19:G:149:G:N9	19:G:150:U:C6	2.72	0.58
19:G:151:C:C5'	19:G:152:C:H5	2.17	0.58
28:3:1204:VAL:O	28:3:1207:LYS:N	2.37	0.58
40:I:108:C:C2'	40:I:109:G:H5'	2.34	0.58
15:t:33:ASP:O	15:t:59:ILE:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:A:570:ASP:C	42:A:572:PHE:N	2.61	0.57
26:1:424:ILE:O	26:1:428:ALA:N	2.36	0.57
32:7:48:ASP:O	32:7:51:ASN:N	2.37	0.57
19:G:125:C:O2'	19:G:126:C:P	2.62	0.57
40:I:113:C:H6	40:I:113:C:O5'	1.88	0.57
19:G:149:G:C4	19:G:150:U:C6	2.93	0.57
42:A:122:ILE:N	42:A:481:PHE:O	2.25	0.57
19:G:150:U:O2	19:G:150:U:O2'	2.22	0.57
20:H:152:G:N2	20:H:153:A:C5	2.73	0.57
39:W:335:GLY:HA2	39:W:340:LYS:O	2.05	0.57
42:A:823:SER:O	42:A:824:PRO:C	2.47	0.57
26:1:929:LEU:O	26:1:930:PRO:C	2.45	0.57
26:1:892:LEU:O	26:1:895:GLY:N	2.37	0.57
35:N:139:GLN:O	35:N:143:SER:N	2.35	0.57
20:H:165:A:C6	20:H:166:G:O6	2.57	0.57
26:1:747:LEU:O	26:1:748:LYS:C	2.48	0.57
40:I:110:G:O5'	40:I:110:G:H8	1.86	0.57
11:F:50:A:H2'	11:F:51:U:H6	1.69	0.57
26:1:578:ILE:O	26:1:581:LEU:N	2.37	0.57
26:1:937:LEU:O	26:1:940:LEU:N	2.38	0.57
40:I:111:C:H2'	40:I:112:A:H8	1.69	0.56
1:B:110:C:H2'	1:B:111:A:H8	1.70	0.56
19:G:146:C:N4	19:G:147:C:H41	2.03	0.56
28:3:287:PHE:CA	28:3:304:GLN:O	2.53	0.56
43:C:682:LYS:O	43:C:797:ALA:N	2.38	0.56
23:u:174:VAL:O	23:u:178:GLY:HA2	2.05	0.56
26:1:849:ILE:O	26:1:852:ARG:N	2.38	0.56
28:3:1160:HIS:O	28:3:1163:PHE:N	2.37	0.56
39:W:341:LYS:CA	39:W:358:LYS:CA	2.83	0.56
40:I:20:A:H2'	40:I:21:U:C5	2.40	0.56
42:A:708:THR:O	42:A:709:ILE:C	2.48	0.56
42:A:1012:LYS:O	42:A:1013:ASN:O	2.23	0.56
11:F:59:G:C4'	40:I:21:U:O3'	2.53	0.56
26:1:699:GLN:O	26:1:700:LYS:C	2.48	0.56
19:G:149:G:C2'	19:G:150:U:C6	2.89	0.56
28:3:15:SER:N	28:3:33:SER:O	2.35	0.56
20:H:141:C:H2'	20:H:142:C:H6	1.71	0.56
28:3:973:GLY:HA3	28:3:976:LYS:C	2.31	0.56
35:N:375:ILE:C	35:N:377:ILE:N	2.63	0.56
42:A:940:ILE:CA	42:A:1090:ARG:O	2.54	0.56
19:G:136:U:C1'	19:G:137:C:P	2.94	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:H:141:C:C2	20:H:142:C:C5	2.93	0.56
42:A:930:ALA:O	42:A:934:ARG:CA	2.54	0.56
1:B:69:A:O2'	1:B:70:A:N3	2.39	0.56
20:H:149:A:H2'	20:H:150:U:H6	1.70	0.56
20:H:152:G:N2	20:H:153:A:C8	2.73	0.56
26:1:716:ALA:O	26:1:719:TYR:N	2.39	0.56
40:I:108:C:H2'	40:I:109:G:C8	2.41	0.56
19:G:151:C:C1'	19:G:152:C:P	2.94	0.56
20:H:150:U:H2'	20:H:151:C:H6	1.71	0.56
28:3:488:GLY:C	28:3:490:THR:H	2.14	0.56
42:A:331:TRP:O	43:C:177:ARG:CA	2.54	0.56
42:A:1787:ARG:O	42:A:1803:ILE:O	2.24	0.56
1:B:61:A:H2'	1:B:62:G:H8	1.69	0.55
26:1:968:GLU:O	26:1:971:MET:N	2.39	0.55
42:A:1520:ASN:C	42:A:1522:GLN:N	2.63	0.55
11:F:50:A:C4	11:F:51:U:C5	2.94	0.55
19:G:149:G:C3'	19:G:150:U:H5''	2.35	0.55
20:H:147:G:C4	20:H:148:C:C5	2.94	0.55
28:3:523:GLY:CA	28:3:536:TRP:O	2.51	0.55
35:N:117:LYS:C	35:N:119:ARG:H	2.12	0.55
20:H:150:U:C2	20:H:151:C:C5	2.94	0.55
26:1:874:LYS:O	26:1:877:GLY:CA	2.54	0.55
26:1:1124:SER:O	26:1:1127:THR:N	2.34	0.55
28:3:931:VAL:O	28:3:935:GLU:N	2.39	0.55
19:G:135:G:N2	20:H:42:G:N9	2.53	0.55
20:H:181:G:H2'	20:H:182:U:H6	1.71	0.55
28:3:303:ALA:O	28:3:310:ILE:CA	2.55	0.55
30:5:98:PHE:O	30:5:100:LYS:N	2.39	0.55
42:A:1488:THR:C	42:A:1537:TRP:O	2.49	0.55
28:3:1194:SER:O	28:3:1199:ARG:N	2.36	0.55
2:D:146:GLU:O	2:D:149:ARG:N	2.40	0.55
19:G:137:C:O2'	19:G:138:A:C5'	2.37	0.55
20:H:183:G:C4	20:H:184:C:C5	2.94	0.55
20:H:183:G:H2'	20:H:184:C:H6	1.71	0.55
25:w:276:GLY:C	25:w:278:LEU:N	2.60	0.55
25:w:411:CYS:O	25:w:414:TYR:N	2.37	0.55
30:5:109:GLN:O	30:5:112:LEU:N	2.39	0.55
40:I:21:U:C2'	40:I:22:C:H5'	2.37	0.55
40:I:59:U:H1'	40:I:60:A:H5'	1.89	0.55
11:F:51:U:H2'	11:F:51:U:O2	2.06	0.55
20:H:181:G:C4	20:H:182:U:C5	2.95	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:3:1195:GLU:C	28:3:1198:ASP:H	2.14	0.55
19:G:151:C:O2'	19:G:151:C:O2	2.24	0.54
2:D:283:GLN:O	2:D:287:ASP:N	2.33	0.54
20:H:149:A:C4	20:H:150:U:C5	2.95	0.54
26:1:517:ARG:O	26:1:520:THR:N	2.41	0.54
26:1:557:ASP:O	26:1:560:LEU:N	2.40	0.54
34:K:250:CYS:O	34:K:251:TRP:C	2.50	0.54
40:I:55:U:H3'	40:I:56:U:C6	2.42	0.54
40:I:55:U:H2'	40:I:55:U:O2	2.07	0.54
40:I:124:U:H1'	9:U:37:HIS:O	2.06	0.54
43:C:664:GLU:O	43:C:785:ARG:N	2.27	0.54
1:B:17:U:O2	1:B:60:G:N2	2.28	0.54
1:B:108:G:H3'	1:B:109:G:H8	1.73	0.54
2:D:1048:VAL:O	2:D:1050:GLU:N	2.40	0.54
11:F:52:U:C6	11:F:52:U:C5'	2.85	0.54
19:G:146:C:C2	20:H:33:G:C2	2.95	0.54
20:H:153:A:C3'	20:H:154:C:C5'	2.86	0.54
43:C:776:GLU:O	43:C:782:GLU:N	2.41	0.54
1:B:26:A:H2	1:B:27:U:C5	2.26	0.54
19:G:146:C:N3	20:H:33:G:O6	2.40	0.54
43:C:470:PRO:C	43:C:499:GLY:HA2	2.29	0.54
1:B:110:C:H2'	1:B:111:A:C8	2.41	0.54
19:G:146:C:C1'	20:H:33:G:N2	2.68	0.54
19:G:151:C:O2'	19:G:152:C:OP1	2.24	0.54
1:B:99:C:H2'	1:B:100:C:C6	2.43	0.54
13:r:48:GLN:C	13:r:50:LEU:H	2.14	0.54
20:H:147:G:H2'	20:H:148:C:C6	2.43	0.54
26:1:1026:ASN:O	26:1:1028:HIS:N	2.41	0.54
26:1:1205:GLU:O	26:1:1208:LEU:N	2.41	0.54
31:6:7:ASP:O	31:6:91:LEU:N	2.39	0.54
42:A:597:LYS:C	42:A:599:MET:H	2.16	0.54
42:A:596:TYR:O	42:A:597:LYS:C	2.50	0.54
19:G:151:C:C5'	19:G:152:C:C5	2.91	0.54
26:1:641:ILE:O	26:1:644:LEU:N	2.40	0.54
37:M:9:LYS:O	37:M:11:TYR:N	2.40	0.54
26:1:981:TYR:O	26:1:984:GLU:N	2.20	0.53
28:3:785:PRO:CA	28:3:800:ILE:O	2.56	0.53
11:F:47:A:H2'	11:F:48:A:H8	1.72	0.53
26:1:1132:LEU:O	26:1:1135:GLU:N	2.41	0.53
42:A:1817:LEU:N	42:A:1917:PHE:O	2.40	0.53
19:G:153:C:H2'	19:G:153:C:O2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:H:153:A:H3'	20:H:154:C:C5'	2.38	0.53
34:K:222:ASN:O	34:K:520:MET:N	2.39	0.53
35:N:159:SER:O	42:A:730:GLY:HA3	2.08	0.53
35:N:142:PHE:O	35:N:144:ASP:N	2.41	0.53
40:I:58:C:H2'	40:I:59:U:H5'	1.85	0.53
40:I:61:A:H2'	40:I:62:U:C6	2.44	0.53
26:1:841:ALA:O	26:1:843:LYS:N	2.42	0.53
43:C:457:VAL:CA	43:C:462:GLY:HA3	2.39	0.53
35:N:160:ILE:CA	42:A:730:GLY:C	2.82	0.53
28:3:1195:GLU:O	28:3:1198:ASP:N	2.41	0.53
35:N:290:ASP:H	42:A:872:ASP:CA	2.21	0.53
42:A:347:LEU:O	42:A:348:PRO:C	2.47	0.53
40:I:55:U:H3'	40:I:56:U:C5	2.44	0.53
11:F:73:A:C2	40:I:2:G:N1	2.75	0.53
19:G:137:C:C2'	19:G:138:A:C5'	2.87	0.52
26:1:939:ARG:O	26:1:940:LEU:C	2.51	0.52
26:1:963:LYS:O	26:1:966:GLN:N	2.30	0.52
2:D:298:ASP:O	2:D:301:GLU:N	2.41	0.52
26:1:244:THR:O	26:1:247:ALA:N	2.42	0.52
33:J:534:LYS:O	33:J:567:LEU:O	2.26	0.52
34:K:206:THR:O	34:K:210:GLN:N	2.37	0.52
26:1:978:LEU:O	26:1:979:TYR:C	2.51	0.52
26:1:1280:LEU:O	26:1:1282:ALA:N	2.42	0.52
35:N:302:ARG:O	35:N:305:ASN:O	2.28	0.52
43:C:366:GLN:O	43:C:367:ARG:C	2.51	0.52
27:2:596:GLU:O	27:2:598:GLU:N	2.43	0.52
26:1:663:THR:O	26:1:666:LYS:N	2.42	0.52
35:N:425:ARG:O	35:N:429:CYS:N	2.38	0.52
26:1:660:ALA:O	26:1:661:ARG:C	2.53	0.52
28:3:430:GLY:O	28:3:433:SER:N	2.31	0.52
28:3:546:LYS:O	28:3:556:ILE:CA	2.58	0.52
39:W:351:GLY:HA2	39:W:367:ALA:C	2.35	0.52
40:I:118:A:H8	40:I:118:A:OP2	1.92	0.52
42:A:1943:LEU:O	42:A:1947:ASN:CA	2.58	0.52
1:B:19:A:H62	42:A:467:GLN:CA	2.22	0.52
1:B:48:A:O5'	42:A:280:GLU:N	2.42	0.52
20:H:46:U:O2'	25:w:394:TYR:CA	2.57	0.52
28:3:589:CYS:O	28:3:608:GLY:N	2.30	0.52
26:1:103:PRO:C	26:1:106:GLU:H	2.18	0.52
40:I:119:A:C2	4:P:103:GLY:C	2.87	0.52
42:A:1439:ARG:O	42:A:1443:LYS:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:G:146:C:H2'	19:G:147:C:H5'	1.91	0.51
20:H:30:A:N3	20:H:30:A:C2'	2.73	0.51
20:H:107:A:C6	20:H:108:G:C5	2.99	0.51
26:1:771:LEU:O	26:1:774:ILE:N	2.44	0.51
26:1:793:LYS:O	26:1:797:GLY:CA	2.54	0.51
26:1:1110:VAL:O	26:1:1113:THR:N	2.43	0.51
32:7:37:ARG:O	32:7:40:TYR:N	2.44	0.51
34:K:340:THR:O	34:K:348:ARG:N	2.40	0.51
35:N:393:LEU:O	35:N:397:LEU:N	2.39	0.51
42:A:617:ASN:CA	42:A:621:VAL:O	2.59	0.51
11:F:52:U:O4	11:F:53:A:N6	2.43	0.51
19:G:152:C:H6	19:G:152:C:H3'	1.76	0.51
28:3:673:VAL:CA	28:3:691:THR:H	2.24	0.51
32:7:36:HIS:O	32:7:37:ARG:C	2.53	0.51
11:F:46:G:H2'	11:F:47:A:C8	2.45	0.51
26:1:667:ILE:O	26:1:668:VAL:C	2.53	0.51
28:3:699:VAL:CA	28:3:715:MET:O	2.59	0.51
39:W:344:ILE:CA	39:W:360:LEU:CA	2.89	0.51
26:1:423:PRO:O	26:1:427:PRO:N	2.43	0.51
1:B:95:G:N3	1:B:95:G:C2'	2.73	0.51
26:1:1025:LYS:O	26:1:1027:ARG:N	2.42	0.51
42:A:838:LEU:O	42:A:841:LEU:N	2.44	0.51
19:G:156:U:H2'	19:G:156:U:O2	2.08	0.51
26:1:705:SER:O	26:1:706:ALA:C	2.54	0.51
30:5:46:ARG:N	30:5:63:VAL:O	2.44	0.51
19:G:126:C:H2'	19:G:126:C:O2	2.09	0.51
40:I:111:C:H2'	40:I:112:A:C8	2.46	0.51
42:A:398:THR:CA	43:C:386:GLY:HA3	2.38	0.51
26:1:974:LEU:O	26:1:975:GLY:C	2.54	0.51
26:1:1035:CYS:O	26:1:1038:LEU:N	2.44	0.51
37:M:59:ASP:O	37:M:60:ALA:C	2.53	0.51
2:D:114:GLU:O	2:D:117:LEU:N	2.44	0.51
20:H:111:G:O3'	20:H:112:G:O4'	2.29	0.51
26:1:1080:THR:O	26:1:1083:TYR:N	2.44	0.51
26:1:1188:ALA:O	26:1:1191:VAL:N	2.44	0.51
26:1:1207:SER:O	26:1:1210:HIS:N	2.43	0.51
26:1:1280:LEU:O	26:1:1281:ILE:C	2.51	0.51
28:3:147:ASP:N	28:3:151:ARG:O	2.42	0.51
28:3:318:ASP:N	28:3:321:MET:O	2.27	0.51
26:1:804:ASN:O	26:1:807:LYS:N	2.44	0.50
40:I:143:U:H2'	40:I:144:G:H5''	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:C:827:LEU:C	43:C:907:VAL:H	2.18	0.50
26:1:1129:LEU:O	26:1:1132:LEU:N	2.44	0.50
32:7:48:ASP:O	32:7:49:LEU:C	2.54	0.50
26:1:629:ALA:O	26:1:632:PHE:N	2.45	0.50
19:G:143:U:C6	19:G:143:U:C5'	2.89	0.50
9:U:18:ARG:N	9:U:81:THR:O	2.40	0.50
1:B:26:A:N3	1:B:26:A:C3'	2.73	0.50
19:G:149:G:H21	19:G:150:U:H5'	1.77	0.50
20:H:143:A:N3	20:H:143:A:C3'	2.73	0.50
40:I:20:A:O2'	40:I:21:U:H5'	2.12	0.50
42:A:332:TYR:CA	43:C:177:ARG:O	2.60	0.50
42:A:570:ASP:O	42:A:571:ALA:C	2.54	0.50
42:A:1520:ASN:C	42:A:1522:GLN:H	2.19	0.50
19:G:146:C:C4	19:G:147:C:N4	2.73	0.50
40:I:58:C:O2'	40:I:59:U:H5''	2.09	0.50
42:A:972:GLU:CA	42:A:1101:PHE:O	2.60	0.50
43:C:452:THR:O	43:C:577:PHE:CA	2.60	0.50
26:1:1268:ILE:O	26:1:1271:SER:N	2.44	0.50
42:A:823:SER:O	42:A:824:PRO:O	2.30	0.50
2:D:159:LEU:C	2:D:161:LEU:N	2.68	0.50
20:H:46:U:HO2'	25:w:394:TYR:H	1.59	0.50
6:l:15:VAL:O	7:n:33:GLY:HA3	2.12	0.50
35:N:360:ALA:O	35:N:364:GLN:N	2.38	0.50
42:A:770:THR:O	42:A:771:VAL:C	2.51	0.50
1:B:100:C:H2'	1:B:101:U:C6	2.46	0.50
1:B:58:U:H2'	1:B:59:G:C8	2.46	0.49
39:W:564:GLY:O	39:W:565:ALA:O	2.29	0.49
26:1:528:ALA:O	26:1:531:LEU:N	2.44	0.49
26:1:862:GLU:O	26:1:863:GLN:C	2.55	0.49
39:W:349:PHE:N	39:W:364:ASP:H	2.10	0.49
42:A:401:GLY:HA3	43:C:385:VAL:O	2.12	0.49
42:A:929:GLU:O	42:A:933:ARG:CA	2.59	0.49
11:F:102:A:O2'	11:F:103:U:C5'	2.60	0.49
26:1:587:TYR:O	26:1:590:ARG:N	2.45	0.49
11:F:47:A:H2'	11:F:48:A:C8	2.47	0.49
26:1:237:GLY:O	26:1:239:ALA:N	2.45	0.49
33:J:446:LYS:CA	40:I:23:G:OP1	2.61	0.49
39:W:334:LEU:CA	39:W:340:LYS:CA	2.90	0.49
1:B:48:A:O5'	42:A:280:GLU:CA	2.60	0.49
20:H:106:G:N2	20:H:107:A:C6	2.72	0.49
