



Full wwPDB EM Validation Report ⓘ

Jul 21, 2026 – 02:58 pm BST

PDB ID : 9S2G / pdb_00009s2g
EMDB ID : EMD-19942
Title : Revised structure of the fission yeast defective B* spliceosome (B*d)
Authors : Boreikaite, V.; Vorlaender, M.K.; Plaschka, C.
Deposited on : 2025-07-21
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

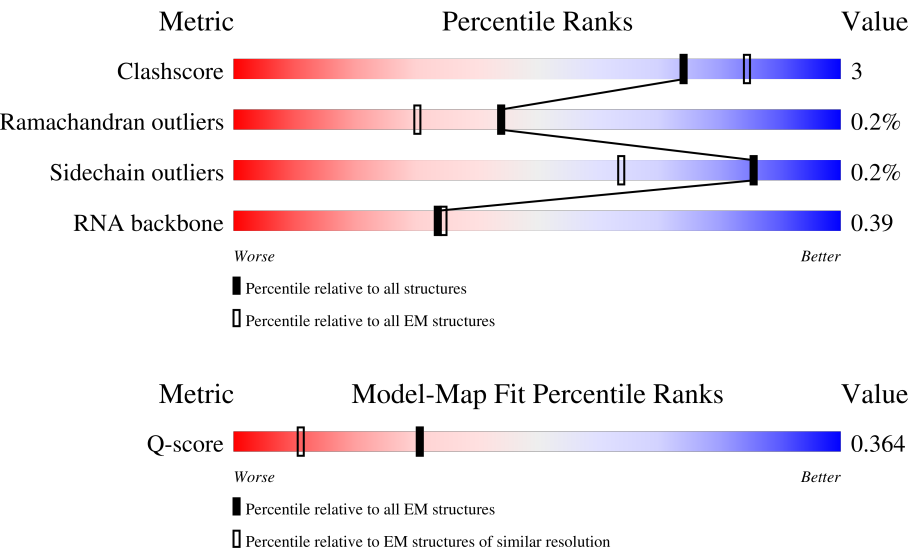
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	1	30	47% 43% 50% . .
2	2	186	7% 9% . . 87%
3	3	384	14% 40% . 57%

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Mol	Chain	Length	Quality of chain
4	35	647	
5	5	120	
6	6	99	
7	A	2363	
8	C	984	
9	CW	887	
10	E	340	
11	GP	534	
12	I	790	
13	J	674	
14	K	187	
15	L	757	
16	LG	198	
17	M	229	
18	N	146	
19	O	354	
20	O2	388	
21	P	265	
22	PX	361	
23	Q	1284	
24	R	557	
25	S	155	
26	SR	293	
27	T	473	
28	TF	797	

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Mol	Chain	Length	Quality of chain
29	W	558	
30	YB	299	
31	Z	142	
32	a	97	
33	b	147	
34	c	117	
35	d	115	
36	e	84	
37	f	78	
38	g	77	
39	q	488	
39	r	488	
39	s	488	
39	t	488	

2 Entry composition

There are 44 unique types of molecules in this entry. The entry contains 99219 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 Pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	30	Total	C	N	O	P	0	0
			563	250	80	203	30		

- Molecule 2 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	24	Total	C	N	O	P	0	0
			500	224	79	173	24		

- Molecule 3 is a protein called Stress response protein bis1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	166	Total	C	N	O	S	0	0
			1329	838	221	268	2		

- Molecule 4 is a protein called Putative pre-mRNA-splicing factor ATP-dependent RNA helicase C20H4.09.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	35	626	Total	C	N	O	S	0	0
			4980	3193	835	933	19		

- Molecule 5 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	102	Total	C	N	O	P	0	0
			2149	963	358	726	102		

- Molecule 6 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	92	Total	C	N	O	P	0	0
			1970	882	365	631	92		

- Molecule 7 is a protein called Pre-mRNA-splicing factor spp42.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	1986	Total	C	N	O	S	0	0
			16424	10532	2887	2938	67		

- Molecule 8 is a protein called Pre-mRNA-splicing factor cwf10.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	918	Total	C	N	O	S	0	0
			7298	4650	1251	1362	35		

- Molecule 9 is a protein called Pre-mRNA-splicing factor cwf22.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	CW	204	Total	C	N	O	S	0	0
			1678	1071	280	315	12		

- Molecule 10 is a protein called Pre-mRNA-splicing factor cwf17.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	E	301	Total	C	N	O	S	0	0
			2328	1460	415	442	11		

- Molecule 11 is a protein called Uncharacterized protein C20H4.06c (GPATCH1).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	GP	222	Total	C	N	O	S	0	0
			1770	1108	305	352	5		

- Molecule 12 is a protein called Pre-mRNA-splicing factor cwf3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	654	Total	C	N	O	S	0	0
			5467	3534	918	996	19		

- Molecule 13 is a protein called Pre-mRNA-splicing factor cwf4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	603	Total	C	N	O	S	0	0
			5108	3280	892	913	23		

- Molecule 14 is a protein called Pre-mRNA-splicing factor cwf7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	155	Total	C	N	O	S	0	0
			1232	766	220	243	3		

- Molecule 15 is a protein called Pre-mRNA-splicing factor cdc5.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L	519	Total	C	N	O	S	0	0
			4302	2688	785	818	11		

- Molecule 16 is a protein called Uncharacterized protein C5E4.10c (LENG1).

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LG	57	Total	C	N	O	S	0	0
			472	296	84	88	4		

- Molecule 17 is a protein called Pre-mRNA-splicing factor syf2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	98	Total	C	N	O	S	0	0
			845	522	157	166			

- Molecule 18 is a protein called Pre-mRNA-splicing factor cwf14.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	144	Total	C	N	O	S	0	0
			1177	733	216	215	13		

- Molecule 19 is a protein called Pre-mRNA-splicing factor cwf5.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	O	234	Total	C	N	O	S	0	0
			1818	1131	329	343	15		

- Molecule 20 is a protein called Pre-mRNA-splicing factor cwf2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	O2	271	Total	C	N	O	S	0	0
			2178	1354	397	416	11		

- Molecule 21 is a protein called Pre-mRNA-splicing factor cwf15.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	P	90	Total	C	N	O	S	0	0
			753	467	146	139	1		

- Molecule 22 is a protein called Uncharacterized protein C17A2.08c (PAXBP1).

Mol	Chain	Residues	Atoms					AltConf	Trace
22	PX	30	Total	C	N	O	S	0	0
			248	153	44	50	1		

- Molecule 23 is a protein called Pre-mRNA-splicing factor cwf11.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Q	1284	Total	C	N	O	S	0	0
			10462	6715	1732	1970	45		

- Molecule 24 is a protein called Pre-mRNA-processing protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	R	286	Total	C	N	O	S	0	0
			2272	1427	419	419	7		

- Molecule 25 is a protein called Peptidyl-prolyl cis-trans isomerase ppi1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	S	154	Total	C	N	O	S	0	0
			1180	750	202	224	4		

- Molecule 26 is a protein called Pre-mRNA-splicing factor cwf21.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	SR	104	Total	C	N	O	S	0	0
			822	503	148	169	2		

- Molecule 27 is a protein called Pre-mRNA-splicing factor prp5.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	T	429	Total	C	N	O	S	0	0
			3343	2104	600	625	14		

- Molecule 28 is a protein called G-patch domain-containing protein C1486.03.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	TF	461	Total	C	N	O	S	0	0
			3813	2488	616	693	16		

- Molecule 29 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	W	152	Total	C	N	O	S	0	0
			1035	644	185	205	1		

- Molecule 30 is a protein called Protein saf4.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	YB	60	Total	C	N	O	0	0
			487	304	89	94		

- Molecule 31 is a protein called Pre-mRNA-splicing factor cwf18.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Z	42	Total	C	N	O	S	0	0
			353	217	65	70	1		

- Molecule 32 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	a	96	Total	C	N	O	S	0	0
			761	470	147	137	7		

- Molecule 33 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	b	97	Total	C	N	O	S	0	0
			726	462	129	130	5		

- Molecule 34 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	c	81	Total	C	N	O	S	0	0
			638	407	109	118	4		

- Molecule 35 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	d	102	Total	C	N	O	S	0	0
			820	516	150	150	4		

- Molecule 36 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	e	80	Total	C	N	O	S	0	0
			653	422	113	116	2		

- Molecule 37 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	f	73	Total	C	N	O	S	0	0
			574	373	95	104	2		

- Molecule 38 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	g	73	Total	C	N	O	S	0	0
			573	366	98	108	1		

- Molecule 39 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	q	132	Total	C	N	O	S	0	0
			1055	664	181	207	3		
39	r	430	Total	C	N	O	S	0	0
			2871	1806	492	564	9		
39	s	131	Total	C	N	O	S	0	0
			1044	655	180	206	3		
39	t	134	Total	C	N	O	S	0	0
			1069	671	183	212	3		

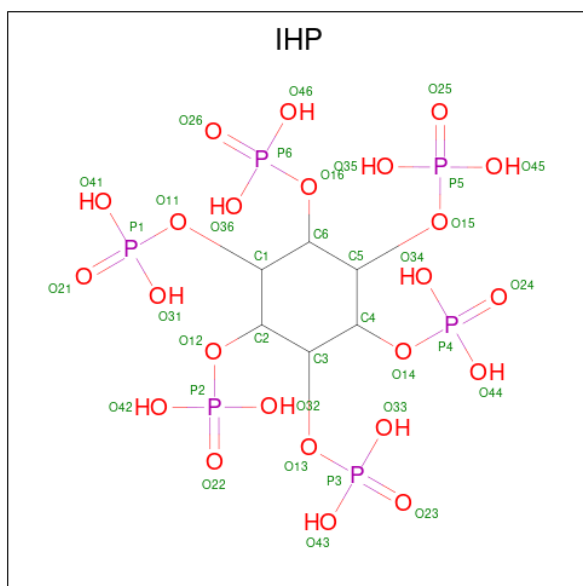
- Molecule 40 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
40	6	3	Total	Mg	0
			3	3	
40	C	1	Total	Mg	0
			1	1	

- Molecule 41 is POTASSIUM ION (CCD ID: K) (formula: K).

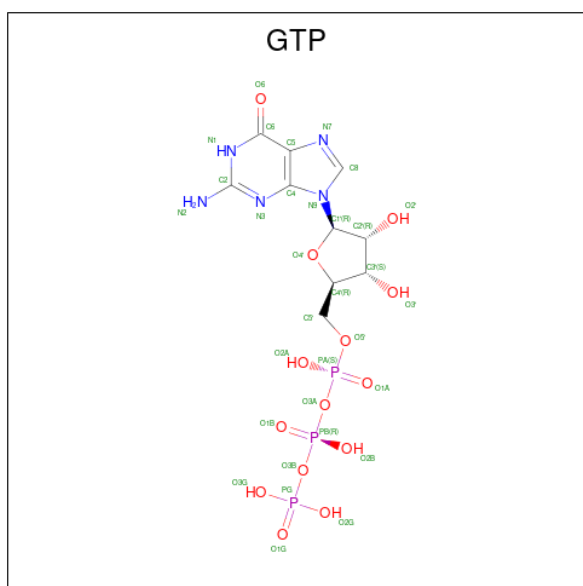
Mol	Chain	Residues	Atoms		AltConf
41	6	1	Total	K	0
			1	1	

- Molecule 42 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$).



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

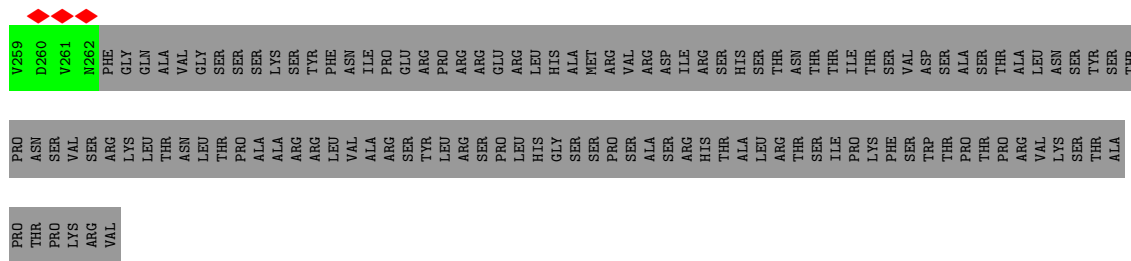
- Molecule 43 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