26:1:408:PHE:O	26:1:409:PRO:C	2.50	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:849:ILE:O	26:1:850:ILE:C	2.54	0.49
20:H:46:U:H5''	20:H:47:U:H2'	1.93	0.49
26:1:1227:ILE:O	26:1:1230:VAL:N	2.46	0.49
28:3:596:PRO:O	28:3:598:GLY:N	2.45	0.49
35:N:289:ASN:N	42:A:871:TYR:C	2.71	0.49
1:B:48:A:H2'	1:B:49:A:H8	1.76	0.49
19:G:149:G:H3'	19:G:149:G:N3	2.28	0.49
26:1:1243:PRO:O	26:1:1244:CYS:C	2.55	0.49
35:N:158:LEU:O	35:N:160:ILE:N	2.44	0.49
11:F:102:A:O2'	11:F:103:U:H5''	2.12	0.49
19:G:146:C:C2	19:G:147:C:H5	2.30	0.49
20:H:40:C:C5'	20:H:40:C:C6	2.92	0.49
26:1:553:VAL:O	26:1:556:ILE:N	2.46	0.49
42:A:1520:ASN:O	42:A:1521:ALA:C	2.56	0.49
26:1:693:GLY:O	26:1:694:LEU:C	2.55	0.49
26:1:708:ALA:O	26:1:709:ILE:C	2.54	0.49
39:W:341:LYS:O	39:W:359:LYS:CA	2.61	0.49
13:r:47:ASP:O	13:r:50:LEU:N	2.39	0.48
19:G:151:C:C1'	19:G:152:C:OP1	2.55	0.48
20:H:107:A:C2	20:H:108:G:C4	3.01	0.48
28:3:930:LEU:C	28:3:934:GLY:HA2	2.38	0.48
42:A:708:THR:O	42:A:710:LEU:N	2.46	0.48
26:1:625:ARG:O	26:1:628:THR:N	2.46	0.48
26:1:631:ALA:O	26:1:634:VAL:N	2.47	0.48
26:1:953:ASP:O	26:1:954:LEU:C	2.56	0.48
43:C:133:THR:O	43:C:225:VAL:CA	2.62	0.48
19:G:135:G:H1	20:H:41:U:H3	1.60	0.48
35:N:560:ARG:C	35:N:564:ALA:H	2.21	0.48
42:A:1197:LEU:O	42:A:1226:ALA:CA	2.62	0.48
19:G:135:G:C2	20:H:42:G:C5	3.02	0.48
26:1:892:LEU:O	26:1:893:ILE:C	2.54	0.48
26:1:177:LYS:O	26:1:180:GLU:N	2.46	0.48
26:1:665:ILE:O	26:1:666:LYS:C	2.55	0.48
26:1:1264:VAL:O	26:1:1265:TYR:C	2.56	0.48
28:3:672:GLY:O	28:3:695:GLY:N	2.46	0.48
42:A:947:PRO:O	42:A:951:LEU:N	2.41	0.48
1:B:72:U:H2'	1:B:73:C:H6	1.78	0.48
26:1:865:ARG:O	26:1:866:LYS:C	2.56	0.48
26:1:955:ILE:O	26:1:956:SER:C	2.57	0.48
27:2:491:LEU:O	27:2:493:ALA:N	2.46	0.48
26:1:629:ALA:O	26:1:630:ARG:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:994:LEU:O	26:1:995:GLY:C	2.56	0.48
26:1:803:ALA:O	26:1:804:ASN:C	2.54	0.48
26:1:1110:VAL:O	26:1:1111:CYS:C	2.57	0.48
2:D:298:ASP:O	2:D:299:ASP:C	2.56	0.48
11:F:73:A:H2	40:I:2:G:H1	1.56	0.48
19:G:152:C:O2'	19:G:153:C:O5'	2.30	0.48
26:1:720:GLY:O	26:1:721:ILE:C	2.54	0.48
26:1:872:ILE:O	26:1:873:GLU:C	2.57	0.48
43:C:263:LEU:O	43:C:268:LYS:N	2.47	0.48
43:C:474:LEU:CA	43:C:498:SER:C	2.86	0.48
1:B:17:U:O4	1:B:60:G:O6	2.31	0.47
1:B:25:C:H42	42:A:420:ARG:H	1.62	0.47
1:B:95:G:N3	1:B:95:G:H2'	2.28	0.47
11:F:49:G:H2'	11:F:50:A:C8	2.48	0.47
19:G:125:C:HO2'	19:G:126:C:P	2.36	0.47
20:H:151:C:C2	20:H:152:G:N7	2.82	0.47
1:B:23:C:H3'	1:B:24:G:H4'	1.96	0.47
19:G:149:G:C2'	19:G:150:U:H6	2.23	0.47
26:1:501:LEU:O	26:1:502:LEU:C	2.55	0.47
26:1:944:SER:O	26:1:946:LYS:N	2.38	0.47
26:1:993:ILE:O	26:1:994:LEU:C	2.57	0.47
28:3:923:GLY:HA3	28:3:947:GLU:O	2.14	0.47
30:5:98:PHE:C	30:5:100:LYS:N	2.72	0.47
40:I:110:G:H2'	40:I:111:C:C6	2.49	0.47
43:C:143:THR:H	45:C:1500:GTP:PB	2.37	0.47
13:r:48:GLN:C	13:r:50:LEU:N	2.69	0.47
16:x:31:ARG:O	16:x:47:GLN:CA	2.63	0.47
26:1:102:ASP:O	26:1:106:GLU:N	2.47	0.47
42:A:597:LYS:C	42:A:599:MET:N	2.72	0.47
3:E:255:MET:C	3:E:257:ASN:H	2.22	0.47
11:F:73:A:N1	40:I:2:G:C6	2.82	0.47
19:G:135:G:O6	20:H:41:U:O4	2.32	0.47
26:1:833:LEU:O	26:1:834:VAL:C	2.56	0.47
28:3:558:LEU:O	28:3:561:GLY:CA	2.63	0.47
40:I:109:G:H2'	40:I:110:G:C8	2.49	0.47
42:A:838:LEU:O	42:A:839:LEU:C	2.57	0.47
20:H:153:A:C2'	20:H:154:C:C5'	2.86	0.47
26:1:226:HIS:O	26:1:229:SER:N	2.47	0.47
26:1:889:GLU:O	26:1:890:GLU:C	2.57	0.47
26:1:935:THR:O	26:1:936:VAL:C	2.58	0.47
28:3:42:ARG:N	28:3:51:HIS:O	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:N:433:SER:O	35:N:437:TRP:N	2.47	0.47
43:C:452:THR:O	43:C:578:ARG:N	2.46	0.47
26:1:663:THR:O	26:1:664:GLY:C	2.56	0.47
28:3:44:ASP:O	28:3:48:GLY:HA2	2.15	0.47
34:K:333:PRO:O	34:K:334:SER:O	2.33	0.47
35:N:410:ALA:O	35:N:413:LEU:CA	2.62	0.47
20:H:153:A:C8	20:H:154:C:H5'	2.50	0.47
20:H:183:G:H2'	20:H:184:C:C6	2.50	0.47
35:N:15:LEU:O	35:N:17:TYR:N	2.48	0.47
42:A:230:PHE:N	42:A:414:ARG:O	2.45	0.47
2:D:355:GLU:O	2:D:359:PHE:N	2.40	0.47
26:1:210:ALA:O	26:1:213:LYS:N	2.48	0.47
26:1:693:GLY:O	26:1:695:VAL:N	2.48	0.47
26:1:831:ARG:O	26:1:832:GLN:C	2.58	0.47
26:1:867:MET:O	26:1:868:VAL:C	2.57	0.47
34:K:307:LEU:O	34:K:316:VAL:N	2.48	0.47
34:K:333:PRO:O	34:K:334:SER:C	2.58	0.47
1:B:111:A:H2'	1:B:112:A:C8	2.49	0.46
11:F:50:A:H2'	11:F:51:U:C6	2.50	0.46
19:G:122:U:H4'	19:G:123:U:OP1	2.14	0.46
26:1:578:ILE:O	26:1:579:GLU:C	2.57	0.46
11:F:66:C:H2'	11:F:67:G:C8	2.50	0.46
26:1:631:ALA:O	26:1:632:PHE:C	2.58	0.46
32:7:42:SER:O	32:7:45:GLY:N	2.48	0.46
42:A:570:ASP:C	42:A:572:PHE:H	2.22	0.46
40:I:61:A:H2'	40:I:62:U:H6	1.80	0.46
13:r:19:ASP:C	13:r:21:ILE:H	2.23	0.46
20:H:107:A:C6	20:H:108:G:C6	3.04	0.46
25:w:404:ILE:N	25:w:417:ARG:O	2.44	0.46
39:W:205:LEU:C	39:W:207:LYS:H	2.23	0.46
19:G:153:C:H4'	19:G:153:C:OP1	2.14	0.46
35:N:557:GLU:O	35:N:561:ALA:N	2.48	0.46
40:I:51:A:C2	40:I:55:U:O2'	2.64	0.46
40:I:126:A:C2	10:V:64:ASN:O	2.60	0.46
40:I:11:A:H2'	40:I:12:G:C8	2.50	0.46
19:G:130:A:H2	25:w:396:LEU:CA	2.29	0.46
25:w:394:TYR:C	25:w:396:LEU:H	2.24	0.46
35:N:391:ARG:O	35:N:395:LYS:N	2.37	0.46
43:C:236:MET:O	43:C:237:LEU:C	2.59	0.46
20:H:141:C:H2'	20:H:142:C:C6	2.50	0.46
20:H:150:U:H2'	20:H:151:C:C6	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:H:168:A:H3'	20:H:169:C:H6	1.80	0.46
31:6:46:CYS:O	31:6:50:ASN:N	2.43	0.46
35:N:117:LYS:C	35:N:119:ARG:N	2.74	0.46
12:q:61:PHE:N	18:z:70:ILE:O	2.45	0.46
20:H:149:A:H2'	20:H:150:U:C6	2.50	0.46
25:w:403:ASN:N	25:w:417:ARG:O	2.49	0.46
26:1:257:THR:O	26:1:259:SER:N	2.49	0.46
26:1:841:ALA:C	26:1:843:LYS:N	2.73	0.46
26:1:1105:GLU:O	26:1:1106:ARG:C	2.59	0.46
32:7:64:VAL:O	32:7:65:ARG:C	2.59	0.46
1:B:26:A:H2	1:B:27:U:C6	2.34	0.46
1:B:99:C:H2'	1:B:100:C:H6	1.79	0.46
20:H:3:C:H2'	20:H:4:G:C8	2.51	0.46
20:H:181:G:H2'	20:H:182:U:C6	2.50	0.46
26:1:708:ALA:O	26:1:711:ALA:N	2.49	0.46
35:N:429:CYS:O	35:N:433:SER:N	2.38	0.46
12:q:73:PRO:O	12:q:75:ASP:N	2.49	0.45
20:H:180:G:H2'	20:H:181:G:C8	2.44	0.45
26:1:830:TYR:O	26:1:831:ARG:C	2.57	0.45
28:3:890:SER:O	28:3:908:GLY:N	2.41	0.45
42:A:331:TRP:O	43:C:177:ARG:C	2.59	0.45
42:A:940:ILE:C	42:A:1090:ARG:O	2.59	0.45
20:H:59:A:H2'	20:H:60:U:O4'	2.17	0.45
28:3:1148:LEU:O	28:3:1149:ARG:C	2.58	0.45
20:H:113:G:H2'	20:H:114:A:H8	1.82	0.45
26:1:547:GLN:O	26:1:548:GLU:C	2.58	0.45
26:1:914:PHE:O	26:1:915:GLY:C	2.58	0.45
26:1:1129:LEU:O	26:1:1130:PRO:C	2.59	0.45
28:3:1141:PHE:O	28:3:1144:VAL:N	2.49	0.45
32:7:62:ALA:O	32:7:65:ARG:N	2.50	0.45
43:C:756:LYS:O	43:C:757:ALA:C	2.58	0.45
20:H:112:G:H2'	20:H:113:G:C8	2.50	0.45
26:1:687:VAL:O	26:1:690:ILE:N	2.50	0.45
26:1:952:ALA:O	26:1:953:ASP:C	2.57	0.45
35:N:554:ASN:O	35:N:558:CYS:N	2.43	0.45
20:H:148:C:H2'	20:H:149:A:H8	1.82	0.45
26:1:745:ALA:O	26:1:746:PHE:C	2.59	0.45
26:1:1128:VAL:O	26:1:1129:LEU:C	2.60	0.45
40:I:125:G:HI'	10:V:63:ASN:O	2.17	0.45
2:D:1349:GLY:HA2	2:D:1491:SER:O	2.16	0.45
32:7:46:HIS:O	32:7:47:PHE:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:U:80:MET:O	10:V:59:SER:N	2.44	0.45
11:F:52:U:C5	11:F:52:U:OP2	2.70	0.45
19:G:149:G:N3	19:G:150:U:H5''	2.31	0.45
26:1:645:LEU:O	26:1:646:PRO:C	2.56	0.45
26:1:1013:ILE:O	26:1:1014:LYS:C	2.60	0.45
28:3:672:GLY:O	28:3:691:THR:N	2.49	0.45
40:I:115:G:H2'	40:I:116:G:C8	2.52	0.45
20:H:142:C:H2'	20:H:143:A:H5'	1.98	0.45
1:B:74:U:H2'	1:B:75:G:C8	2.52	0.45
26:1:1031:VAL:O	26:1:1032:GLN:C	2.60	0.45
28:3:215:LEU:O	28:3:218:ASN:N	2.50	0.45
43:C:133:THR:O	43:C:226:VAL:N	2.46	0.45
26:1:1119:VAL:O	26:1:1122:THR:N	2.49	0.45
28:3:663:LEU:O	28:3:678:VAL:CA	2.65	0.45
28:3:1191:LYS:O	28:3:1192:ASN:C	2.59	0.45
26:1:810:ILE:O	26:1:811:LEU:C	2.59	0.44
26:1:1165:TYR:O	26:1:1166:ILE:C	2.59	0.44
26:1:1223:SER:O	26:1:1224:PRO:C	2.60	0.44
39:W:346:THR:N	39:W:359:LYS:C	2.75	0.44
40:I:118:A:OP2	40:I:118:A:C8	2.71	0.44
42:A:350:PHE:O	43:C:268:LYS:O	2.35	0.44
42:A:1519:THR:C	42:A:1521:ALA:H	2.22	0.44
1:B:98:G:OP2	1:B:98:G:C8	2.70	0.44
19:G:127:U:O2'	19:G:127:U:O2	2.31	0.44
19:G:147:C:N3	20:H:31:G:O6	2.50	0.44
19:G:150:U:O2'	19:G:151:C:C5	2.71	0.44
26:1:749:ALA:O	26:1:750:ILE:C	2.60	0.44
26:1:937:LEU:O	26:1:938:TRP:C	2.59	0.44
42:A:989:ASP:O	42:A:993:LEU:N	2.41	0.44
11:F:102:A:C2'	11:F:103:U:C5'	2.93	0.44
20:H:114:A:H2'	20:H:115:G:H8	1.81	0.44
20:H:152:G:O2'	20:H:153:A:H1'	2.16	0.44
26:1:567:VAL:O	26:1:568:ARG:C	2.58	0.44
35:N:149:LEU:O	35:N:151:GLU:N	2.51	0.44
26:1:606:LEU:O	26:1:609:MET:N	2.51	0.44
26:1:916:THR:O	26:1:917:VAL:C	2.61	0.44
26:1:948:ARG:O	26:1:949:GLN:C	2.60	0.44
40:I:91:A:H2'	40:I:92:C:C6	2.53	0.44
4:P:109:VAL:N	5:Q:63:LEU:O	2.42	0.44
26:1:791:VAL:O	26:1:792:VAL:C	2.60	0.44
34:K:374:HIS:O	34:K:377:GLY:N	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:U:H2'	1:B:11:U:C6	2.52	0.44
19:G:148:U:O3'	19:G:149:G:O4'	2.35	0.44
20:H:178:A:C5'	20:H:179:C:OP2	2.66	0.44
20:H:182:U:H2'	20:H:183:G:H8	1.81	0.44
26:1:429:ARG:C	26:1:432:THR:H	2.26	0.44
26:1:874:LYS:O	26:1:875:ILE:C	2.61	0.44
42:A:570:ASP:O	42:A:574:LEU:N	2.38	0.44
42:A:1676:ILE:C	42:A:1678:ARG:N	2.75	0.44
2:D:121:GLN:O	2:D:125:GLY:N	2.40	0.44
11:F:52:U:C6	11:F:52:U:OP2	2.71	0.44
11:F:90:G:H2'	11:F:91:A:H8	1.82	0.44
11:F:91:A:H2'	11:F:92:A:C8	2.53	0.44
19:G:149:G:C5	19:G:150:U:C4	3.05	0.44
26:1:950:GLN:O	26:1:951:ALA:C	2.61	0.44
28:3:676:ARG:O	28:3:686:LEU:CA	2.65	0.44
39:W:334:LEU:O	39:W:340:LYS:O	2.35	0.44
40:I:59:U:O2	40:I:60:A:C8	2.70	0.44
7:S:22:ASN:N	7:S:66:SER:O	2.49	0.44
1:B:61:A:H2'	1:B:62:G:C8	2.50	0.44
19:G:126:C:C2	19:G:126:C:OP2	2.70	0.44
20:H:142:C:O2'	20:H:143:A:H5'	2.18	0.44
20:H:143:A:OP2	20:H:143:A:C2	2.71	0.44
43:C:257:ILE:O	43:C:310:SER:O	2.36	0.44
26:1:710:ALA:O	26:1:711:ALA:C	2.61	0.44
35:N:160:ILE:C	42:A:730:GLY:O	2.61	0.44
26:1:102:ASP:O	26:1:105:ALA:C	2.61	0.43
26:1:792:VAL:O	26:1:793:LYS:C	2.59	0.43
26:1:889:GLU:O	26:1:892:LEU:N	2.51	0.43
26:1:1078:VAL:O	26:1:1081:PHE:N	2.50	0.43
28:3:672:GLY:C	28:3:691:THR:H	2.25	0.43
28:3:1148:LEU:O	28:3:1151:GLU:N	2.51	0.43
28:3:430:GLY:O	28:3:431:PRO:C	2.61	0.43
40:I:21:U:C5	40:I:21:U:OP2	2.70	0.43
42:A:770:THR:O	42:A:772:CYS:N	2.51	0.43
42:A:1512:SER:O	42:A:1515:TRP:C	2.61	0.43
26:1:625:ARG:O	26:1:626:ASN:C	2.61	0.43
26:1:723:SER:C	26:1:725:ASP:H	2.26	0.43
26:1:928:TYR:O	26:1:929:LEU:C	2.61	0.43
27:2:504:TRP:C	27:2:506:PHE:H	2.27	0.43
1:B:95:G:N3	1:B:95:G:C3'	2.81	0.43
26:1:471:ASP:O	26:1:472:ILE:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:682:HIS:O	26:1:683:LEU:C	2.61	0.43
26:1:1230:VAL:O	26:1:1233:ALA:N	2.52	0.43
40:I:110:G:O5'	40:I:110:G:C8	2.70	0.43
1:B:31:U:H2'	1:B:32:C:C6	2.54	0.43
1:B:72:U:H2'	1:B:73:C:C6	2.53	0.43
20:H:98:G:H5'	20:H:104:U:OP2	2.19	0.43
25:w:394:TYR:C	25:w:396:LEU:N	2.75	0.43
26:1:1082:GLY:O	26:1:1083:TYR:C	2.61	0.43
26:1:1090:PRO:O	26:1:1091:HIS:C	2.62	0.43
39:W:205:LEU:C	39:W:207:LYS:N	2.76	0.43
42:A:708:THR:C	42:A:710:LEU:N	2.76	0.43
20:H:154:C:O2'	20:H:155:C:C5'	2.66	0.43
26:1:1029:GLU:O	26:1:1032:GLN:N	2.51	0.43
28:3:5:ASN:O	28:3:1176:GLY:HA3	2.19	0.43
28:3:1141:PHE:O	28:3:1142:GLN:C	2.61	0.43
35:N:560:ARG:O	35:N:564:ALA:O	2.33	0.43
20:H:64:A:H2'	20:H:65:U:C6	2.54	0.43
20:H:157:G:H2'	20:H:158:G:O4'	2.19	0.43
42:A:84:ASP:O	42:A:88:TYR:CA	2.66	0.43
42:A:379:GLU:O	43:C:355:LYS:CA	2.67	0.43
42:A:1502:PHE:O	42:A:1503:TRP:O	2.36	0.43
26:1:981:TYR:C	26:1:983:GLY:N	2.75	0.43
26:1:998:LYS:O	26:1:1001:VAL:N	2.51	0.43
26:1:1205:GLU:O	26:1:1206:ASP:C	2.62	0.43
9:f:18:ARG:N	9:f:81:THR:O	2.39	0.43
11:F:48:A:H2'	11:F:49:G:H8	1.84	0.43
11:F:91:A:H2'	11:F:92:A:H8	1.82	0.43
26:1:658:TRP:O	26:1:659:GLN:C	2.60	0.43
26:1:1279:ALA:O	26:1:1280:LEU:C	2.61	0.43
11:F:89:U:H2'	11:F:90:G:C8	2.53	0.42
20:H:3:C:H2'	20:H:4:G:H8	1.84	0.42
26:1:594:ARG:O	26:1:595:GLU:C	2.61	0.42
26:1:665:ILE:O	26:1:668:VAL:N	2.52	0.42
42:A:1805:GLY:O	42:A:1822:ILE:N	2.45	0.42
19:G:128:U:H2'	19:G:129:G:H8	1.84	0.42
19:G:130:A:H2	25:w:395:TRP:C	2.26	0.42
19:G:149:G:C8	19:G:150:U:O4	2.70	0.42
19:G:152:C:C2'	19:G:153:C:O5'	2.67	0.42
26:1:627:THR:O	26:1:630:ARG:N	2.52	0.42
26:1:706:ALA:O	26:1:707:LEU:C	2.61	0.42
19:G:137:C:H2'	19:G:138:A:C5'	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:981:TYR:O	26:1:983:GLY:N	2.52	0.42
26:1:997:LEU:O	26:1:998:LYS:C	2.62	0.42
26:1:1262:ARG:O	26:1:1263:ASP:C	2.61	0.42
28:3:1211:ILE:O	28:3:1212:ARG:C	2.63	0.42
40:I:21:U:OP2	40:I:21:U:H5	2.03	0.42
42:A:597:LYS:O	42:A:599:MET:N	2.51	0.42
11:F:92:A:H2'	11:F:93:G:C8	2.54	0.42
20:H:179:C:H2'	20:H:180:G:H8	1.83	0.42
40:I:90:G:H2'	40:I:91:A:C8	2.55	0.42
19:G:152:C:O2'	19:G:153:C:O4'	2.38	0.42
20:H:178:A:N3	20:H:178:A:H2'	2.34	0.42
26:1:429:ARG:O	26:1:432:THR:N	2.46	0.42
26:1:951:ALA:O	26:1:952:ALA:C	2.61	0.42
28:3:1189:LYS:O	28:3:1190:GLN:C	2.62	0.42
42:A:770:THR:C	42:A:772:CYS:N	2.76	0.42
1:B:31:U:H2'	1:B:32:C:H6	1.84	0.42
11:F:92:A:H2'	11:F:93:G:H8	1.83	0.42
25:w:34:ARG:O	25:w:35:ASP:C	2.62	0.42
30:5:51:GLY:HA3	30:5:56:THR:O	2.20	0.42
1:B:59:G:C2	1:B:60:G:C8	3.08	0.42
11:F:71:G:N2	40:I:4:U:O2	2.33	0.42
11:F:89:U:H2'	11:F:90:G:H8	1.84	0.42
20:H:107:A:N1	20:H:108:G:C5	2.88	0.42
26:1:647:PHE:O	26:1:648:LEU:C	2.63	0.42
26:1:854:VAL:O	26:1:856:ASP:N	2.52	0.42
26:1:1016:LEU:O	26:1:1017:LEU:C	2.62	0.42
26:1:1149:LYS:O	26:1:1150:SER:C	2.63	0.42
26:1:1256:HIS:O	26:1:1257:PRO:C	2.58	0.42
40:I:125:G:N3	10:V:63:ASN:O	2.53	0.42
1:B:98:G:OP2	1:B:98:G:H8	2.03	0.42
19:G:155:U:O4'	19:G:156:U:C5	2.73	0.42
29:4:77:ILE:C	29:4:84:ILE:H	2.19	0.42
35:N:462:THR:O	35:N:466:ILE:N	2.38	0.42
40:I:14:G:H2'	40:I:15:G:C8	2.55	0.42
1:B:55:C:O2'	42:A:642:ARG:O	2.23	0.42
2:D:441:GLY:O	2:D:693:THR:N	2.36	0.42
2:D:1583:ASP:C	2:D:1585:GLN:H	2.26	0.42
19:G:135:G:C2	20:H:42:G:N1	2.87	0.42
26:1:1018:PRO:O	26:1:1019:ARG:C	2.63	0.42
42:A:1507:SER:O	42:A:1511:GLU:N	2.48	0.42
43:C:909:GLY:HA3	43:C:930:ALA:N	2.29	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:A:HO2'	1:B:52:U:H6	1.68	0.42
20:H:168:A:H3'	20:H:169:C:C6	2.54	0.42
26:1:546:ASP:O	26:1:547:GLN:C	2.63	0.42
26:1:704:ILE:O	26:1:705:SER:C	2.61	0.42
26:1:1115:ALA:O	26:1:1116:ILE:C	2.61	0.42
26:1:1188:ALA:O	26:1:1189:SER:C	2.63	0.42
39:W:344:ILE:CA	39:W:360:LEU:N	2.81	0.42
40:I:51:A:HO2'	40:I:56:U:C5'	2.25	0.42
20:H:155:C:H2'	20:H:156:U:H5''	2.02	0.41
26:1:669:GLN:O	26:1:670:GLN:C	2.60	0.41
26:1:1078:VAL:O	26:1:1079:ASN:C	2.63	0.41
36:L:278:ASP:O	36:L:281:GLN:N	2.53	0.41
39:W:405:LYS:CA	42:A:789:GLU:CA	2.98	0.41
26:1:301:ARG:O	26:1:302:ASP:C	2.63	0.41
42:A:378:PHE:O	43:C:355:LYS:C	2.61	0.41
42:A:1593:LEU:O	42:A:1596:VAL:N	2.53	0.41
1:B:38:C:N4	1:B:39:C:N3	2.68	0.41
11:F:66:C:H2'	11:F:67:G:H8	1.85	0.41
20:H:153:A:H62	20:H:177:A:H2	1.67	0.41
26:1:318:ARG:O	26:1:321:ASP:N	2.52	0.41
26:1:408:PHE:C	26:1:409:PRO:O	2.63	0.41
26:1:806:ILE:O	26:1:807:LYS:C	2.62	0.41
26:1:834:VAL:O	26:1:835:ASP:C	2.60	0.41
26:1:887:LYS:O	26:1:888:LEU:C	2.63	0.41
26:1:1046:GLY:O	26:1:1048:GLU:N	2.52	0.41
26:1:1270:ASN:O	26:1:1271:SER:C	2.64	0.41
39:W:338:LYS:O	39:W:339:LYS:O	2.38	0.41
39:W:405:LYS:C	42:A:789:GLU:CA	2.93	0.41
19:G:125:C:OP2	19:G:125:C:C2	2.73	0.41
20:H:112:G:H8	20:H:112:G:O5'	2.04	0.41
28:3:1143:HIS:O	28:3:1144:VAL:C	2.64	0.41
42:A:1502:PHE:C	42:A:1503:TRP:O	2.63	0.41
1:B:26:A:N7	42:A:423:ASP:CA	2.83	0.41
20:H:152:G:H2'	20:H:153:A:C1'	2.51	0.41
26:1:310:TRP:O	26:1:311:ALA:C	2.62	0.41
26:1:758:ASP:O	26:1:761:TYR:N	2.54	0.41
26:1:1246:MET:O	26:1:1247:LEU:C	2.59	0.41
28:3:437:VAL:O	28:3:776:GLN:CA	2.69	0.41
26:1:600:LEU:O	26:1:604:ALA:N	2.35	0.41
26:1:671:ILE:O	26:1:672:ALA:C	2.62	0.41
32:7:52:TYR:O	32:7:53:PHE:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:W:206:ASP:C	39:W:208:GLN:H	2.29	0.41
42:A:2332:ASP:C	42:A:2334:TYR:H	2.28	0.41
20:H:153:A:H2'	20:H:154:C:H5''	1.99	0.41
26:1:763:ASN:O	26:1:764:TYR:C	2.64	0.41
1:B:26:A:N3	1:B:26:A:C5'	2.80	0.41
19:G:148:U:O2'	19:G:149:G:C8	2.70	0.41
20:H:103:U:C3'	20:H:104:U:H5'	2.50	0.41
20:H:183:G:C6	20:H:184:C:N4	2.89	0.41
26:1:301:ARG:O	26:1:304:PRO:N	2.53	0.41
1:B:5:U:H2'	1:B:6:C:C6	2.56	0.41
1:B:75:G:H2'	1:B:76:A:C8	2.55	0.41
2:D:577:LYS:O	2:D:581:SER:N	2.54	0.41
2:D:1481:ILE:C	2:D:1483:ARG:H	2.28	0.41
3:E:255:MET:O	3:E:257:ASN:N	2.54	0.41
19:G:145:U:C3'	19:G:146:C:H5'	2.42	0.41
19:G:146:C:N3	19:G:147:C:N4	2.69	0.41
20:H:171:U:H2'	20:H:172:C:O4'	2.21	0.41
21:o:160:LYS:O	21:o:161:MET:C	2.63	0.41
26:1:574:ILE:O	26:1:575:LEU:C	2.63	0.41
26:1:742:GLY:O	26:1:743:LEU:C	2.63	0.41
26:1:750:ILE:O	26:1:753:LEU:N	2.54	0.41
26:1:871:THR:O	26:1:872:ILE:C	2.63	0.41
26:1:912:ASN:O	26:1:913:GLY:C	2.63	0.41
26:1:1169:VAL:O	26:1:1172:LEU:N	2.54	0.41
26:1:1182:LEU:O	26:1:1183:VAL:C	2.63	0.41
28:3:127:GLY:O	28:3:128:ARG:C	2.63	0.41
28:3:215:LEU:O	28:3:216:GLY:C	2.64	0.41
36:L:310:GLU:O	36:L:311:SER:C	2.64	0.41
38:O:52:VAL:O	38:O:53:LYS:C	2.62	0.41
42:A:1317:TYR:O	42:A:1318:THR:C	2.63	0.41
42:A:1952:VAL:O	42:A:1956:PRO:N	2.54	0.41
26:1:862:GLU:O	26:1:864:TYR:N	2.53	0.41
26:1:1211:LEU:O	26:1:1212:LEU:C	2.64	0.41
28:3:488:GLY:C	28:3:490:THR:N	2.79	0.41
40:I:107:U:H2'	40:I:108:C:H6	1.85	0.41
1:B:101:U:H2'	1:B:102:U:C6	2.56	0.40
2:D:642:THR:C	2:D:644:GLU:H	2.30	0.40
9:f:15:TYR:O	9:f:31:PHE:N	2.40	0.40
26:1:854:VAL:C	26:1:856:ASP:H	2.28	0.40
43:C:684:LYS:O	43:C:795:VAL:N	2.45	0.40
13:r:19:ASP:C	13:r:21:ILE:N	2.77	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:549:ARG:O	26:1:550:HIS:C	2.64	0.40
26:1:750:ILE:O	26:1:751:GLY:C	2.63	0.40
28:3:1193:VAL:O	28:3:1196:GLU:N	2.54	0.40
32:7:55:ILE:O	32:7:56:ALA:C	2.63	0.40
35:N:736:LEU:O	35:N:740:PRO:N	2.54	0.40
38:O:30:PHE:O	38:O:79:CYS:CA	2.69	0.40
40:I:60:A:P	40:I:61:A:OP1	2.79	0.40
26:1:782:GLU:O	26:1:783:GLU:C	2.62	0.40
26:1:1020:LEU:O	26:1:1021:THR:C	2.64	0.40
29:4:20:LEU:O	29:4:55:GLY:HA2	2.21	0.40
31:6:30:CYS:N	31:6:35:SER:O	2.38	0.40
43:C:684:LYS:N	43:C:795:VAL:O	2.55	0.40
1:B:71:C:H2'	1:B:72:U:C6	2.55	0.40
11:F:90:G:H2'	11:F:91:A:C8	2.57	0.40
26:1:632:PHE:O	26:1:633:ALA:C	2.59	0.40
26:1:897:LEU:O	26:1:898:TYR:C	2.64	0.40
26:1:1038:LEU:O	26:1:1039:VAL:C	2.62	0.40
26:1:1162:GLY:C	26:1:1164:ASP:N	2.79	0.40
26:1:1236:GLY:O	26:1:1237:LEU:C	2.64	0.40
35:N:289:ASN:N	42:A:871:TYR:O	2.54	0.40
42:A:954:LYS:O	42:A:958:GLY:N	2.46	0.40
2:D:606:THR:C	2:D:608:LEU:H	2.30	0.40
19:G:149:G:C4	19:G:150:U:C5	3.09	0.40
20:H:152:G:H2'	20:H:152:G:N3	2.36	0.40
20:H:166:G:N3	20:H:166:G:H2'	2.37	0.40
26:1:712:LEU:O	26:1:713:ALA:C	2.64	0.40
26:1:874:LYS:O	26:1:877:GLY:HA3	2.21	0.40
40:I:14:G:H2'	40:I:15:G:H8	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	1868/2136 (88%)	1770 (95%)	93 (5%)	5 (0%)	36	72
3	E	297/357 (83%)	272 (92%)	16 (5%)	9 (3%)	3	22
4	P	70/118 (59%)	68 (97%)	2 (3%)	0	100	100
4	a	74/118 (63%)	71 (96%)	3 (4%)	0	100	100
4	k	81/118 (69%)	78 (96%)	3 (4%)	0	100	100
5	Q	69/86 (80%)	67 (97%)	2 (3%)	0	100	100
5	b	71/86 (83%)	70 (99%)	1 (1%)	0	100	100
5	m	72/86 (84%)	68 (94%)	4 (6%)	0	100	100
6	R	76/92 (83%)	70 (92%)	6 (8%)	0	100	100
6	c	76/92 (83%)	70 (92%)	6 (8%)	0	100	100
6	l	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
7	S	71/76 (93%)	67 (94%)	4 (6%)	0	100	100
7	d	67/76 (88%)	63 (94%)	4 (6%)	0	100	100
7	n	64/76 (84%)	62 (97%)	2 (3%)	0	100	100
8	T	69/126 (55%)	69 (100%)	0	0	100	100
8	e	76/126 (60%)	73 (96%)	3 (4%)	0	100	100
8	h	76/126 (60%)	75 (99%)	1 (1%)	0	100	100
9	U	60/231 (26%)	57 (95%)	3 (5%)	0	100	100
9	f	60/231 (26%)	57 (95%)	3 (5%)	0	100	100
9	i	69/231 (30%)	68 (99%)	1 (1%)	0	100	100
10	V	80/119 (67%)	76 (95%)	4 (5%)	0	100	100
10	g	89/119 (75%)	84 (94%)	5 (6%)	0	100	100
10	j	80/119 (67%)	77 (96%)	3 (4%)	0	100	100
12	q	88/95 (93%)	77 (88%)	7 (8%)	4 (4%)	2	16
13	r	71/102 (70%)	66 (93%)	3 (4%)	2 (3%)	4	24
14	s	70/139 (50%)	64 (91%)	5 (7%)	1 (1%)	9	39
15	t	71/91 (78%)	64 (90%)	4 (6%)	3 (4%)	2	17
16	x	68/80 (85%)	66 (97%)	2 (3%)	0	100	100
17	y	61/103 (59%)	56 (92%)	5 (8%)	0	100	100
18	z	57/96 (59%)	52 (91%)	4 (7%)	1 (2%)	6	33
21	o	160/255 (63%)	146 (91%)	12 (8%)	2 (1%)	9	41
22	p	92/225 (41%)	90 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	u	118/793 (15%)	106 (90%)	6 (5%)	6 (5%)	1	14
24	v	91/464 (20%)	66 (72%)	16 (18%)	9 (10%)	0	7
25	w	431/501 (86%)	385 (89%)	41 (10%)	5 (1%)	10	43
26	1	1014/1304 (78%)	821 (81%)	171 (17%)	22 (2%)	5	28
27	2	174/895 (19%)	155 (89%)	14 (8%)	5 (3%)	3	23
28	3	1160/1217 (95%)	1062 (92%)	90 (8%)	8 (1%)	18	55
29	4	76/424 (18%)	74 (97%)	2 (3%)	0	100	100
30	5	106/125 (85%)	83 (78%)	20 (19%)	3 (3%)	4	24
31	6	87/110 (79%)	76 (87%)	11 (13%)	0	100	100
32	7	64/86 (74%)	55 (86%)	8 (12%)	1 (2%)	7	37
33	J	159/683 (23%)	148 (93%)	7 (4%)	4 (2%)	4	25
34	K	335/522 (64%)	295 (88%)	26 (8%)	14 (4%)	2	17
35	N	541/941 (58%)	475 (88%)	41 (8%)	25 (5%)	2	16
36	L	222/499 (44%)	214 (96%)	8 (4%)	0	100	100
37	M	123/128 (96%)	117 (95%)	6 (5%)	0	100	100
38	O	137/142 (96%)	126 (92%)	9 (7%)	2 (2%)	8	39
39	W	461/565 (82%)	327 (71%)	77 (17%)	57 (12%)	0	4
41	X	402/820 (49%)	393 (98%)	8 (2%)	1 (0%)	43	77
42	A	2213/2335 (95%)	2046 (92%)	100 (4%)	67 (3%)	3	22
43	C	814/972 (84%)	751 (92%)	40 (5%)	23 (3%)	4	24
All	All	13158/19749 (67%)	11964 (91%)	915 (7%)	279 (2%)	8	29