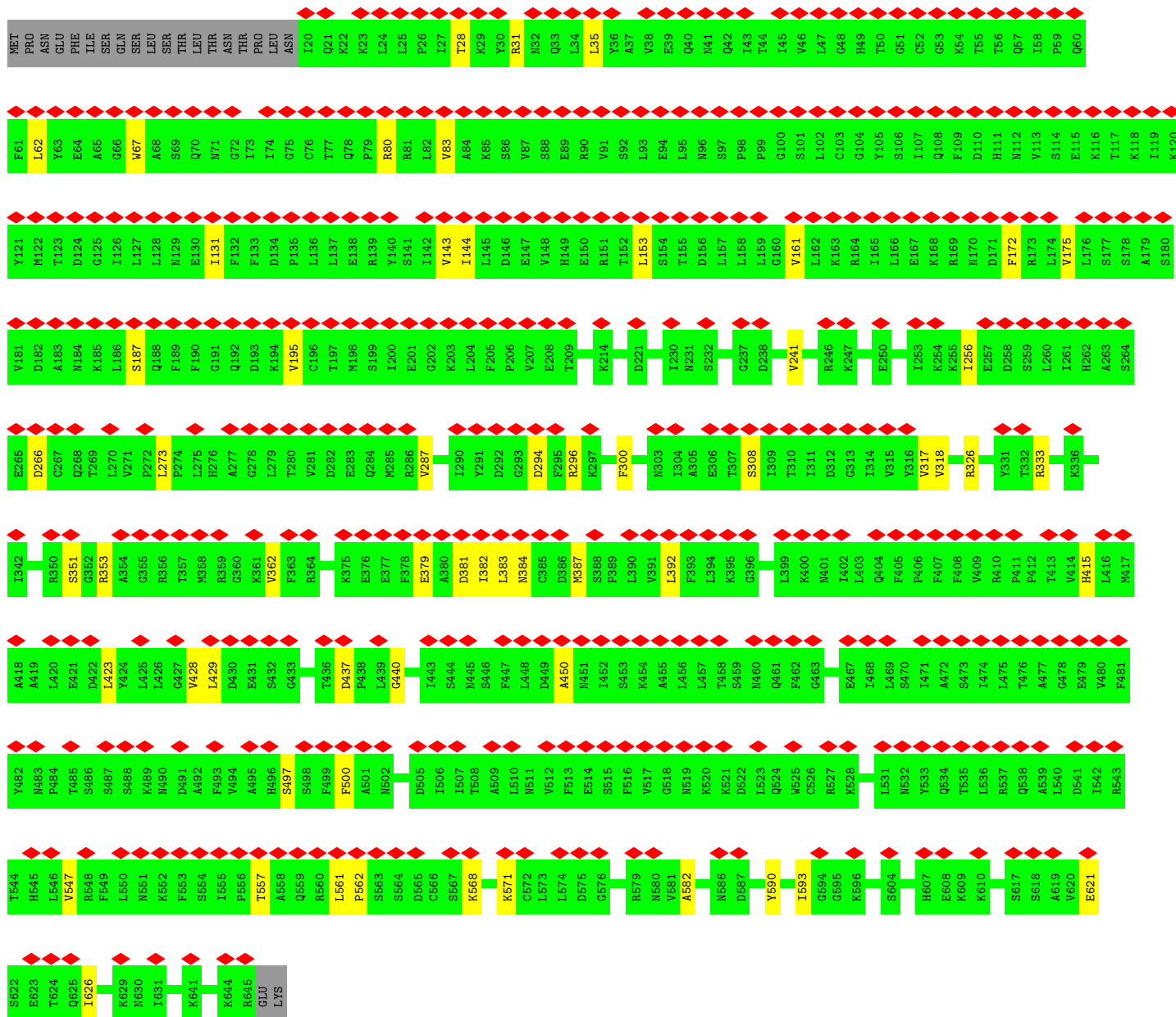
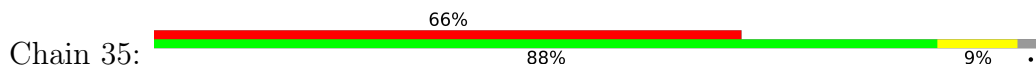
Mol	Chain	Residues	Atoms					AltConf
43	C	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 44 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
44	N	3	Total	Zn	0
			3	3	
44	O	2	Total	Zn	0
			2	2	
44	O2	1	Total	Zn	0
			1	1	

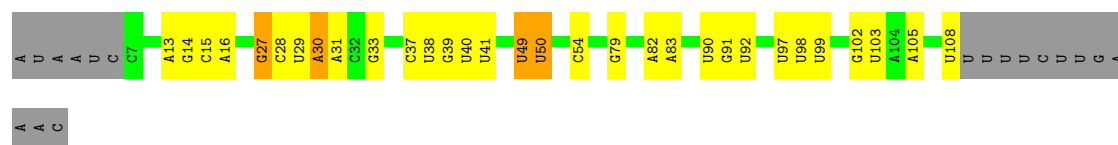


- Molecule 4: Putative pre-mRNA-splicing factor ATP-dependent RNA helicase C20H4.09



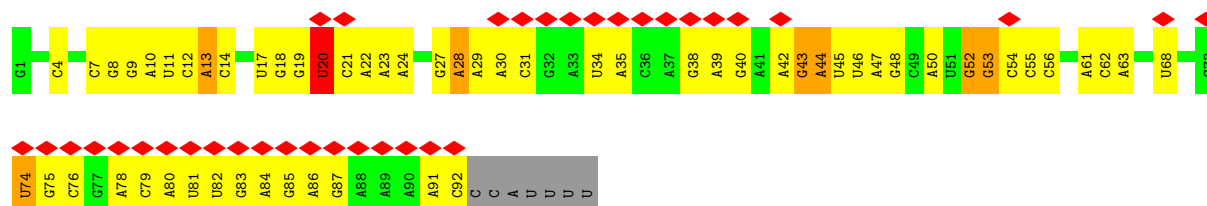
- Molecule 5: U5 snRNA

Chain 5: 



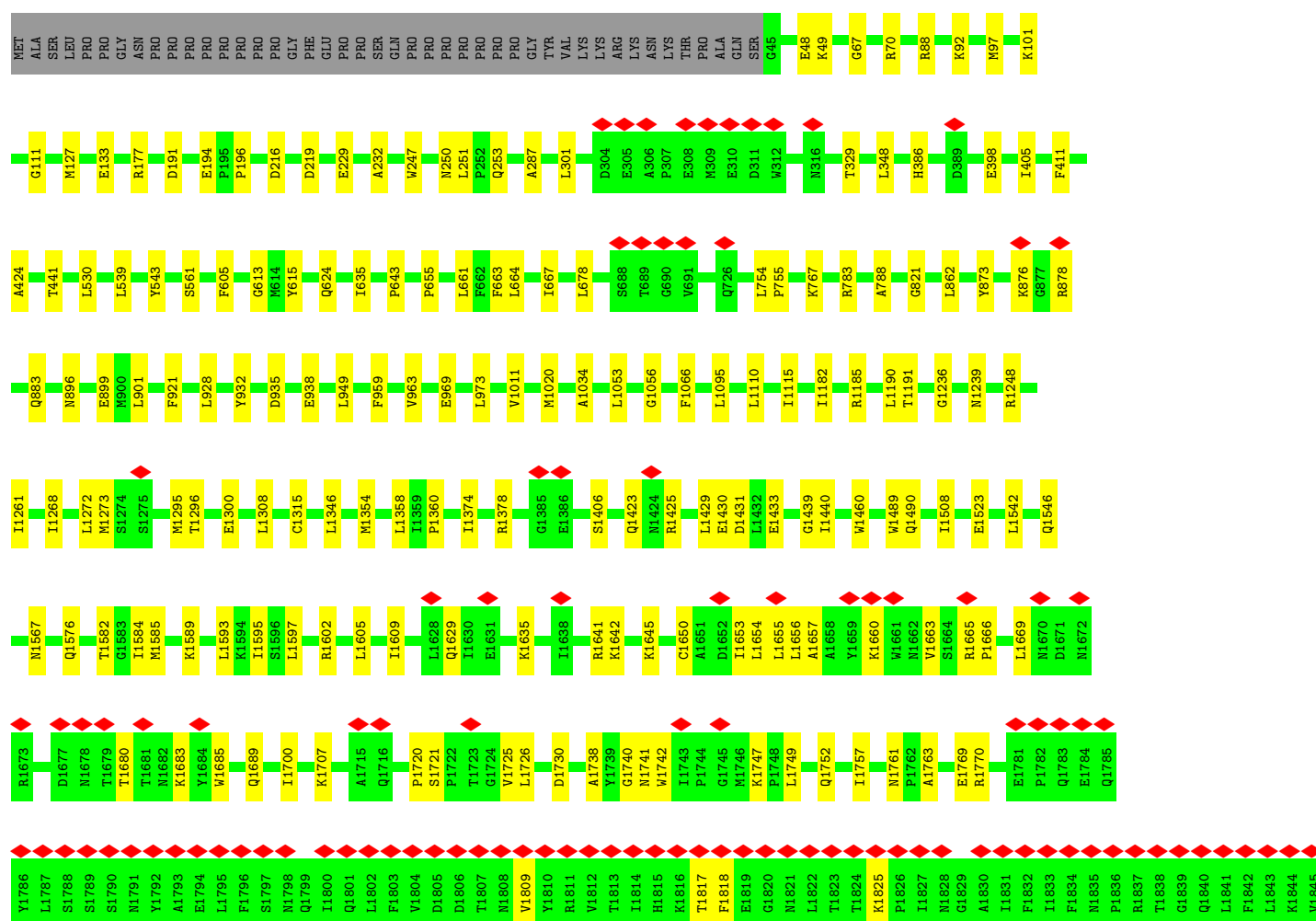
• Molecule 6: U6 snRNA

Chain 6: 

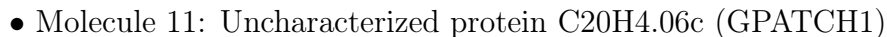


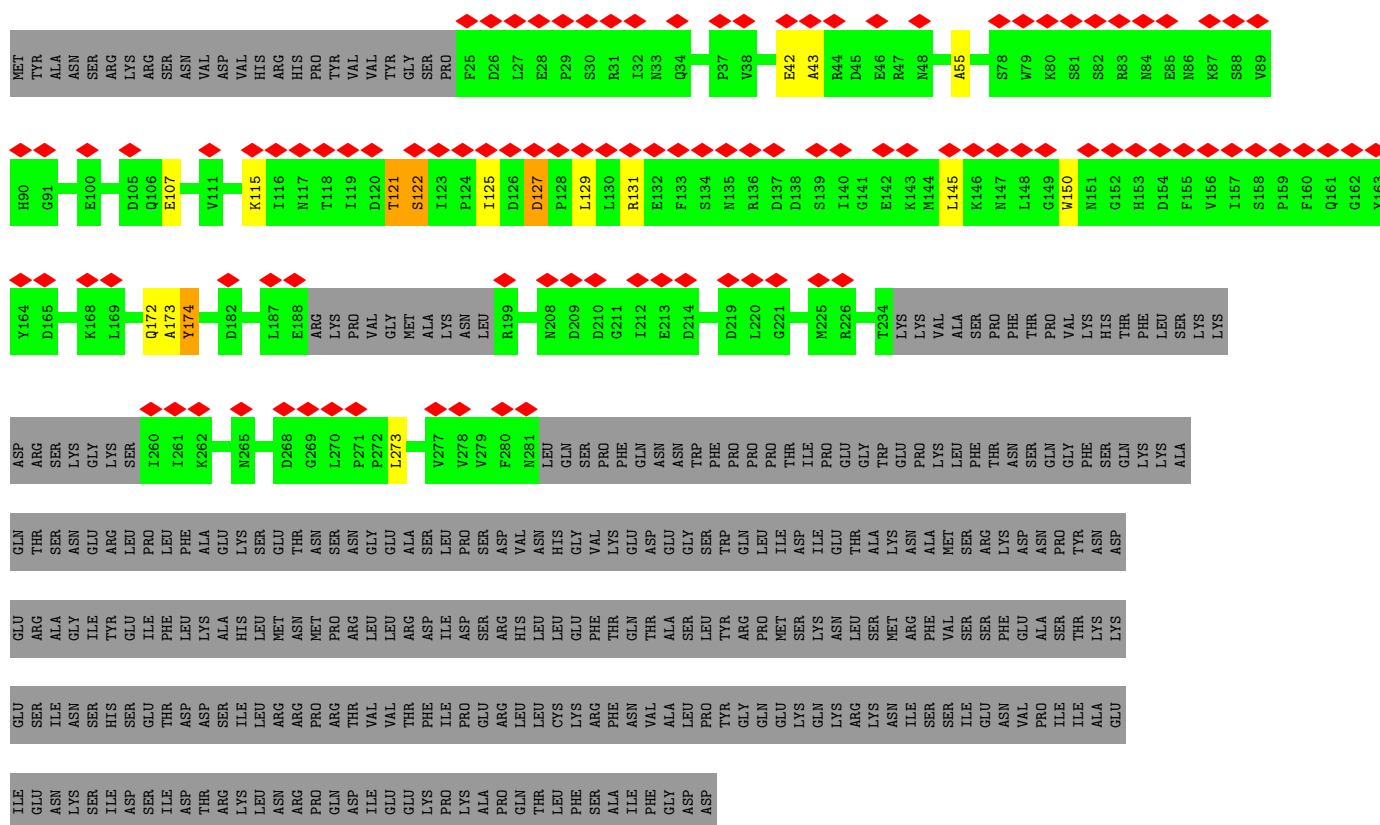
• Molecule 7: Pre-mRNA-splicing factor spp42

Chain A: 