All (279) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	354	PRO
2	D	957	VAL
2	D	1584	ILE
3	E	193	THR
12	q	55	LEU
15	t	60	THR
15	t	61	PRO
15	t	70	ASP
23	u	301	PRO
24	v	139	PRO

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Mol	Chain	Res	Type
24	v	160	GLU
24	v	161	PRO
24	v	162	PRO
24	v	165	ARG
24	v	218	PRO
25	w	284	ARG
26	1	113	ALA
26	1	208	PRO
26	1	416	PRO
26	1	418	PRO
26	1	456	VAL
26	1	941	ASN
26	1	1105	GLU
26	1	1110	VAL
27	2	597	PHE
28	3	406	PRO
30	5	99	GLN
33	J	541	VAL
34	K	171	PRO
34	K	227	GLN
34	K	334	SER
34	K	480	PRO
34	K	514	ARG
35	N	12	PRO
35	N	163	VAL
35	N	355	GLY
35	N	370	PRO
35	N	420	ARG
35	N	741	HIS
35	N	841	PRO
35	N	918	ASP
39	W	146	ARG
39	W	178	ASN
39	W	183	ASP
39	W	206	ASP
39	W	207	LYS
39	W	208	GLN
39	W	231	LYS
39	W	265	PRO
39	W	307	SER
39	W	340	LYS
39	W	345	VAL

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Mol	Chain	Res	Type
39	W	350	GLN
39	W	355	ILE
39	W	360	LEU
39	W	361	PRO
39	W	364	ASP
39	W	394	ASP
39	W	406	GLU
39	W	411	PRO
39	W	414	PRO
39	W	415	LEU
39	W	419	LEU
39	W	458	THR
39	W	479	ASP
39	W	484	LEU
39	W	486	GLU
39	W	532	LEU
39	W	556	ASP
42	A	63	PRO
42	A	166	PHE
42	A	308	ILE
42	A	331	TRP
42	A	363	HIS
42	A	371	LEU
42	A	373	ASP
42	A	424	ILE
42	A	425	PRO
42	A	442	LYS
42	A	471	TYR
42	A	571	ALA
42	A	598	LEU
42	A	629	PHE
42	A	631	ALA
42	A	697	MET
42	A	698	PRO
42	A	799	PRO
42	A	1013	ASN
42	A	1124	ASN
42	A	1186	LEU
42	A	1202	THR
42	A	1511	GLU
42	A	1520	ASN
42	A	1521	ALA

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Mol	Chain	Res	Type
42	A	1604	LEU
42	A	1760	GLU
42	A	2016	ILE
42	A	2018	ALA
43	C	333	ASP
43	C	388	VAL
43	C	427	PHE
43	C	444	GLY
43	C	457	VAL
43	C	458	ASP
43	C	475	MET
43	C	516	LEU
43	C	572	GLU
43	C	825	PRO
2	D	151	LYS
12	q	74	ALA
13	r	97	PRO
14	s	12	ASN
21	o	160	LYS
23	u	223	LYS
23	u	280	VAL
25	w	277	THR
28	3	772	ALA
30	5	104	LYS
34	K	198	LEU
34	K	265	LEU
35	N	150	ALA
35	N	824	PRO
35	N	840	ASP
39	W	105	CYS
39	W	107	TYR
39	W	186	LEU
39	W	211	LEU
39	W	339	LYS
39	W	341	LYS
39	W	365	LEU
39	W	380	GLN
39	W	395	LEU
39	W	457	PHE
39	W	462	PHE
39	W	502	ASN
39	W	531	ASP

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Mol	Chain	Res	Type
41	X	666	PRO
42	A	531	THR
42	A	729	PRO
42	A	767	VAL
42	A	1015	VAL
42	A	1092	ILE
42	A	1126	VAL
42	A	1185	LEU
42	A	1308	PRO
43	C	156	GLU
43	C	354	ARG
43	C	367	ARG
43	C	440	SER
43	C	824	THR
43	C	868	LEU
3	E	60	MET
3	E	88	ARG
3	E	256	ASP
25	w	177	ARG
25	w	393	PRO
26	1	437	PRO
27	2	510	TYR
34	K	261	PRO
35	N	143	SER
35	N	774	PRO
38	O	74	GLU
39	W	400	LEU
39	W	410	ILE
39	W	417	ASN
39	W	466	LYS
39	W	509	PRO
42	A	212	PRO
42	A	376	GLU
42	A	381	PRO
42	A	709	ILE
42	A	734	PRO
42	A	824	PRO
42	A	1203	SER
42	A	1204	TYR
42	A	1503	TRP
42	A	1677	GLU
42	A	1758	PRO

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Mol	Chain	Res	Type
42	A	1947	ASN
43	C	237	LEU
43	C	615	PRO
3	E	162	ARG
13	r	96	ALA
21	o	32	PRO
23	u	300	THR
26	1	112	ILE
26	1	523	ALA
26	1	909	VAL
26	1	1006	MET
27	2	463	ALA
27	2	599	THR
28	3	529	ALA
28	3	578	THR
30	5	75	ASP
33	J	535	GLU
33	J	536	ASP
33	J	615	ASP
34	K	229	GLY
34	K	259	SER
34	K	405	GLY
35	N	324	LYS
35	N	374	ARG
35	N	777	PRO
35	N	809	ASN
35	N	855	ARG
39	W	176	PRO
39	W	376	ASN
39	W	418	ILE
39	W	425	ILE
39	W	491	VAL
42	A	188	LEU
42	A	380	LEU
42	A	526	PRO
42	A	903	SER
42	A	1305	SER
43	C	856	HIS
3	E	159	PRO
12	q	73	PRO
24	v	141	ILE
24	v	217	PRO

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Mol	Chain	Res	Type
26	1	1075	ARG
26	1	1186	GLN
28	3	95	SER
28	3	229	GLU
35	N	421	ILE
39	W	337	THR
39	W	434	LYS
42	A	349	ALA
42	A	437	ALA
42	A	1206	GLU
43	C	360	ALA
43	C	573	GLU
3	E	270	LYS
18	z	34	ILE
24	v	220	PRO
26	1	326	THR
26	1	932	ILE
26	1	1047	ALA
28	3	407	ILE
35	N	307	HIS
35	N	325	LEU
38	O	77	ASP
39	W	357	THR
39	W	413	VAL
42	A	370	PRO
42	A	619	GLY
42	A	1198	PRO
42	A	1275	ARG
42	A	1955	LYS
42	A	2012	LEU
43	C	361	PRO
3	E	149	GLY
26	1	417	PRO
34	K	459	PRO
34	K	479	HIS
35	N	739	CYS
39	W	222	PRO
39	W	262	ILE
42	A	771	VAL
23	u	221	PRO
26	1	223	THR
42	A	358	PRO

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Mol	Chain	Res	Type
42	A	1118	PRO
25	w	229	TRP
26	1	409	PRO
27	2	586	ILE
28	3	1204	VAL
34	K	446	PRO
35	N	323	GLY
35	N	369	LEU
2	D	585	ILE
3	E	324	PRO
23	u	298	PRO
26	1	1031	VAL
32	7	64	VAL
42	A	894	VAL
12	q	52	PRO
35	N	743	THR
43	C	778	PRO

5.3.2 Protein sidechains [i](#)

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

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	114/117 (97%)	38 (33%)	2 (1%)
11	F	65/107 (60%)	10 (15%)	2 (3%)
19	G	41/274 (14%)	28 (68%)	9 (21%)
20	H	105/188 (55%)	25 (23%)	2 (1%)
40	I	112/144 (77%)	31 (27%)	4 (3%)
All	All	437/830 (52%)	132 (30%)	19 (4%)

All (132) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B	8	G
1	B	10	U
1	B	20	G
1	B	21	A
1	B	22	U
1	B	23	C

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Mol	Chain	Res	Type
1	B	24	G
1	B	25	C
1	B	26	A
1	B	27	U
1	B	34	U
1	B	36	C
1	B	38	C
1	B	39	C
1	B	41	U
1	B	42	U
1	B	45	C
1	B	48	A
1	B	52	U
1	B	53	U
1	B	54	U
1	B	57	G
1	B	68	C
1	B	69	A
1	B	70	A
1	B	79	C
1	B	80	U
1	B	83	A
1	B	88	A
1	B	90	U
1	B	92	U
1	B	93	U
1	B	94	U
1	B	95	G
1	B	96	A
1	B	97	G
1	B	98	G
1	B	109	G
11	F	6	C
11	F	7	G
11	F	9	U
11	F	51	U
11	F	52	U
11	F	53	A
11	F	70	A
11	F	103	U
11	F	104	U
11	F	106	U

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Mol	Chain	Res	Type
19	G	123	U
19	G	124	U
19	G	125	C
19	G	126	C
19	G	127	U
19	G	128	U
19	G	129	G
19	G	130	A
19	G	135	G
19	G	136	U
19	G	137	C
19	G	140	A
19	G	144	A
19	G	145	U
19	G	146	C
19	G	147	C
19	G	148	U
19	G	149	G
19	G	150	U
19	G	151	C
19	G	152	C
19	G	154	U
19	G	156	U
19	G	157	U
19	G	159	U
19	G	161	U
19	G	162	C
19	G	163	C
20	H	31	G
20	H	37	U
20	H	40	C
20	H	45	C
20	H	47	U
20	H	51	A
20	H	65	U
20	H	105	G
20	H	106	G
20	H	112	G
20	H	143	A
20	H	147	G
20	H	152	G
20	H	153	A

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Mol	Chain	Res	Type
20	H	154	C
20	H	156	U
20	H	157	G
20	H	164	C
20	H	166	G
20	H	167	U
20	H	168	A
20	H	169	C
20	H	177	A
20	H	178	A
20	H	179	C
40	I	21	U
40	I	25	A
40	I	26	G
40	I	36	U
40	I	41	C
40	I	44	A
40	I	45	G
40	I	56	U
40	I	58	C
40	I	59	U
40	I	60	A
40	I	61	A
40	I	62	U
40	I	84	C
40	I	85	G
40	I	90	G
40	I	100	A
40	I	103	A
40	I	109	G
40	I	114	U
40	I	115	G
40	I	118	A
40	I	119	A
40	I	120	U
40	I	121	U
40	I	122	U
40	I	124	U
40	I	125	G
40	I	126	A
40	I	127	C
40	I	144	G