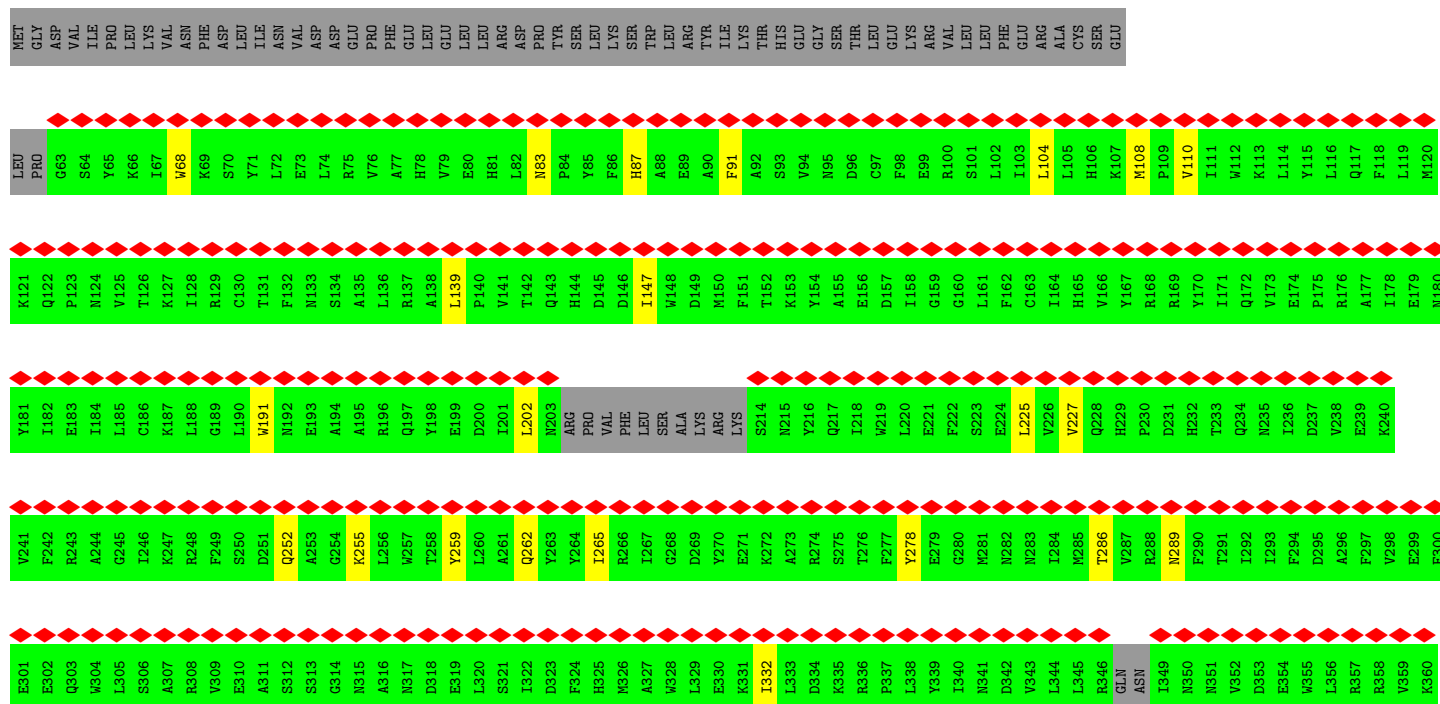
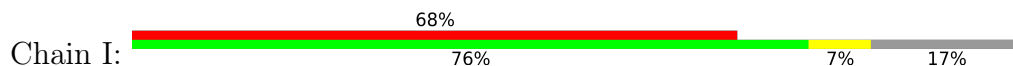


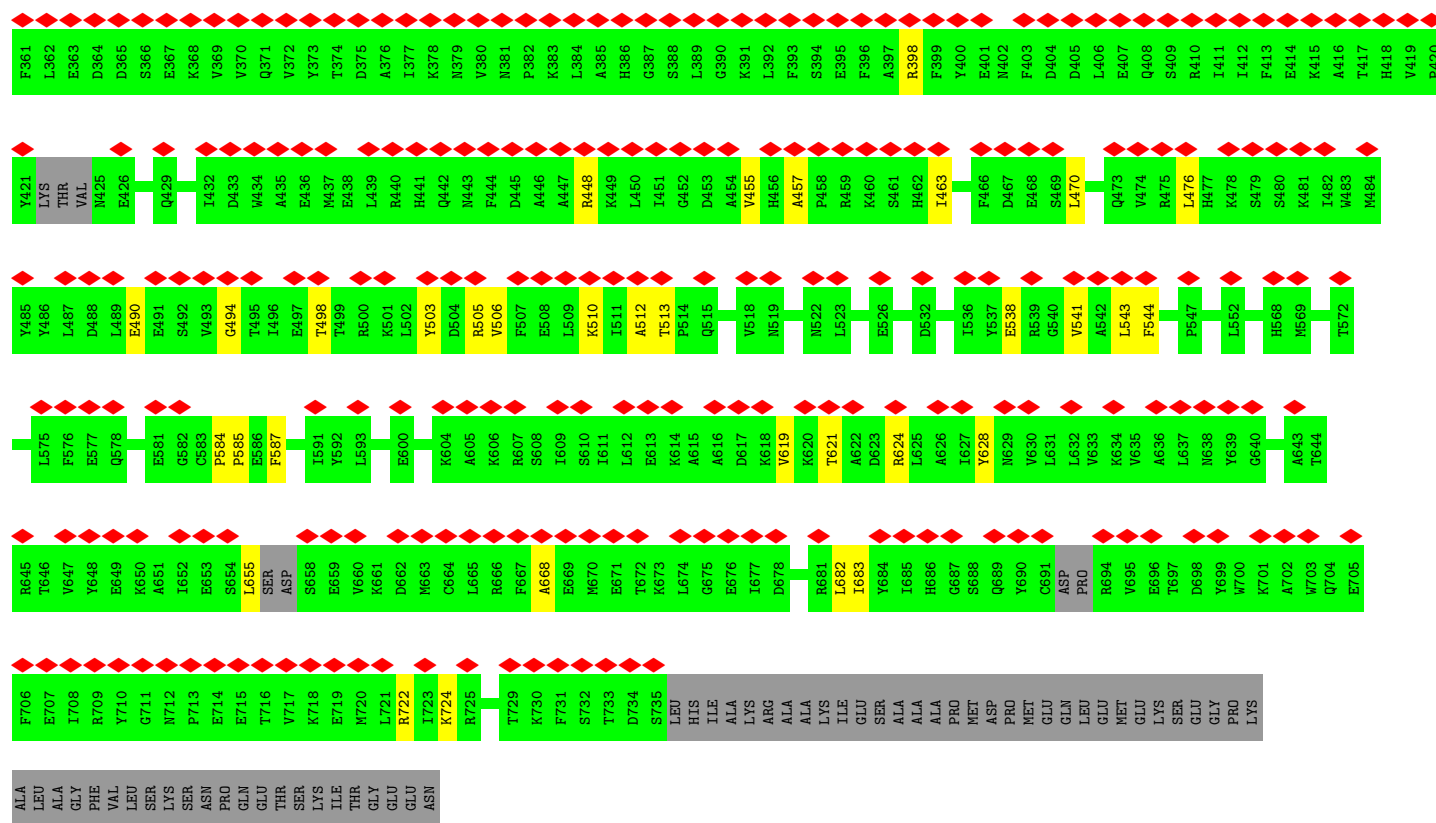
WORLDWIDE
PDB
PROTEIN DATA BANK



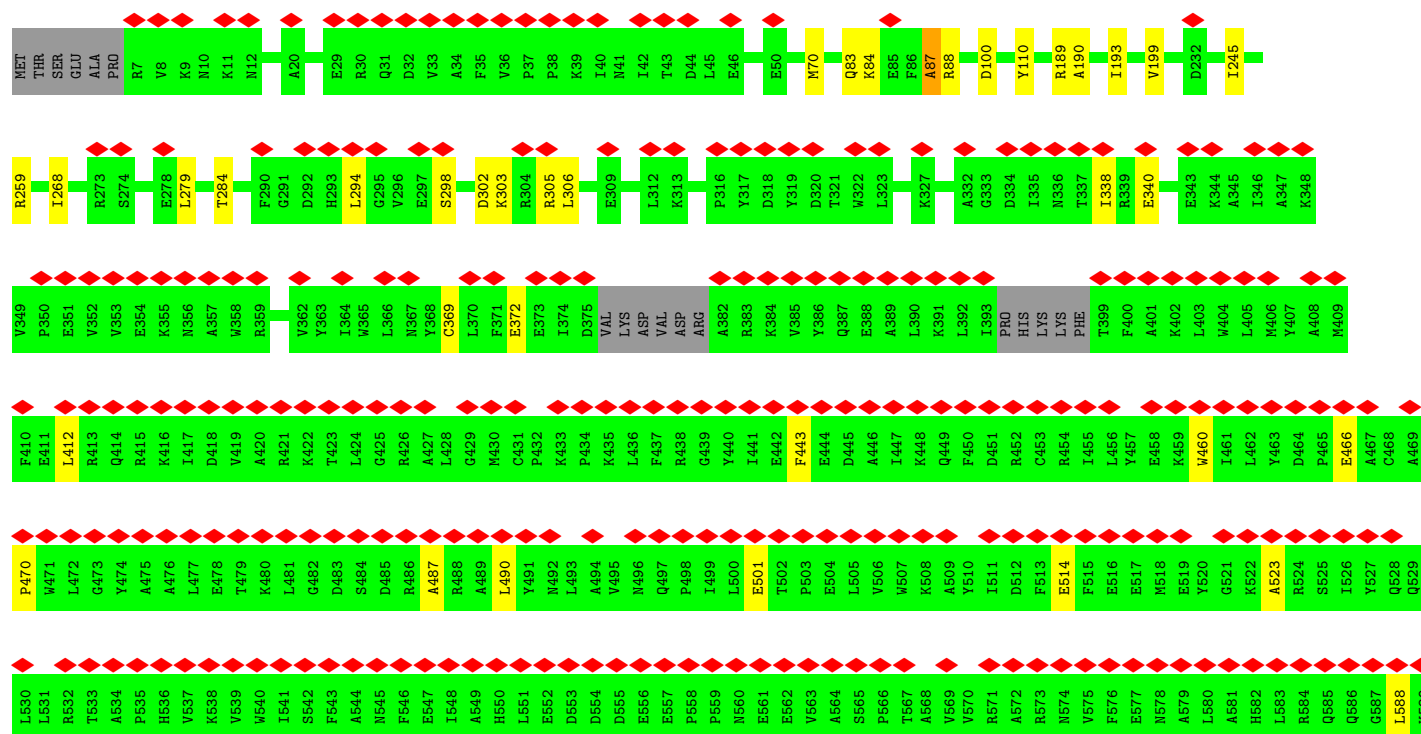
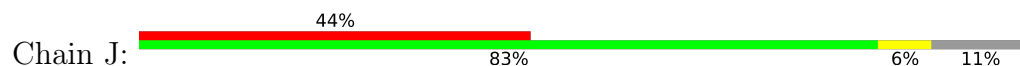


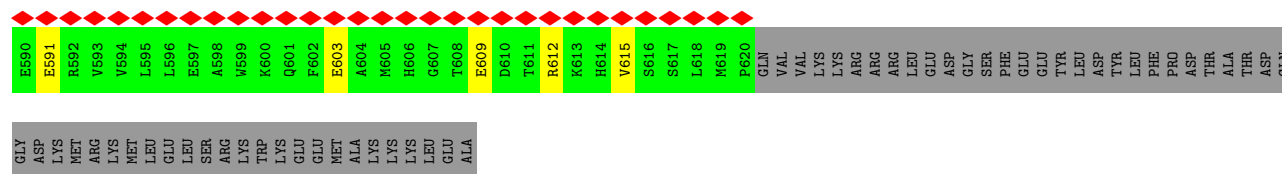
● Molecule 12: Pre-mRNA-splicing factor cwf3



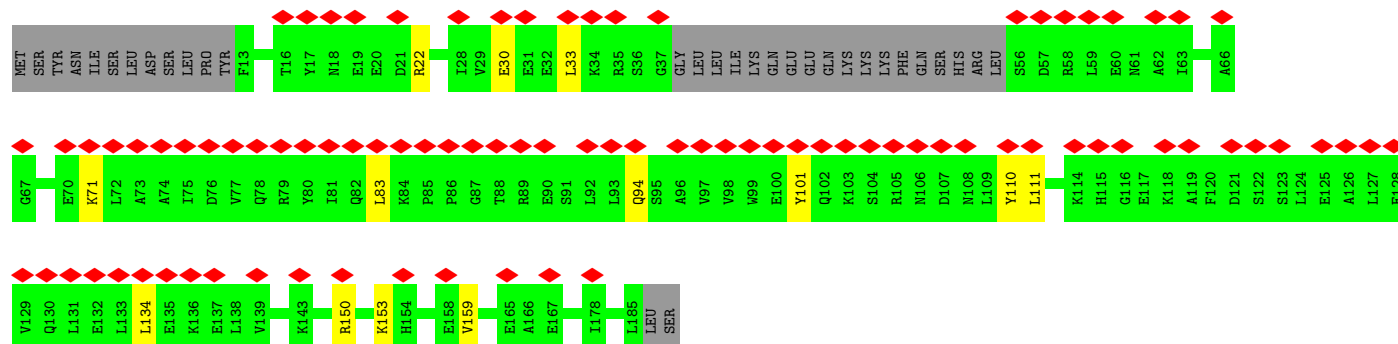
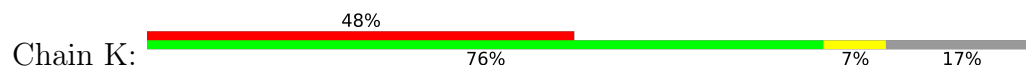


• Molecule 13: Pre-mRNA-splicing factor cwf4

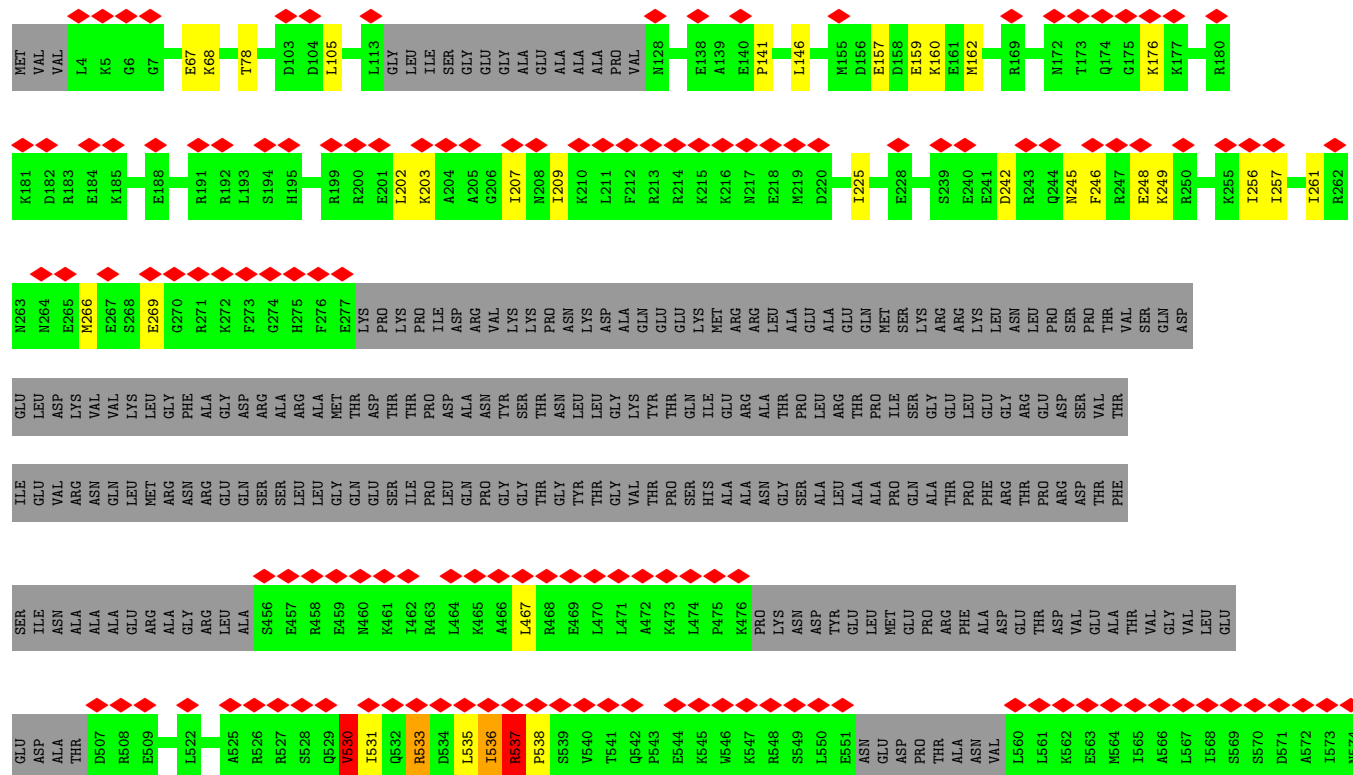


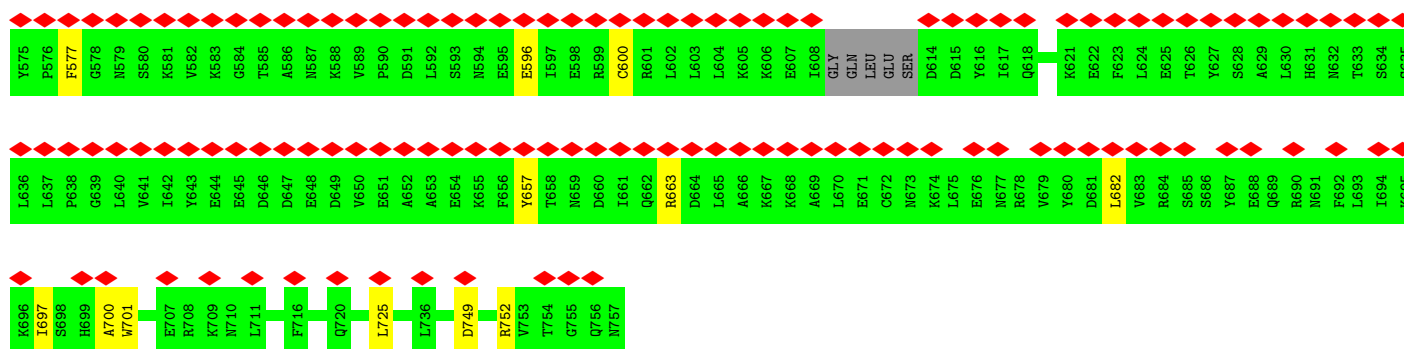


• Molecule 14: Pre-mRNA-splicing factor cwf7

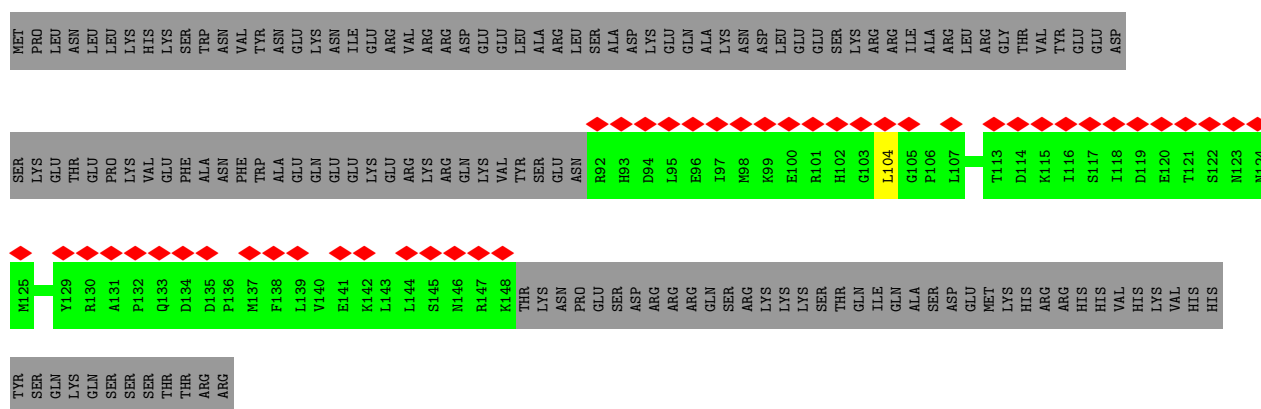


• Molecule 15: Pre-mRNA-splicing factor cdc5

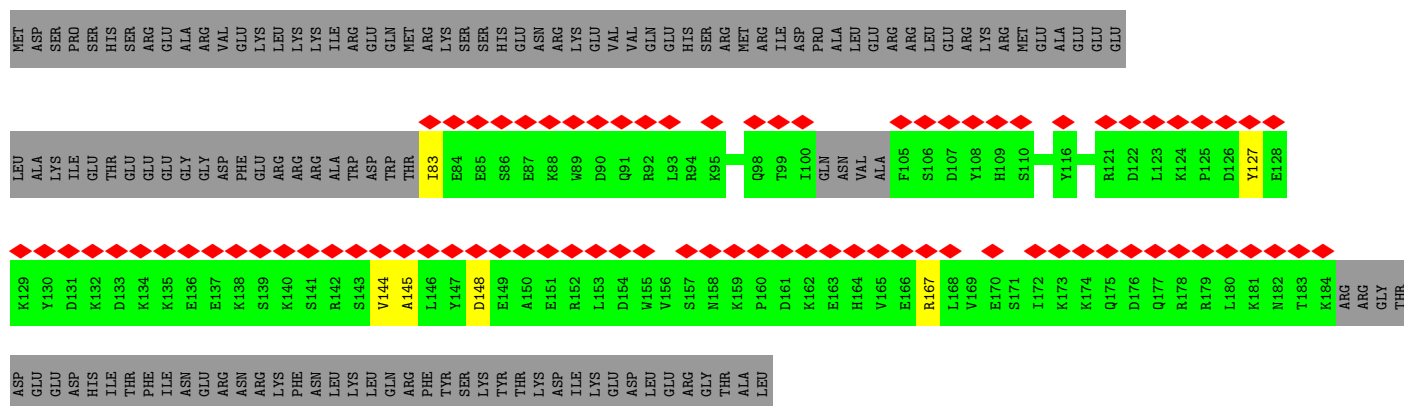
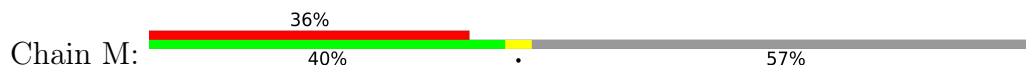




• Molecule 16: Uncharacterized protein C5E4.10c (LENG1)



• Molecule 17: Pre-mRNA-splicing factor syf2



• Molecule 18: Pre-mRNA-splicing factor cwf14



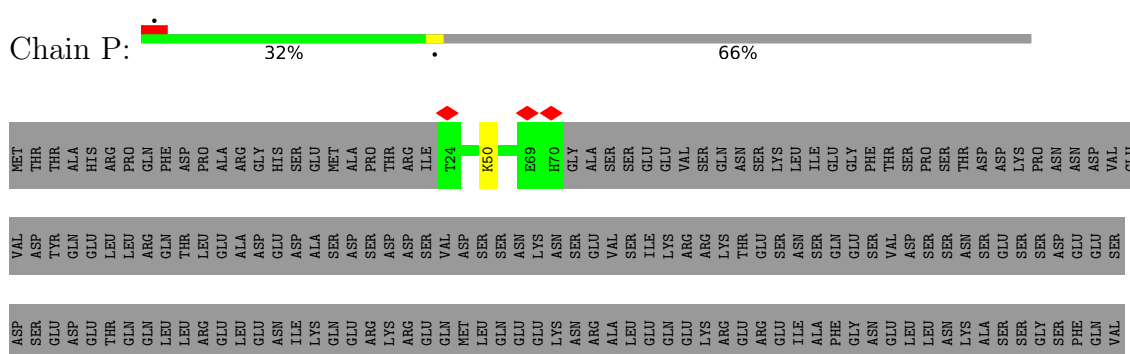
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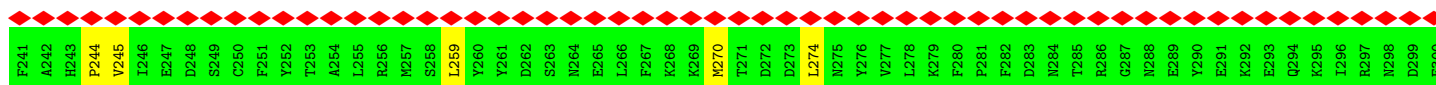


Chain O2:

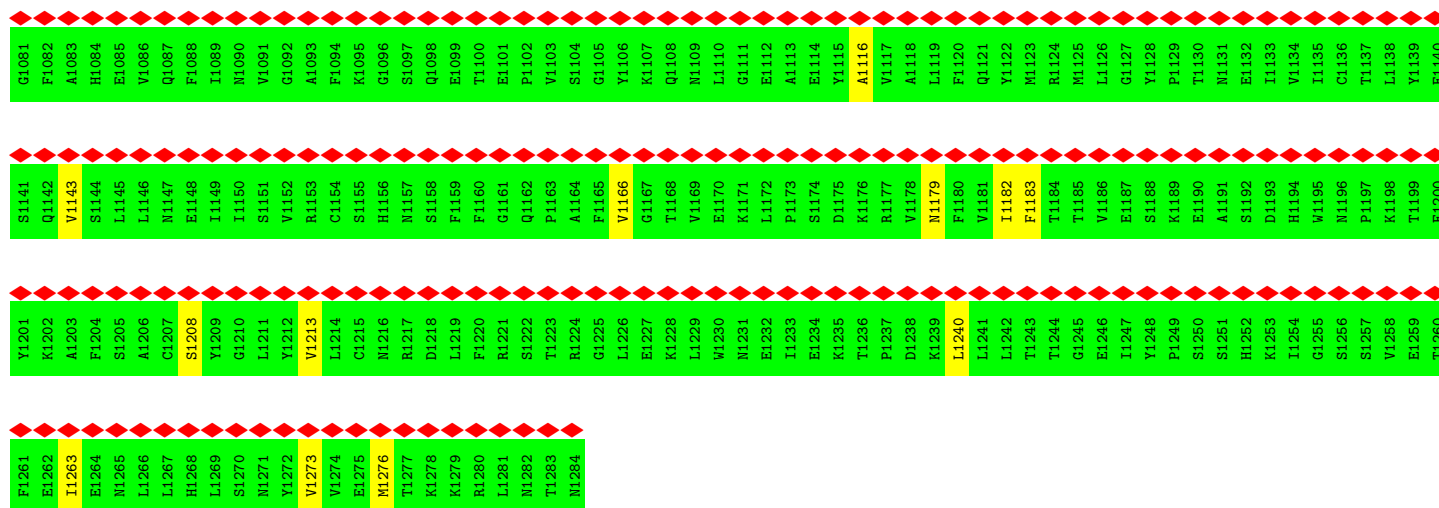


Chain P:

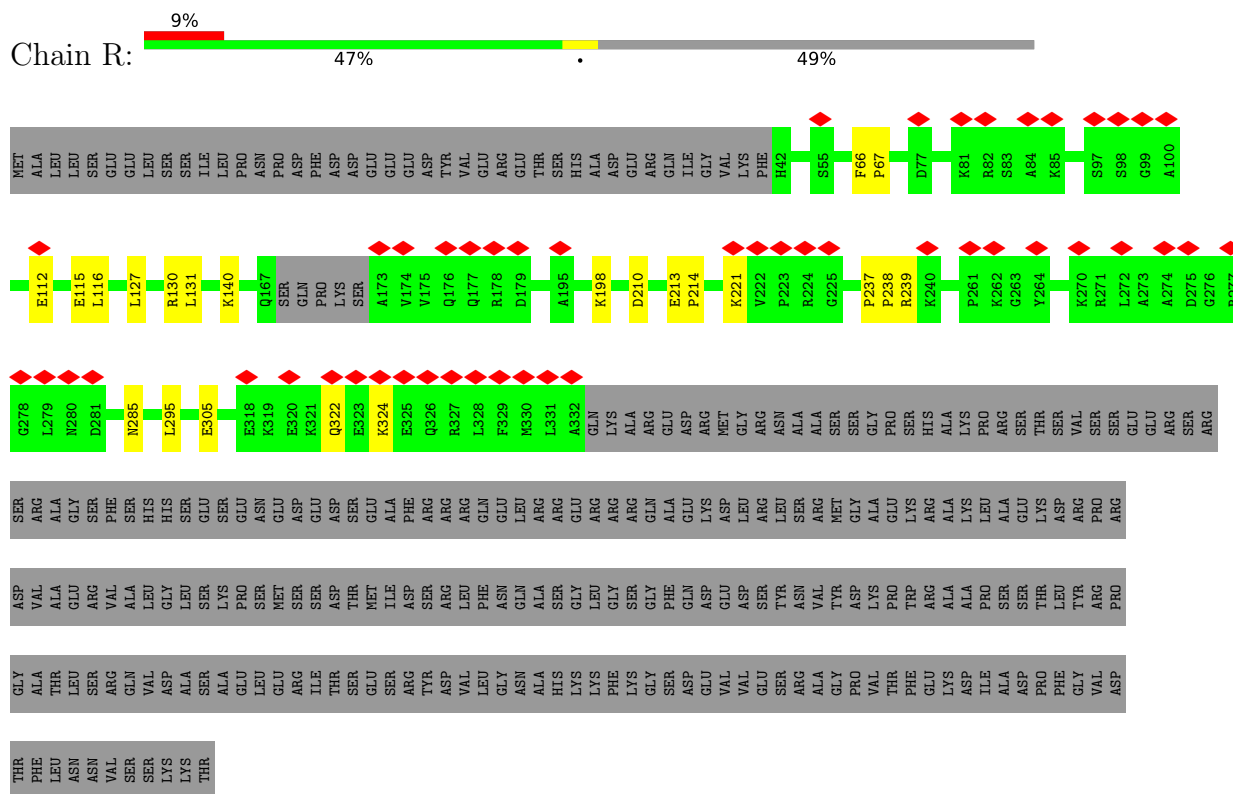




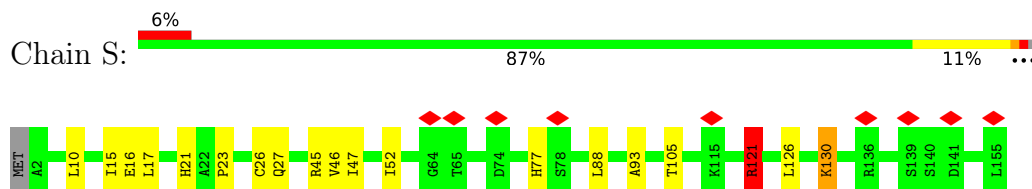
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T961	R962	L963	G964	T965	L966	K967	E968	R969	G970	F971	C972	F973	N974	N975	L976	I977	V978	M979	N980	S981	Q982	N983	I984	S985	E986	S987	S988	I989	T990	S991	I992	L993	L994	S995	N996	C997	E998	S999	T1000	G1001	F1002	D1003	R1004	L1005	V1006	L1007	L1008	G1009	S1010	Q1011	Y1012	L1013	T1014	S1015	G1016	Y1017	Q1018	D1019	I1020
T841	Q842	A843	P844	D845	S846	H847	D848	A849	S850	P851	D852	T853	A854	L855	Y856	F857	R858	D859	A860	Y861	T862	K863	R864	L865	R866	E867	K868	Y869	L870	M871	T872	H873	D874	D875	K876	D877	S878	V879	D880	A881	H882	N883	R884	F885	P886	F887	H888	S889	Y890	F891	C892	D893	K894	S895	K896	R897	P898	T899	E900
T841	Q842	A843	P844	D845	S846	H847	D848	A849	S850	P851	D852	T853	A854	L855	Y856	F857	R858	D859	A860	Y861	T862	K863	R864	L865	R866	E867	K868	Y869	L870	M871	T872	H873	D874	D875	K876	D877	S878	V879	D880	A881	H882	N883	R884	F885	P886	F887	H888	S889	Y890	F891	C892	D893	K894	S895	K896	R897	P898	T899	E900
T781	F782	S783	M784	N785	T786	L787	F788	T789	L790	L791	E792	K793	A794	R795	C796	F797	H798	Q799	G800	H801	L802	L803	Y804	L805	S806	D807	E808	G809	L810	E811	S812	T813	L814	E815	R816	Y817	F818	C819	L820	S821	S822	N823	T824	S825	K826	L827	P828	G829	L830	L831	C832	E833	T834	G835	R836	L837	A838	E839	S840
T721	N722	R723	L724	Y725	T726	Y727	N728	D729	K730	Q731	L732	E733	S734	I735	L736	R737	G738	S739	Q740	P741	G742	L743	T744	N745	V746	M747	G748	P749	T750	R751	C752	G753	K754	H755	V756	L757	F758	C759	K760	L761	L762	E763	V764	L765	Q766	D767	T768	S769	P770	N771	T772	R773	T774	V775	V776	L777	S778	D779	S780
G661	L662	N663	S664	T665	Y666	A667	R668	N669	L670	F671	N672	T673	V674	E675	Q676	L677	Q678	S679	V680	L681	P682	N683	C684	H685	V686	P687	S688	N689	L690	S691	T692	E693	S694	L695	L696	I697	K698	F699	Y700	T701	L702	S703	Q704	D705	L706	S707	A708	D709	G710	T711	P712	A713	D714	C715	H716	F717	L718	L719	P720
Y601	R602	P603	K604	Q605	L606	K607	F608	N609	F610	A611	L612	G613	L614	S615	P616	E617	A618	N619	K620	Y621	N622	L623	D624	L625	N626	I627	L628	V629	S630	L631	L632	N633	R634	A635	K636	E637	F638	P639	K640	W641	E642	F643	E644	L645	F646	L647	G648	F649	G650	T651	P652	H653	I654	C655	A656	F657	P658	N659	A660
K541	L542	L543	H544	G545	N546	A547	L548	D549	P550	L551	E552	G553	V554	T555	D556	F557	T558	I559	A560	T561	I562	C563	N564	D565	D566	V567	G568	M569	F570	Q571	S572	D573	H574	S575	S576	D577	S578	D579	N580	K581	S582	I583	N584	V585	Y586	L587	S588	P589	F590	Y591	Y592	H593	S594	L595	A596	G597	L598	G599	E600
M481	N482	F483	K484	V485	T486	S487	V488	A489	P490	P491	Q492	T493	G494	Q495	V496	L497	P498	Q499	F500	V501	K502	C503	Q504	M505	G506	L507	S508	R509	P510	G511	P512	F513	H514	S515	A516	L517	R518	D519	L520	K521	N522	S523	I524	K525	S526	P527	F528	L529	C530	L531	I532	Y533	I534	S535	K536	D537	M538	E539	Y540
Q421	N422	T423	A424	I425	Q426	Y427	L428	A429	I430	A431	F432	F433	M434	R435	Q436	Q437	S438	K439	A440	Y441	K442	K443	L444	L445	L446	R447	S448	L449	Y450	A451	E452	L453	L454	N455	F456	S457	E458	Q459	Y460	R461	R462	L463	S464	L465	K466	N467	A468	T469	Q470	N471	L472	T473	K474	D475	N476	F477	F478	S479	L480
P361	E362	K363	Y364	A365	L366	K367	V368	D369	F370	E371	F372	L373	K374	N375	V376	F377	I378	N379	T380	Y381	D382	R383	T384	R385	L386	V387	N388	D389	Y390	D391	E392	I393	I394	N395	F396	T397	L398	K399	D400	V401	L402	G403	E404	R405	S406	V407	M408	D409	Q410	E411	N412	S413	L414	T415	N416	Y417	F418	L419	L420
L301	V302	Y303	Y304	H305	L306	Q307	L308	T309	L310	F311	S312	D313	F314	Q315	K316	E317	L318	G319	D320	L321	V322	F323	C324	T325	Q326	T327	S328	L329	Q330	Q331	R332	Q333	K334	L335	E336	E337	I338	T339	S340	F341	L342	S343	F344	N345	S346	L347	K348	S349	L350	C351	S352	K353	C354	Y355	L356	R357	T358	S359	F360



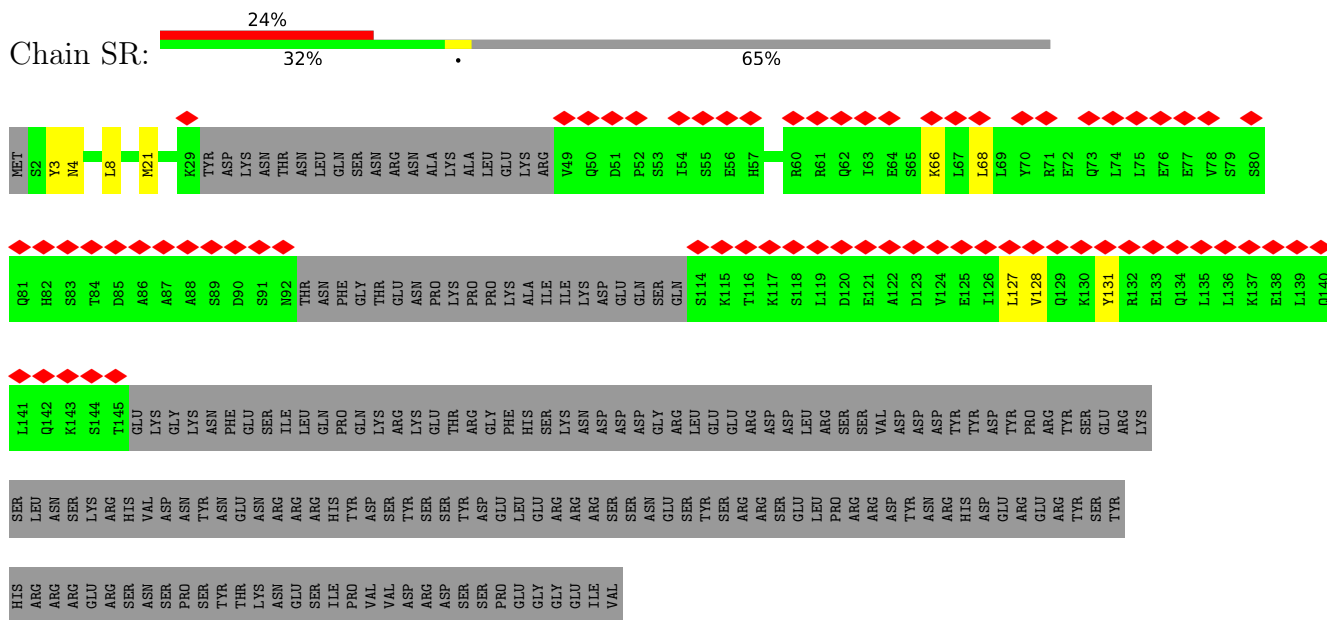
• Molecule 24: Pre-mRNA-processing protein 45



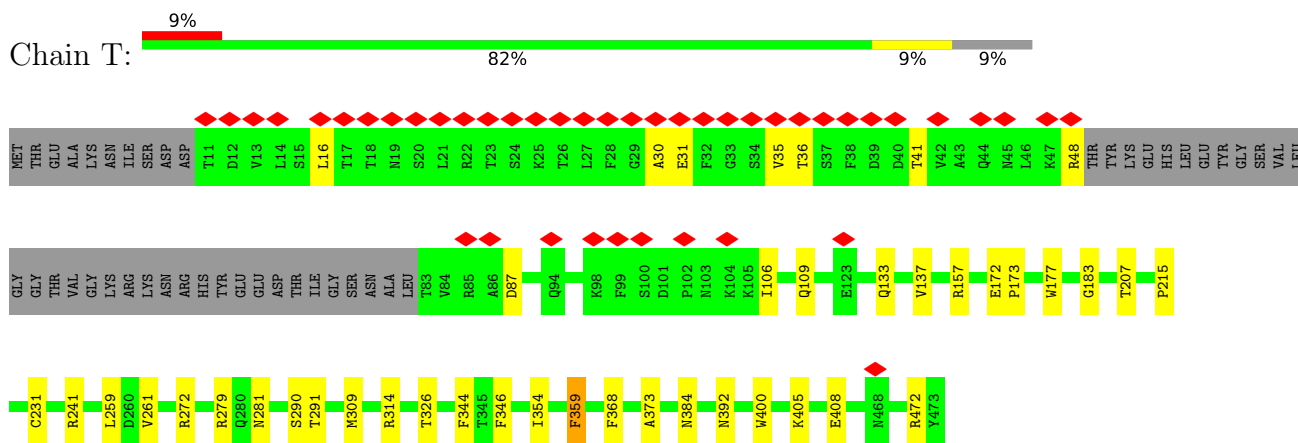
• Molecule 25: Peptidyl-prolyl cis-trans isomerase pp1l