All (19) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	B	78	U
1	B	94	U
11	F	51	U
11	F	52	U
19	G	123	U
19	G	136	U
19	G	143	U
19	G	148	U
19	G	150	U
19	G	151	C
19	G	153	C
19	G	155	U
19	G	156	U
20	H	156	U
20	H	168	A
40	I	43	G
40	I	58	C
40	I	99	C
40	I	114	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is 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
45	GTP	C	1500	46	33,34,34	1.54	5 (15%)	50,54,54	1.66	6 (12%)
44	IHP	A	3000	-	36,36,36	0.82	0	60,60,60	1.26	3 (5%)

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
45	GTP	C	1500	46	-	3/22/38/38	0/3/3/3
44	IHP	A	3000	-	-	5/30/54/54	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	C	1500	GTP	PA-O3A	4.30	1.64	1.59
45	C	1500	GTP	C6-N1	-3.44	1.32	1.38
45	C	1500	GTP	C5-C4	2.70	1.46	1.38
45	C	1500	GTP	C4-N9	-2.28	1.32	1.38
45	C	1500	GTP	C5-N7	-2.24	1.34	1.39

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	C	1500	GTP	C5-C4-N3	-5.94	118.94	128.39
45	C	1500	GTP	C2-N3-C4	4.78	120.53	112.30
45	C	1500	GTP	N9-C4-N3	3.82	133.58	125.95
44	A	3000	IHP	C6-C5-C4	3.79	118.73	110.43
45	C	1500	GTP	C6-C5-N7	3.28	136.26	130.29
44	A	3000	IHP	P5-O15-C5	-2.79	115.98	123.43
45	C	1500	GTP	C4-C5-N7	-2.51	106.70	110.67
44	A	3000	IHP	C5-C4-C3	2.45	115.80	110.43
45	C	1500	GTP	O4'-C1'-N9	2.04	112.98	108.36

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	C	1500	GTP	C5'-O5'-PA-O3A
44	A	3000	IHP	C3-O13-P3-O23

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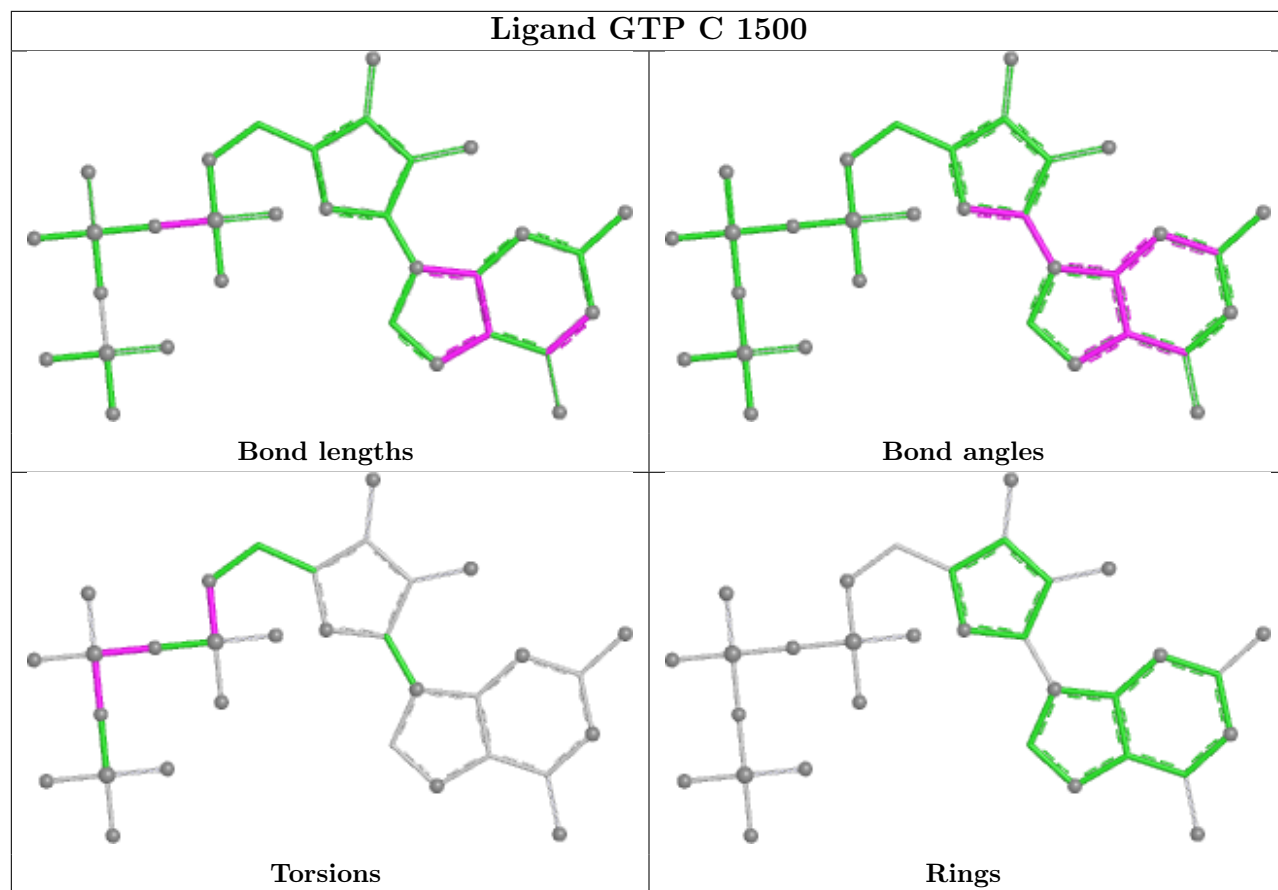
Mol	Chain	Res	Type	Atoms
44	A	3000	IHP	C2-O12-P2-O42
44	A	3000	IHP	C5-O15-P5-O25
45	C	1500	GTP	PG-O3B-PB-O2B
44	A	3000	IHP	C6-O16-P6-O46
44	A	3000	IHP	C1-O11-P1-O21
45	C	1500	GTP	PA-O3A-PB-O2B

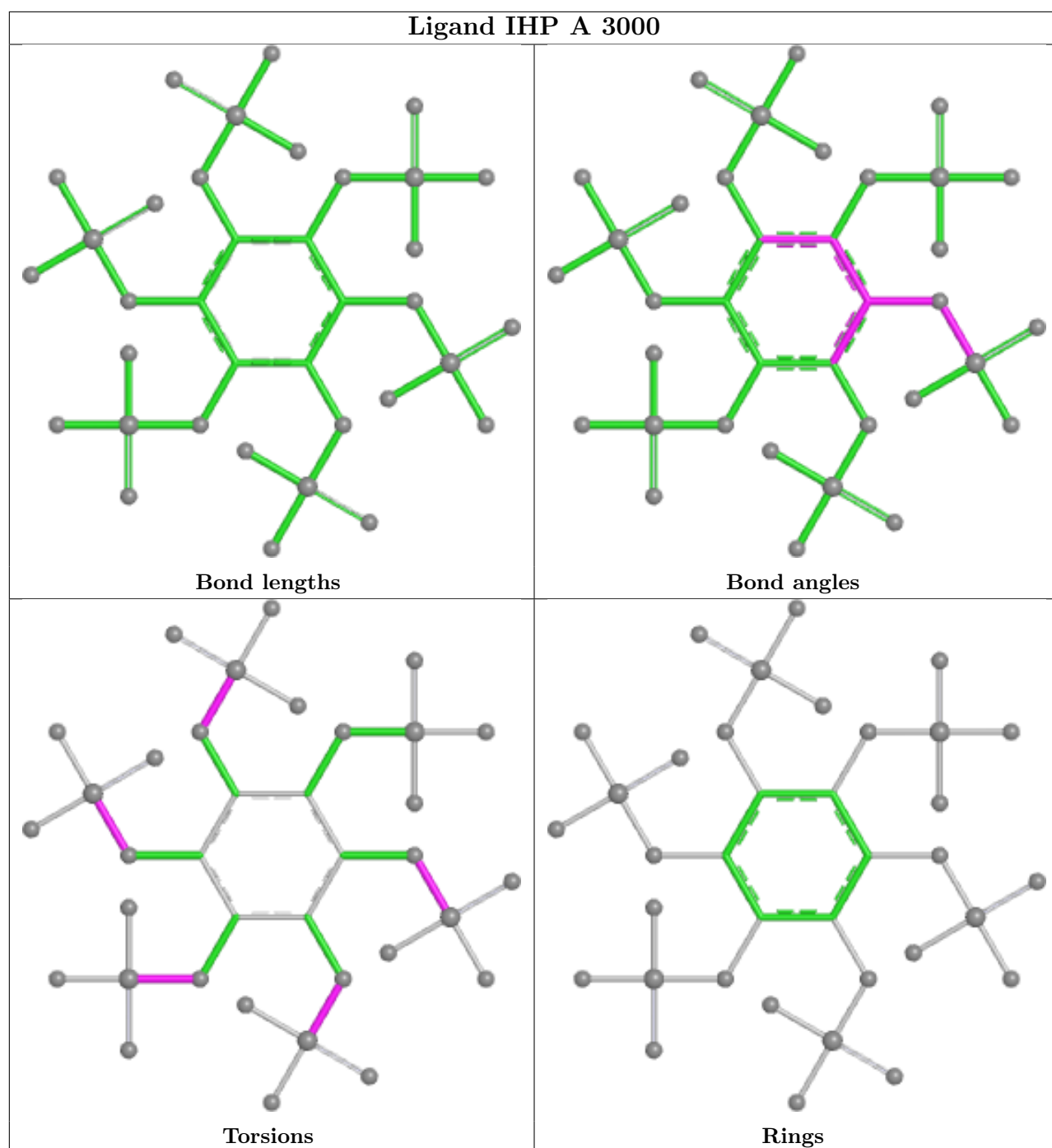
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	C	1500	GTP	4	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.

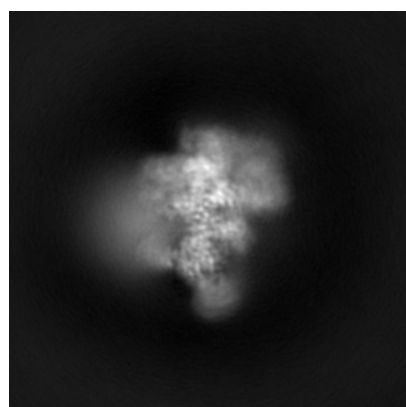
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9621. These allow visual inspection of the internal detail of the map and identification of artifacts.

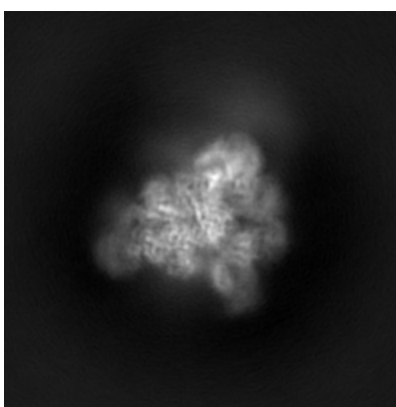
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

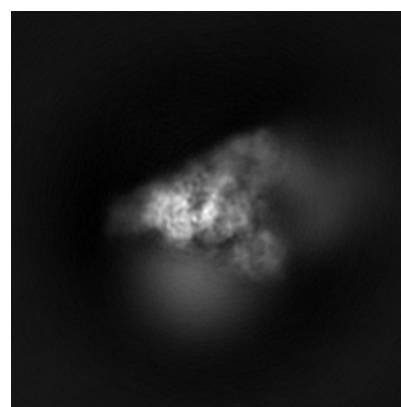
6.1.1 Primary map



X



Y

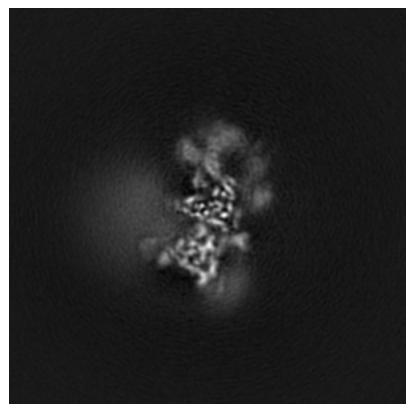


Z

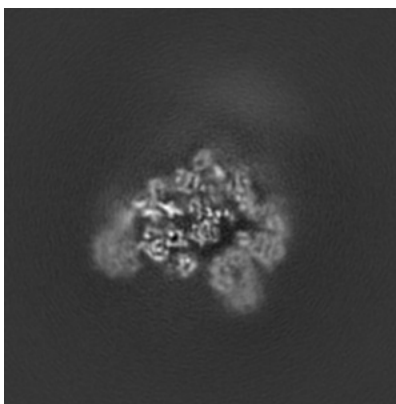
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

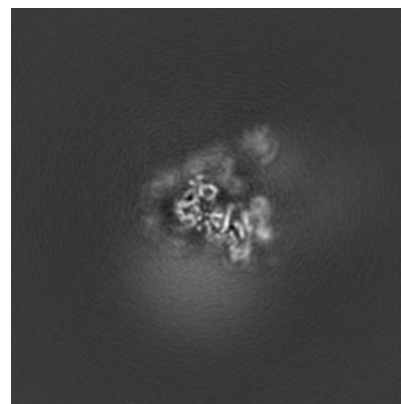
6.2.1 Primary map



X Index: 200



Y Index: 200

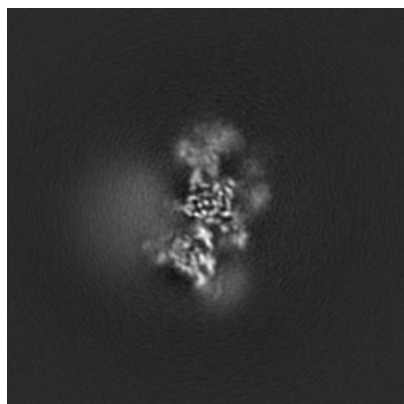


Z Index: 200

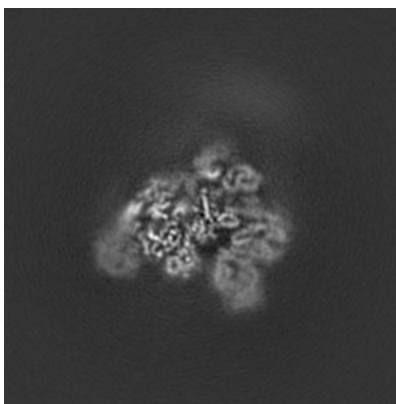
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