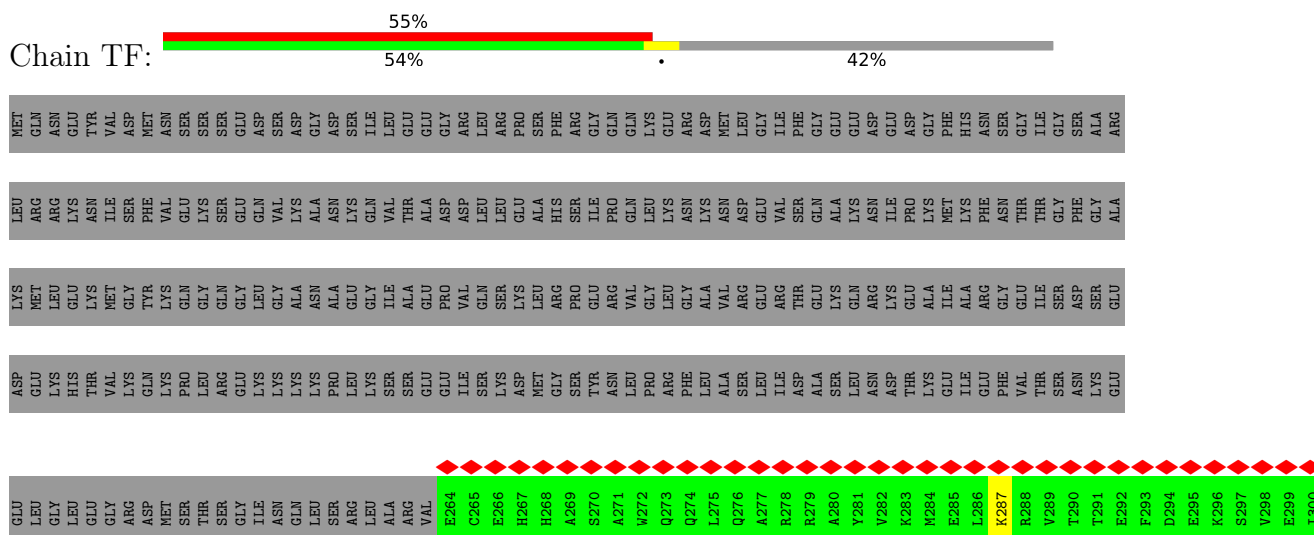
• Molecule 26: Pre-mRNA-splicing factor cwf21

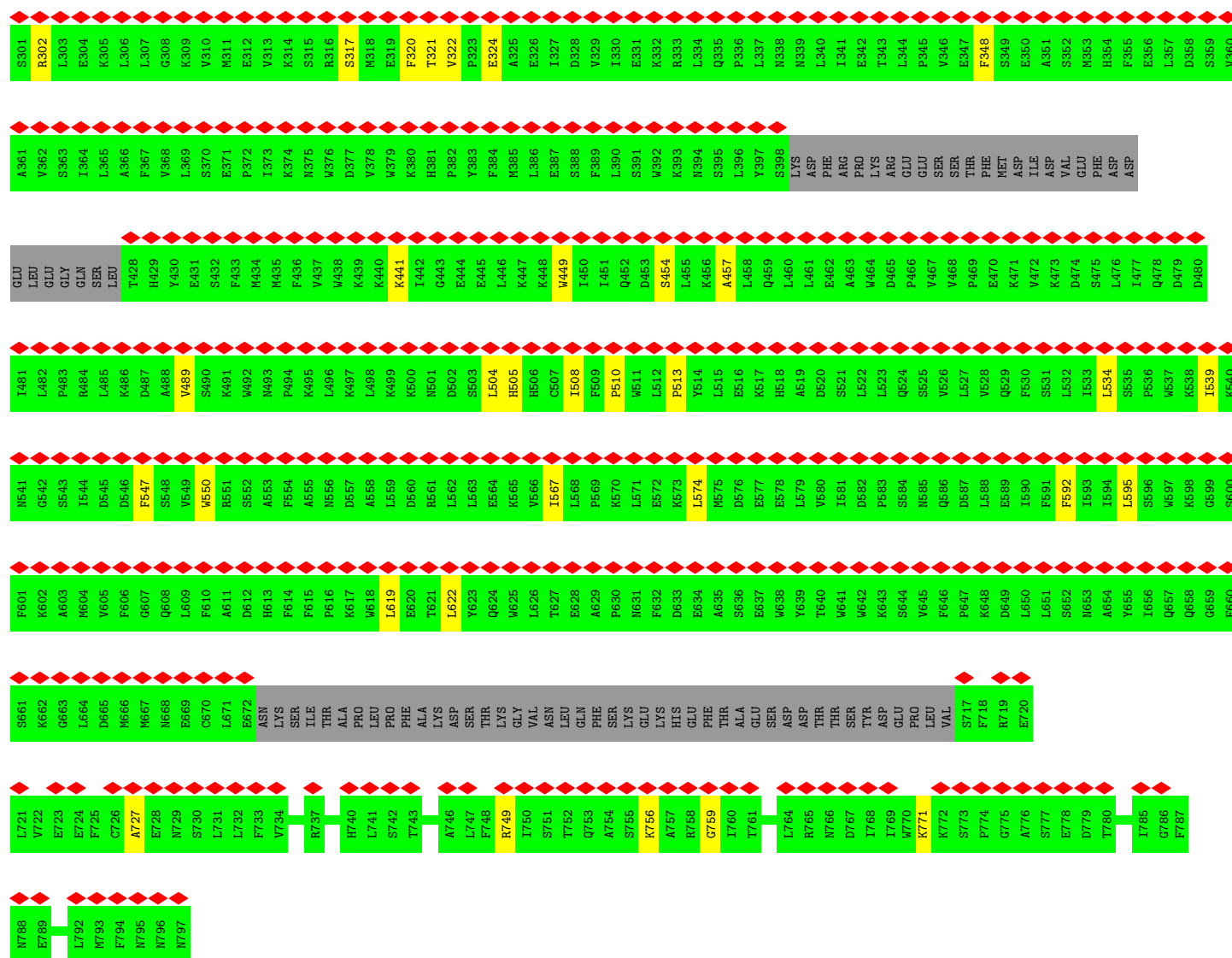


- Molecule 27: Pre-mRNA-splicing factor prp5

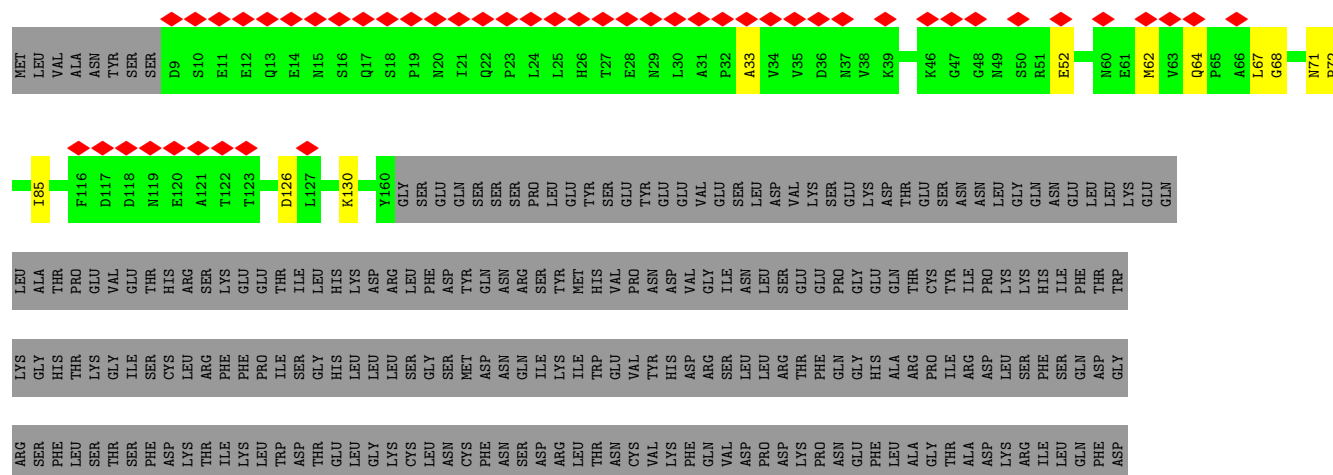


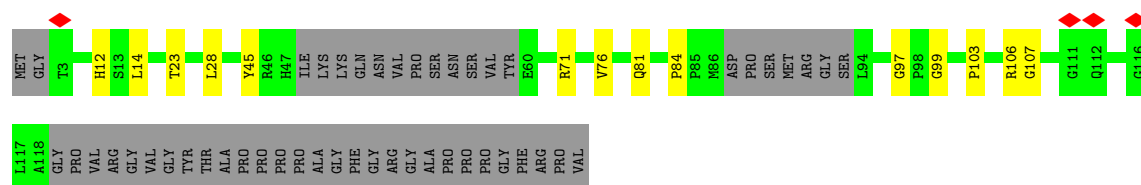
- Molecule 28: G-patch domain-containing protein C1486.03



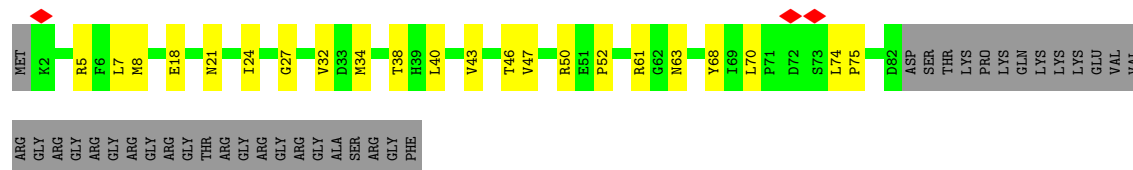


• Molecule 29: Pre-mRNA-processing factor 17

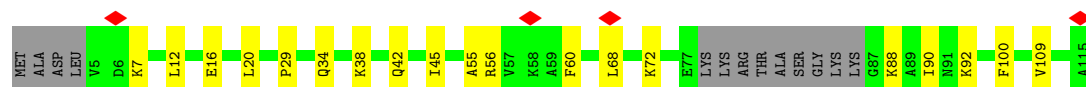




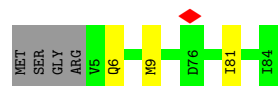
- Molecule 34: Small nuclear ribonucleoprotein Sm D1



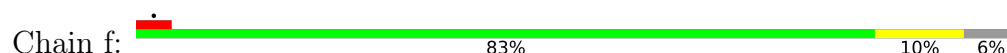
- Molecule 35: Small nuclear ribonucleoprotein Sm D2



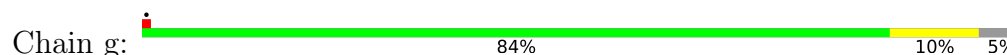
- Molecule 36: Small nuclear ribonucleoprotein E