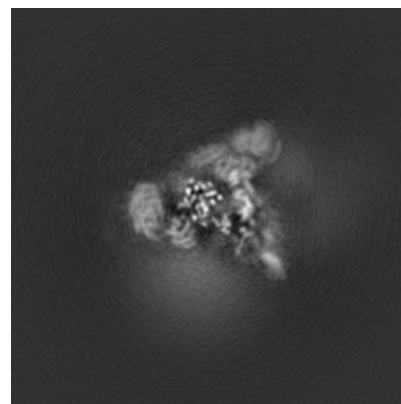
6.3.1 Primary map



X Index: 197



Y Index: 193

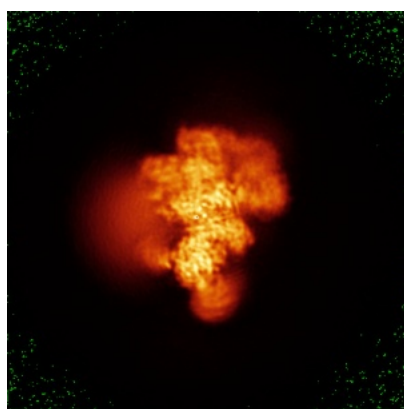


Z Index: 213

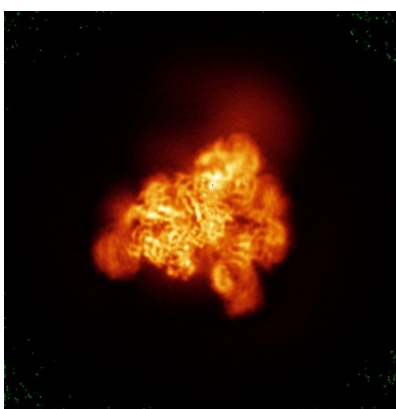
The images above show the largest variance slices of the map in three orthogonal directions.

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

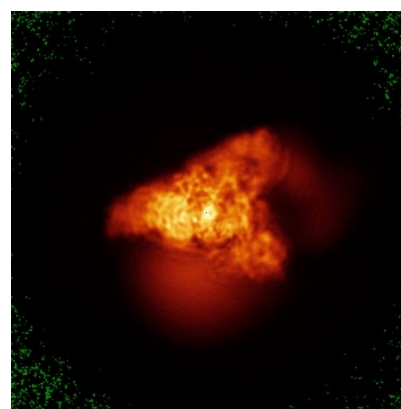
6.4.1 Primary map



X



Y

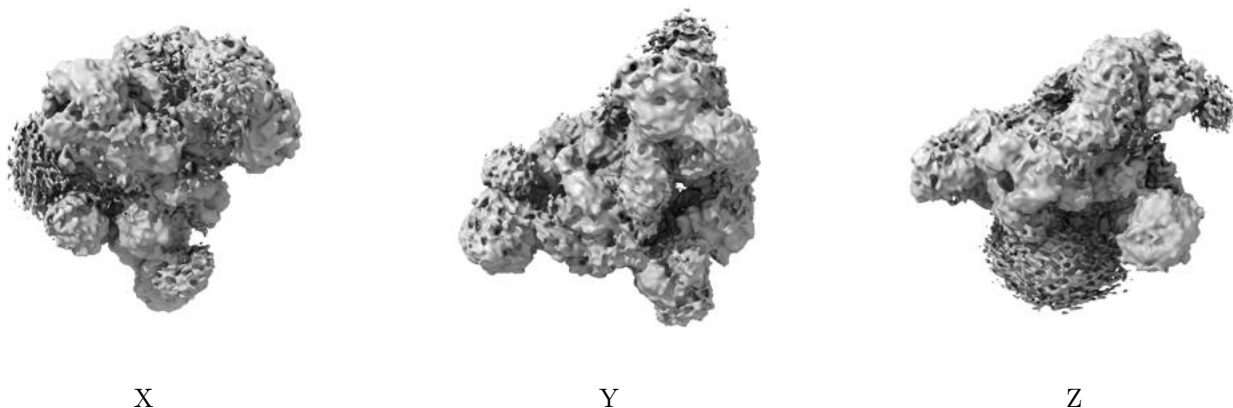


Z

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.

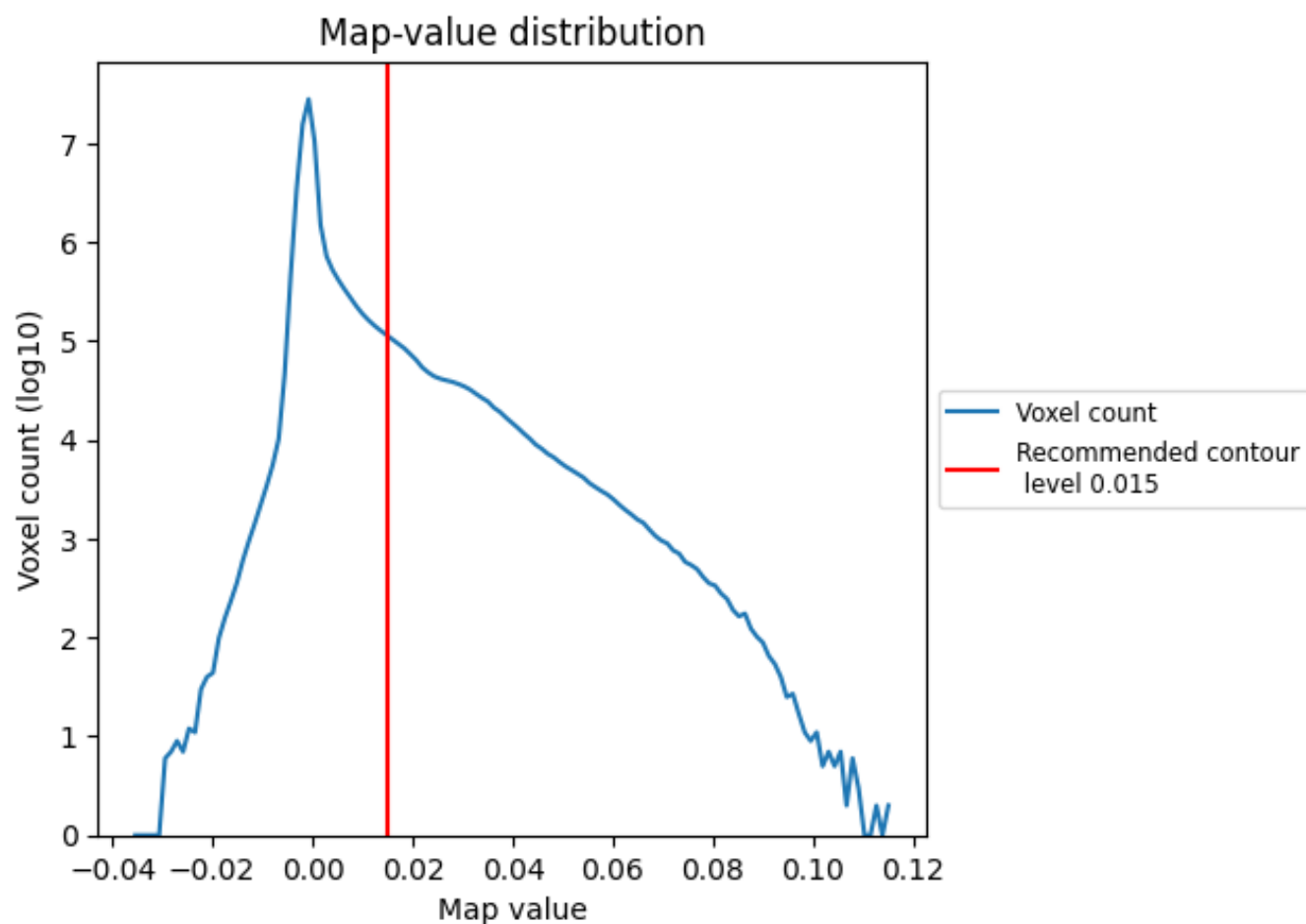
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

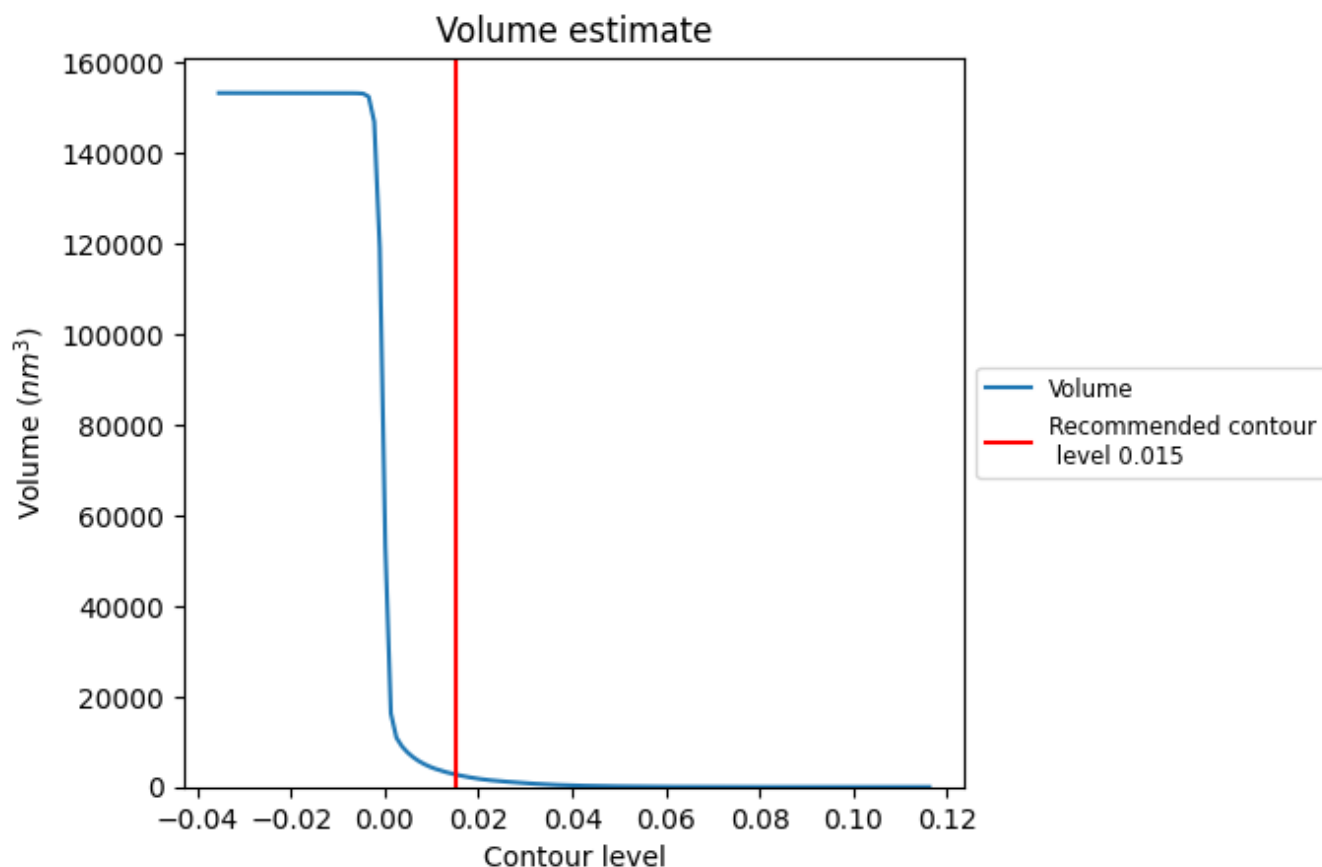
This section contains the results of statistical analysis of the map.

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.