- Molecule 37: Small nuclear ribonucleoprotein F

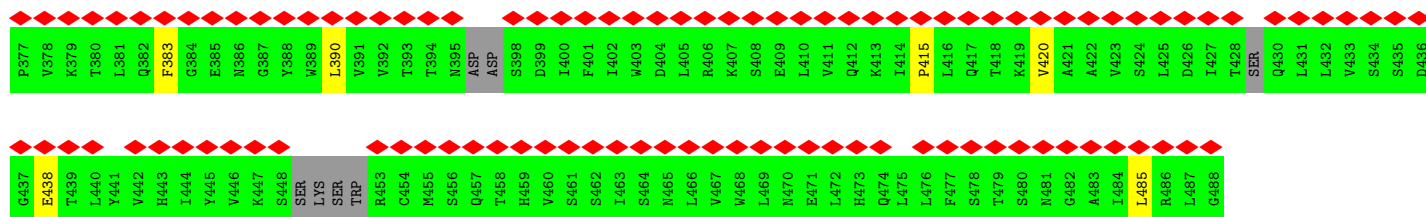


- Molecule 38: Small nuclear ribonucleoprotein G

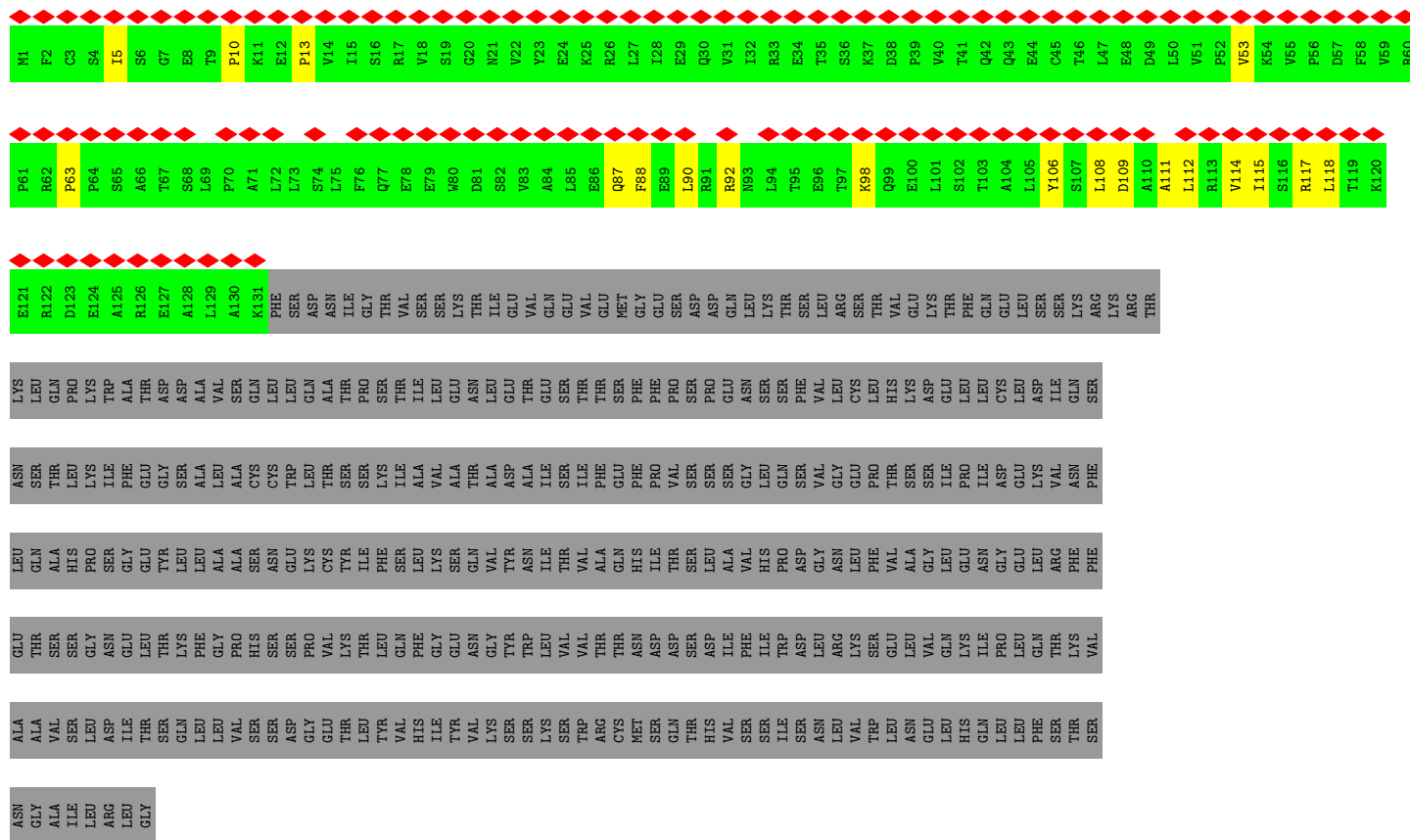


- Molecule 39: Pre-mRNA-processing factor 19

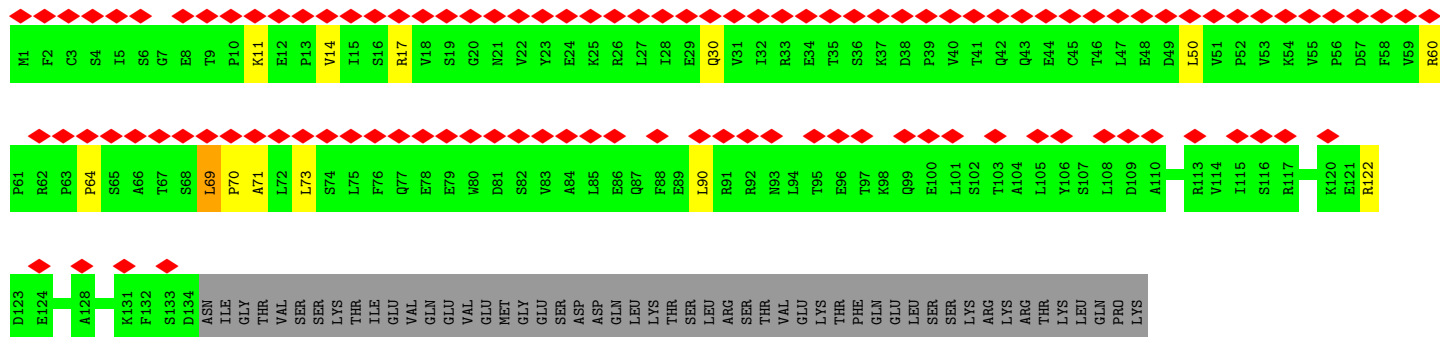




• Molecule 39: Pre-mRNA-processing factor 19



• Molecule 39: Pre-mRNA-processing factor 19





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	72631	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49.4	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	37.664	Depositor
Minimum map value	-23.068	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.904	Depositor
Recommended contour level	3.2	Depositor
Map size (Å)	460.32, 460.32, 460.32	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.822, 0.822, 0.822	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	1	0.60	0/626	0.87	2/970 (0.2%)
2	2	0.43	0/554	0.54	0/856
3	3	0.32	0/1354	0.67	0/1831
4	35	0.30	0/5079	0.66	0/6875
5	5	0.74	0/2397	0.55	1/3727 (0.0%)
6	6	0.45	0/2207	0.74	4/3438 (0.1%)
7	A	0.72	0/16857	0.71	1/22848 (0.0%)
8	C	0.69	0/7459	0.73	0/10117
9	CW	0.64	0/1711	0.78	0/2312
10	E	0.49	0/2376	0.75	0/3216
11	GP	0.40	0/1809	0.88	3/2440 (0.1%)
12	I	0.29	0/5599	0.68	0/7566
13	J	0.41	0/5235	0.70	0/7067
14	K	0.28	0/1244	0.73	0/1667
15	L	0.41	0/4363	0.78	3/5843 (0.1%)
16	LG	0.30	0/482	0.78	0/646
17	M	0.28	0/857	0.71	0/1138
18	N	0.63	0/1200	0.72	0/1609
19	O	0.42	0/1841	0.79	0/2468
20	O2	0.41	0/2222	0.80	0/2991
21	P	0.57	0/768	0.71	0/1028
22	PX	0.22	0/247	0.52	0/327
23	Q	0.24	0/10691	0.55	0/14463
24	R	0.49	0/2324	0.78	0/3137
25	S	0.44	0/1207	0.83	1/1636 (0.1%)
26	SR	0.48	0/829	0.66	0/1111
27	T	0.75	0/3422	0.82	1/4644 (0.0%)
28	TF	0.28	0/3916	0.61	0/5300
29	W	0.45	0/1055	0.75	0/1443
30	YB	0.32	0/491	0.66	0/654
31	Z	0.25	0/358	0.65	0/479
32	a	0.66	0/773	0.73	0/1038

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	b	0.50	0/737	0.70	0/993
34	c	0.51	0/646	0.92	0/875
35	d	0.43	0/830	0.87	0/1111
36	e	0.47	0/663	0.84	0/894
37	f	0.46	0/585	0.94	0/794
38	g	0.59	0/578	0.79	0/774
39	q	0.36	1/1072 (0.1%)	0.75	0/1453
39	r	0.27	0/2898	0.62	0/3914
39	s	0.33	0/1060	0.78	0/1437
39	t	0.32	0/1086	0.70	0/1472
All	All	0.51	1/101708 (0.0%)	0.71	16/138602 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	35	0	3
6	6	0	1
11	GP	0	1
13	J	0	1
15	L	0	3
20	O2	0	1
25	S	0	1
All	All	0	11

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	q	55	VAL	C-N	5.71	1.47	1.33

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	6	20	U	N1-C1'-C2'	9.10	127.64	114.00
1	1	0	G	P-O3'-C3'	7.15	130.93	120.20
15	L	533	ARG	CA-C-N	6.54	132.10	122.82
15	L	533	ARG	C-N-CA	6.54	132.10	122.82
25	S	130	LYS	CA-CB-CG	-6.48	101.14	114.10
27	T	359	PHE	N-CA-C	5.98	120.31	112.17
5	5	27	G	P-O3'-C3'	5.64	128.67	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	0	G	C2'-C3'-O3'	5.58	117.88	109.50
15	L	530	VAL	CA-CB-CG2	5.54	119.82	110.40
6	6	13	A	P-O3'-C3'	5.22	128.03	120.20
6	6	74	U	P-O3'-C3'	5.21	128.02	120.20
11	GP	174	TYR	N-CA-C	5.18	121.84	110.80
6	6	13	A	C2'-C3'-O3'	5.14	121.41	113.70
7	A	1273	MET	CA-CB-CG	5.11	124.32	114.10
11	GP	173	ALA	CA-C-N	5.08	131.25	121.54
11	GP	173	ALA	C-N-CA	5.08	131.25	121.54

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	35	296	ARG	Sidechain
4	35	326	ARG	Sidechain
4	35	353	ARG	Sidechain
6	6	20	U	Sidechain
11	GP	122	SER	Peptide
13	J	110	TYR	Sidechain
15	L	533	ARG	Sidechain
15	L	537	ARG	Sidechain
15	L	657	TYR	Peptide
20	O2	205	ARG	Sidechain
25	S	121	ARG	Sidechain

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	1	563	0	281	3	0
2	2	500	0	257	4	0
3	3	1329	0	1293	12	0
4	35	4980	0	5047	28	0
5	5	2149	0	1085	7	0
6	6	1970	0	994	20	0
7	A	16424	0	16380	115	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	7298	0	7336	54	0
9	CW	1678	0	1659	12	0
10	E	2328	0	2276	23	0
11	GP	1770	0	1669	7	0
12	I	5467	0	5372	34	0
13	J	5108	0	5024	25	0
14	K	1232	0	1242	10	0
15	L	4302	0	4350	36	0
16	LG	472	0	472	1	0
17	M	845	0	842	5	0
18	N	1177	0	1167	7	0
19	O	1818	0	1821	14	0
20	O2	2178	0	2101	18	0
21	P	753	0	729	4	0
22	PX	248	0	262	0	0
23	Q	10462	0	10412	53	0
24	R	2272	0	2283	15	0
25	S	1180	0	1169	12	0
26	SR	822	0	820	7	0
27	T	3343	0	3299	28	0
28	TF	3813	0	3794	20	0
29	W	1035	0	837	9	0
30	YB	487	0	515	6	0
31	Z	353	0	344	1	0
32	a	761	0	776	7	0
33	b	726	0	750	13	0
34	c	638	0	682	14	0
35	d	820	0	845	13	0
36	e	653	0	680	3	0
37	f	574	0	591	5	0
38	g	573	0	602	7	0
39	q	1055	0	1075	18	0
39	r	2871	0	2403	22	0
39	s	1044	0	1066	18	0
39	t	1069	0	1084	11	0
40	6	3	0	0	0	0
40	C	1	0	0	0	0
41	6	1	0	0	0	0
42	A	36	0	6	0	0
43	C	32	0	12	1	0
44	N	3	0	0	0	0
44	O	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	O2	1	0	0	0	0
All	All	99219	0	95704	616	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 3.