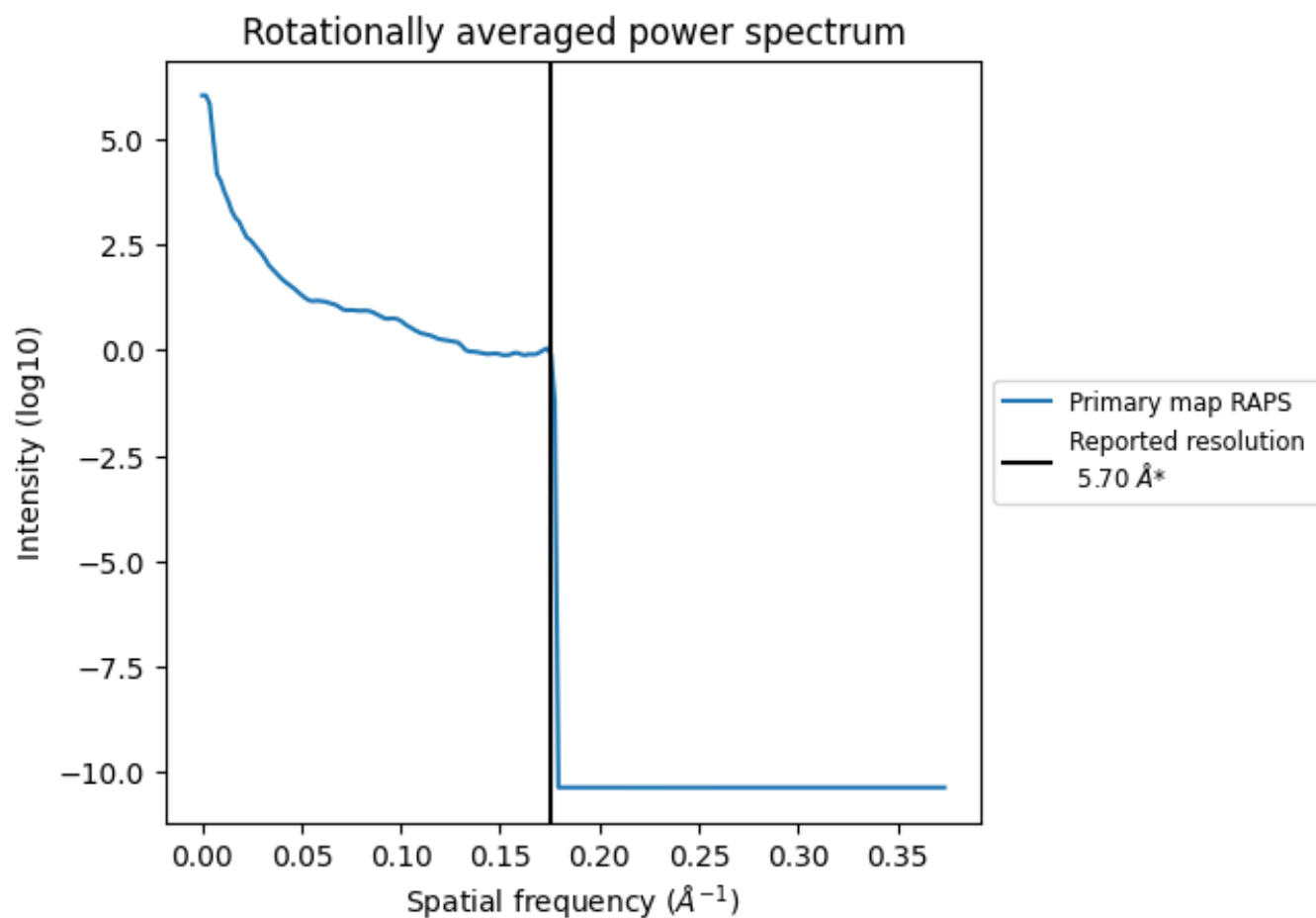
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2784 nm³; this corresponds to an approximate mass of 2515 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 0.175 Å⁻¹

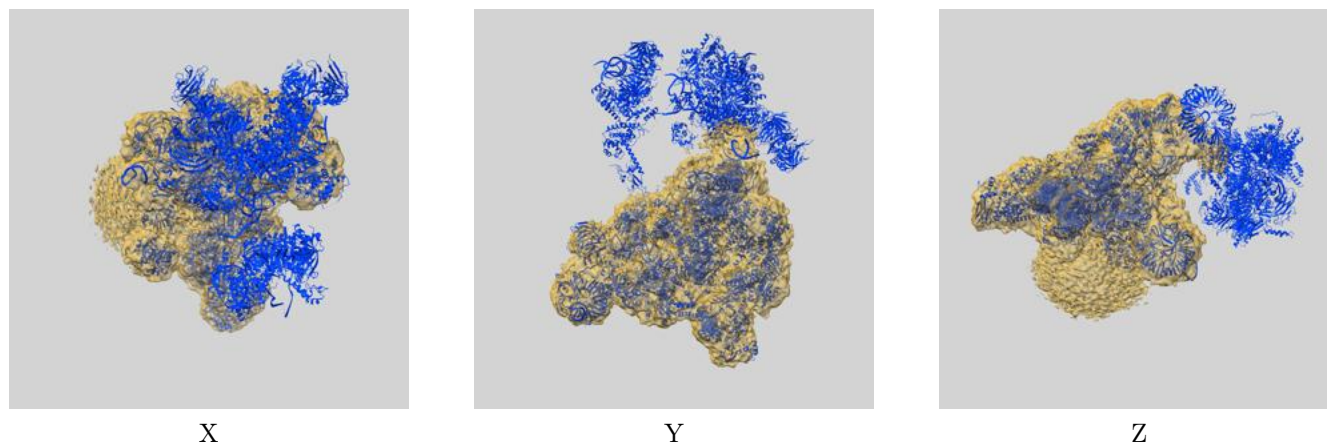
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

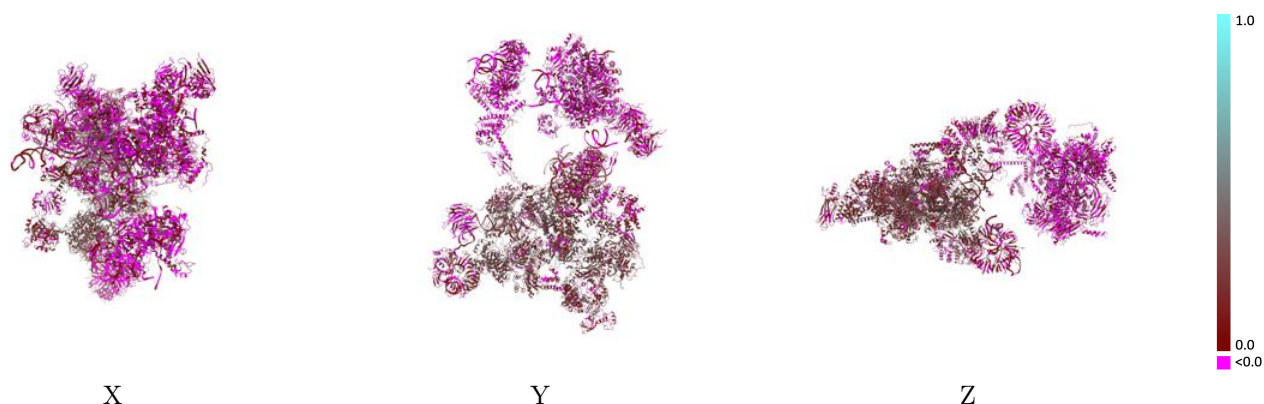
This section contains information regarding the fit between EMDB map EMD-9621 and PDB model 6AH0. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

9.1 Map-model overlay [i](#)



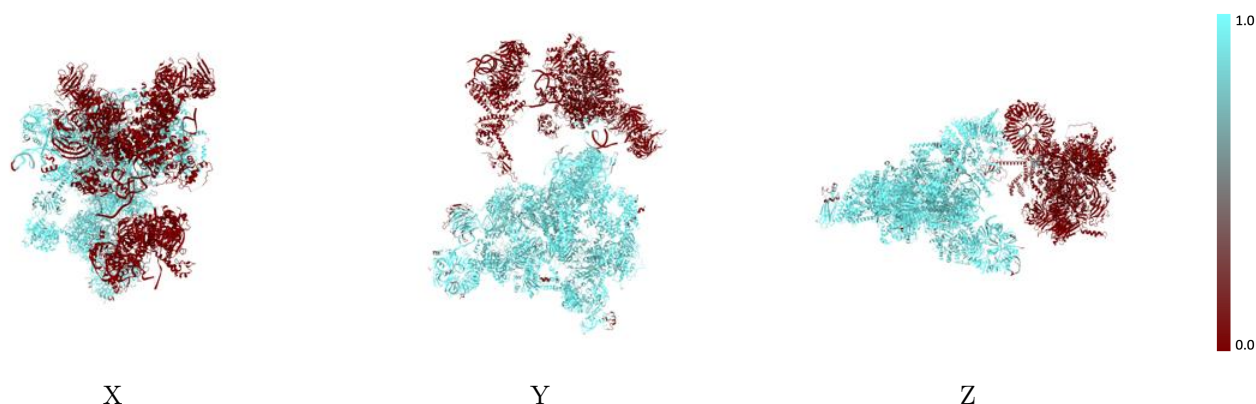
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



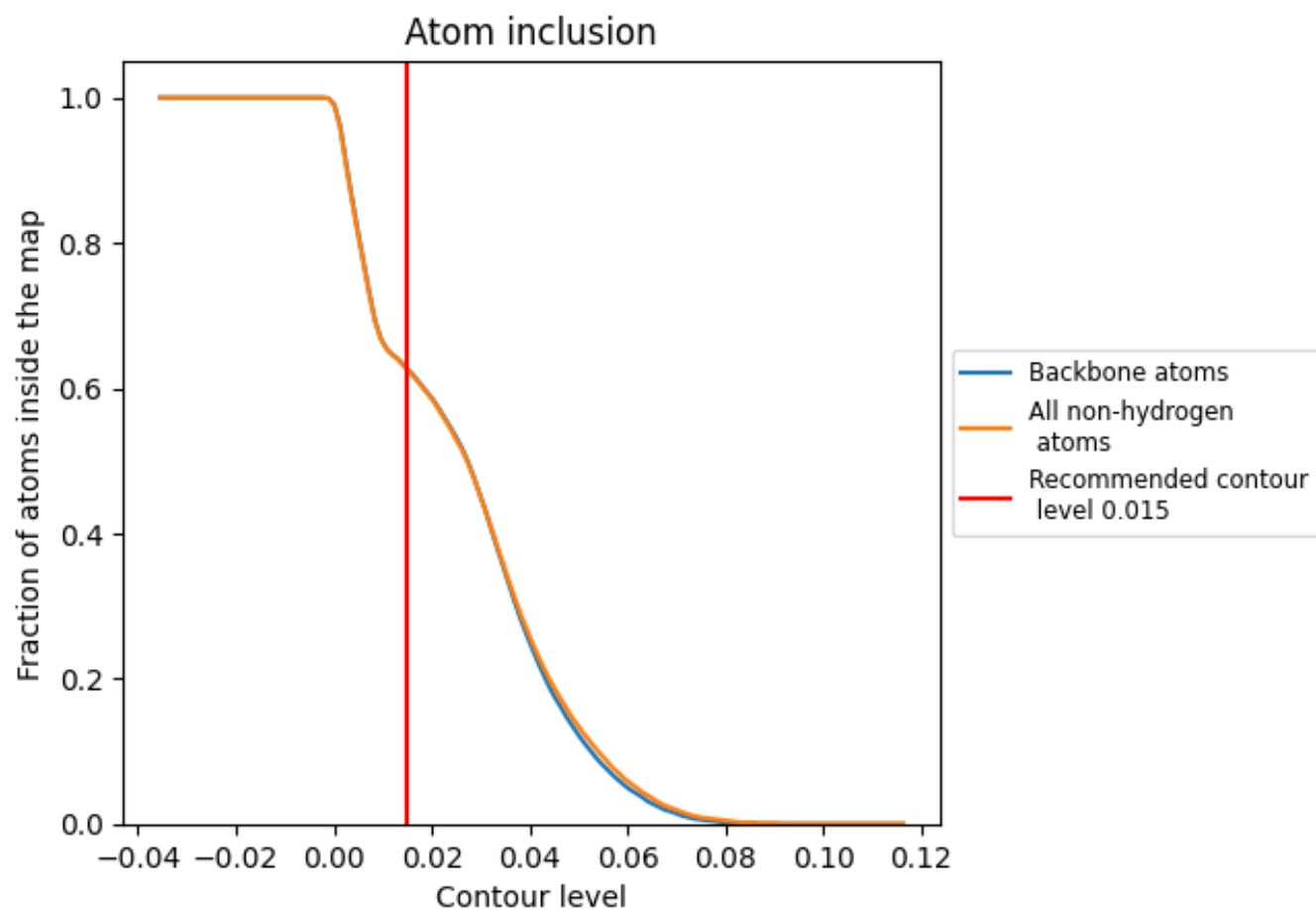
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



At the recommended contour level, 63% of all backbone atoms, 63% 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	 0.6260	 0.1190
1	 0.0190	 0.0020
2	 0.0360	 0.0050
3	 0.0000	 -0.0030
4	 0.0000	 -0.0090
5	 0.0000	 -0.0110
6	 0.0000	 -0.0050
7	 0.0000	 0.0920
A	 0.9900	 0.2830
B	 0.9360	 0.1220
C	 1.0000	 0.2810
D	 0.9740	 0.1980
E	 0.7270	 -0.0190
F	 0.7860	 0.1010
G	 0.0000	 0.0150
H	 0.0530	 -0.0000
I	 0.9330	 0.1200
J	 0.9580	 0.0740
K	 0.9940	 0.0920
L	 0.9870	 0.1530
M	 0.9900	 0.2130
N	 0.9580	 0.1260
O	 0.9750	 0.2170
P	 0.9570	 0.1190
Q	 0.9210	 0.0870
R	 0.8920	 0.0800
S	 0.9230	 0.1050
T	 0.9060	 0.0760
U	 0.9100	 0.0820
V	 0.9550	 0.1500
W	 0.9250	 0.1840
X	 0.9610	 0.1200
a	 0.9650	 0.1010
b	 0.8400	 0.0480
c	 0.9040	 0.0990



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Chain	Atom inclusion	Q-score
d	 0.8760	 0.1480
e	 1.0000	 0.2090
f	 1.0000	 0.1490
g	 0.9290	 0.1560
h	 0.0000	 0.0120
i	 0.0000	 -0.0140
j	 0.0000	 -0.0180
k	 0.0000	 0.0390
l	 0.0000	 0.0120
m	 0.0000	 0.0380
n	 0.0000	 0.0170
o	 0.0000	 -0.0050
p	 0.0000	 0.0060
q	 0.0000	 0.0370
r	 0.0000	 0.0420
s	 0.0000	 -0.0520
t	 0.0000	 -0.0050
u	 0.0000	 0.0100
v	 0.0000	 0.0170
w	 0.0000	 -0.0140
x	 0.0000	 0.0050
y	 0.0000	 0.0190
z	 0.0000	 -0.0140