All (616) 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)
6:6:20:U:N3	6:6:28:A:H8	1.32	1.27
6:6:20:U:N3	6:6:28:A:C8	2.02	1.26
6:6:20:U:O2	6:6:28:A:N7	2.16	0.79
32:a:64:SER:HA	33:b:71:ARG:HH21	1.52	0.76
6:6:20:U:C4	6:6:28:A:H8	2.05	0.75
12:I:490:GLU:HG3	12:I:494:GLY:HA3	1.67	0.74
6:6:20:U:C2	6:6:28:A:N7	2.56	0.72
39:q:122:ARG:HH21	39:s:114:VAL:HG13	1.54	0.71
4:35:568:LYS:HA	4:35:571:LYS:HG2	1.72	0.71
35:d:7:LYS:HB2	35:d:20:LEU:HD21	1.74	0.70
7:A:1605:LEU:HD22	7:A:1770:ARG:HH11	1.57	0.70
7:A:1665:ARG:HE	7:A:1666:PRO:HD2	1.58	0.69
12:I:510:LYS:HZ3	17:M:83:ILE:HB	1.58	0.69
27:T:106:ILE:HG12	27:T:109:GLN:HG2	1.74	0.69
7:A:1757:ILE:HG23	7:A:1761:ASN:HD21	1.59	0.67
6:6:20:U:C2	6:6:28:A:C8	2.83	0.67
18:N:101:CYS:HB3	18:N:142:CYS:SG	2.36	0.66
23:Q:206:SER:HB3	23:Q:225:ILE:HD13	1.76	0.66
27:T:106:ILE:HG21	27:T:137:VAL:HA	1.78	0.66
7:A:1236:GLY:HA2	7:A:1300:GLU:HG3	1.77	0.65
3:3:256:TYR:HB3	9:CW:601:ARG:HH22	1.60	0.65
39:q:92:ARG:HH21	39:s:5:ILE:HG12	1.62	0.65
12:I:621:THR:HA	12:I:624:ARG:HE	1.61	0.65
7:A:1888:THR:HG22	7:A:1915:LEU:HB2	1.78	0.65
7:A:1892:MET:HE2	7:A:1896:LEU:HD21	1.79	0.65
35:d:45:ILE:HG12	35:d:109:VAL:HG12	1.79	0.65
20:O2:268:ASN:HA	20:O2:271:LYS:HE3	1.79	0.64
7:A:1576:GLN:HB3	7:A:1585:MET:HE1	1.78	0.64
9:CW:520:GLU:HA	9:CW:567:PRO:HG3	1.79	0.64
39:q:122:ARG:HE	39:s:114:VAL:HG22	1.61	0.64
1:1:-4:A:H5'	7:A:1589:LYS:HG3	1.79	0.64
24:R:210:ASP:HB3	24:R:213:GLU:HG2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1700:ILE:HD12	7:A:1730:ASP:HB2	1.80	0.63
13:J:88:ARG:HB3	15:L:225:ILE:HD12	1.79	0.63
13:J:259:ARG:HH12	27:T:87:ASP:HA	1.64	0.62
34:c:46:THR:HG22	34:c:52:PRO:HB3	1.82	0.62
10:E:328:CYS:HA	10:E:334:ILE:HG22	1.82	0.62
8:C:245:GLU:HB3	8:C:248:MET:HE2	1.82	0.62
39:r:272:ILE:HD13	39:r:301:LEU:HD13	1.81	0.61
7:A:1635:LYS:HB2	7:A:1653:ILE:HG22	1.83	0.61
8:C:678:GLU:HG2	8:C:793:LEU:HB3	1.83	0.61
10:E:203:ILE:HD11	10:E:215:LEU:HG	1.82	0.61
30:YB:186:LEU:HA	30:YB:189:ARG:HE	1.65	0.61
4:35:387:MET:HE2	4:35:415:HIS:HB3	1.83	0.60
5:5:15:C:H2'	5:5:16:A:H8	1.67	0.60
15:L:207:ILE:HG12	15:L:209:ILE:H	1.64	0.60
25:S:45:ARG:HE	25:S:47:ILE:HD11	1.66	0.60
24:R:115:GLU:HG2	24:R:116:LEU:HD12	1.82	0.60
7:A:1609:ILE:HG12	7:A:1763:ALA:HB1	1.84	0.60
39:r:357:LEU:HB2	39:r:371:PHE:HB2	1.84	0.60
15:L:245:ASN:HB2	15:L:248:GLU:HB2	1.82	0.59
7:A:1809:VAL:HG11	7:A:1861:ALA:HB1	1.84	0.59
10:E:41:VAL:HG11	33:b:103:PRO:HB3	1.82	0.59
25:S:16:GLU:HG2	25:S:121:ARG:HB3	1.85	0.59
4:35:333:ARG:HH22	11:GP:121:THR:HG22	1.66	0.59
12:I:668:ALA:HB2	12:I:683:ILE:HD11	1.83	0.59
39:r:191:ALA:HB3	39:r:485:LEU:HB3	1.85	0.59
12:I:191:TRP:HB3	12:I:225:LEU:HD13	1.84	0.59
29:W:62:MET:HA	29:W:64:GLN:HE21	1.68	0.59
9:CW:569:LEU:HD22	9:CW:572:LEU:HD12	1.85	0.58
20:O2:117:CYS:SG	20:O2:135:HIS:HD2	2.16	0.58
20:O2:198:TRP:HE1	20:O2:230:MET:HE3	1.67	0.58
3:3:132:PHE:HE1	15:L:68:LYS:HG3	1.69	0.58
19:O:75:ARG:HG3	29:W:85:ILE:HD11	1.85	0.58
35:d:109:VAL:HG22	37:f:64:LEU:HB3	1.85	0.58
7:A:1976:LEU:HA	7:A:1979:ARG:HG2	1.85	0.58
19:O:68:GLN:HG3	20:O2:147:ASN:HD22	1.68	0.58
23:Q:529:LEU:HD11	23:Q:611:ALA:HB1	1.85	0.58
34:c:27:GLY:HA3	34:c:43:VAL:HG12	1.84	0.58
39:q:110:ALA:HA	39:q:113:ARG:HE	1.68	0.58
35:d:55:ALA:HB3	35:d:68:LEU:HD12	1.86	0.58
15:L:141:PRO:HB2	15:L:146:LEU:HD21	1.86	0.57
7:A:1689:GLN:HE22	7:A:1726:LEU:HD21	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1960:LEU:HA	7:A:1963:ILE:HD12	1.86	0.57
12:I:262:GLN:HA	12:I:265:ILE:HD12	1.86	0.57
12:I:584:PRO:HD2	12:I:587:PHE:HB2	1.85	0.57
39:r:14:VAL:HG12	39:r:51:VAL:HB	1.85	0.57
23:Q:665:ILE:HD11	23:Q:740:GLN:HG2	1.86	0.57
8:C:254:ILE:HD13	8:C:597:MET:HE1	1.86	0.57
12:I:139:LEU:HD13	12:I:147:ILE:HG23	1.87	0.57
23:Q:306:LEU:HD23	23:Q:329:LEU:HD23	1.86	0.57
10:E:77:TRP:HH2	33:b:99:GLY:HA3	1.70	0.57
8:C:225:ASP:HB3	8:C:629:PRO:HB2	1.86	0.56
13:J:487:ALA:HA	13:J:490:LEU:HD12	1.87	0.56
3:3:256:TYR:HE2	9:CW:595:ALA:HA	1.71	0.56
8:C:741:LEU:H	26:SR:66:LYS:HG2	1.70	0.56
12:I:538:GLU:HA	12:I:541:VAL:HG12	1.87	0.56
24:R:324:LYS:HE2	28:TF:513:PRO:HA	1.87	0.56
19:O:148:GLU:HG3	20:O2:282:LEU:HD21	1.87	0.56
15:L:246:PHE:HA	15:L:249:LYS:HG2	1.85	0.56
19:O:102:LEU:HD23	19:O:103:VAL:HG23	1.87	0.56
36:e:9:MET:HE3	38:g:34:TYR:H	1.70	0.56
4:35:187:SER:HA	4:35:195:VAL:HG21	1.88	0.56
3:3:51:LEU:HD13	24:R:305:GLU:HG2	1.87	0.55
2:2:24:A:H5'	2:2:25:G:H5''	1.88	0.55
3:3:216:THR:HG22	21:P:234:THR:HA	1.88	0.55
7:A:251:LEU:HD21	7:A:424:ALA:HB2	1.87	0.55
20:O2:98:VAL:HG12	20:O2:101:ARG:HH11	1.70	0.55
23:Q:694:SER:HB3	23:Q:713:SER:HB3	1.88	0.55
7:A:1582:THR:HG22	7:A:1584:ILE:H	1.71	0.55
32:a:17:THR:HG22	32:a:27:ARG:HD2	1.88	0.55
7:A:67:GLY:HA3	7:A:70:ARG:HD2	1.89	0.55
15:L:203:LYS:HA	15:L:207:ILE:HB	1.88	0.55
3:3:204:HIS:HB3	8:C:76:GLN:HB2	1.88	0.55
4:35:379:GLU:HB2	4:35:383:LEU:HD22	1.89	0.55
15:L:202:LEU:HG	15:L:207:ILE:HA	1.88	0.55
12:I:457:ALA:H	12:I:505:ARG:HH22	1.54	0.54
27:T:290:SER:HB2	27:T:309:MET:HB3	1.87	0.54
26:SR:128:VAL:HA	26:SR:131:TYR:HD2	1.71	0.54
29:W:52:GLU:H	33:b:107:GLY:HA2	1.71	0.54
39:s:106:TYR:HA	39:s:109:ASP:HB2	1.88	0.54
7:A:1602:ARG:HE	7:A:1770:ARG:HH21	1.55	0.54
6:6:42:A:H5''	15:L:176:LYS:HG3	1.89	0.54
7:A:1095:LEU:HD22	7:A:1110:LEU:HD22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1268:ILE:HG21	7:A:1315:CYS:HB2	1.90	0.54
18:N:101:CYS:CB	18:N:142:CYS:SG	2.94	0.54
39:q:102:SER:HA	39:q:105:LEU:HD12	1.90	0.54
39:t:69:LEU:HD12	39:t:71:ALA:H	1.73	0.53
14:K:22:ARG:HH11	39:r:112:LEU:HD22	1.73	0.53
28:TF:489:VAL:HG22	28:TF:504:LEU:HD11	1.90	0.53
8:C:531:GLU:HA	28:TF:756:LYS:HD2	1.90	0.53
23:Q:226:ILE:HG23	23:Q:274:LEU:HD12	1.89	0.53
25:S:15:ILE:HG12	25:S:88:LEU:HD22	1.90	0.53
8:C:267:LEU:HB3	8:C:319:VAL:HG22	1.89	0.53
15:L:697:ILE:HD11	39:q:61:PRO:HG2	1.90	0.53
11:GP:145:LEU:HD12	11:GP:150:TRP:HB2	1.90	0.53
23:Q:357:ARG:HH21	23:Q:361:PRO:HD3	1.73	0.53
10:E:308:GLY:HA3	33:b:106:ARG:HG2	1.90	0.53
23:Q:666:TYR:HB2	23:Q:768:THR:HA	1.91	0.53
24:R:67:PRO:HD2	25:S:121:ARG:HH22	1.74	0.53
7:A:287:ALA:HA	7:A:301:LEU:HD23	1.91	0.53
19:O:91:LEU:HD13	19:O:95:LEU:HD22	1.89	0.53
38:g:21:LEU:HB2	38:g:25:ARG:HB2	1.91	0.53
7:A:539:LEU:HD11	7:A:561:SER:HB2	1.91	0.52
28:TF:454:SER:HB3	28:TF:510:PRO:HG2	1.90	0.52
10:E:306:LEU:HD13	33:b:106:ARG:HE	1.73	0.52
12:I:68:TRP:HE1	12:I:104:LEU:HD23	1.74	0.52
15:L:536:ILE:HG22	15:L:537:ARG:H	1.73	0.52
37:f:45:LEU:HB2	37:f:63:ILE:HB	1.91	0.52
12:I:543:LEU:HD13	17:M:83:ILE:HD11	1.91	0.52
23:Q:151:ILE:HG12	23:Q:245:VAL:HG21	1.91	0.52
3:3:183:LYS:HG2	3:3:184:SER:H	1.74	0.52
12:I:108:MET:HE3	12:I:110:VAL:HB	1.90	0.52
23:Q:1273:VAL:HA	23:Q:1276:MET:HE2	1.91	0.52
7:A:635:ILE:HD11	7:A:655:PRO:HG2	1.90	0.52
12:I:512:ALA:HB2	17:M:83:ILE:HG13	1.91	0.52
28:TF:749:ARG:HE	28:TF:759:GLY:HA3	1.75	0.52
20:O2:190:ILE:HG22	20:O2:193:ARG:HH22	1.73	0.52
13:J:284:THR:HG21	13:J:306:LEU:HD22	1.92	0.52
23:Q:748:GLY:HA3	23:Q:1042:LEU:HD12	1.92	0.52
8:C:222:ASP:HB3	8:C:650:TYR:HB2	1.92	0.51
13:J:609:GLU:HA	13:J:612:ARG:HD2	1.92	0.51
7:A:932:TYR:HB2	7:A:1056:GLY:HA3	1.90	0.51
8:C:221:VAL:HG21	8:C:912:GLN:HB3	1.91	0.51
34:c:40:LEU:HB3	34:c:43:VAL:HG11	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:t:70:PRO:HA	39:t:73:LEU:HG	1.91	0.51
4:35:241:VAL:HG12	4:35:318:VAL:HB	1.93	0.51
39:r:336:ILE:HA	39:r:352:LEU:HA	1.91	0.51
39:r:383:PHE:HD1	39:r:390:LEU:HD22	1.75	0.51
4:35:428:VAL:HG23	4:35:440:GLY:HA2	1.93	0.51
27:T:231:CYS:HB3	27:T:241:ARG:HB2	1.92	0.51
28:TF:539:ILE:HD11	28:TF:574:LEU:HD13	1.92	0.51
13:J:338:ILE:HG23	13:J:340:GLU:H	1.76	0.51
13:J:412:LEU:HD13	13:J:443:PHE:HE1	1.75	0.51
27:T:373:ALA:HB1	27:T:392:ASN:HD21	1.76	0.51
30:YB:192:LEU:HD11	30:YB:194:ILE:HG22	1.93	0.51
7:A:216:ASP:HB3	7:A:219:ASP:HB3	1.93	0.51
37:f:25:LYS:HA	37:f:71:LEU:HD12	1.93	0.51
37:f:49:GLU:HG3	37:f:56:LYS:HD3	1.93	0.51
7:A:1430:GLU:HA	7:A:1433:GLU:HG2	1.93	0.51
10:E:74:ILE:HB	10:E:89:LEU:HB2	1.93	0.51
14:K:111:LEU:HD21	27:T:48:ARG:HE	1.75	0.51
23:Q:483:PHE:HE1	23:Q:505:MET:HE3	1.76	0.51
27:T:183:GLY:HA2	27:T:207:THR:HG23	1.91	0.51
8:C:85:TYR:HB3	8:C:89:VAL:HG21	1.91	0.50
14:K:159:VAL:HG21	15:L:725:LEU:HD13	1.92	0.50
34:c:18:GLU:HG3	34:c:24:ILE:HG13	1.93	0.50
35:d:42:GLN:HG2	35:d:56:ARG:HH12	1.75	0.50
4:35:547:VAL:HG22	4:35:557:THR:HG21	1.92	0.50
5:5:29:U:H4'	5:5:30:A:H5'	1.93	0.50
6:6:52:G:H2'	6:6:53:G:C8	2.46	0.50
8:C:821:GLN:HG3	28:TF:727:ALA:HB1	1.93	0.50
13:J:245:ILE:HD11	13:J:279:LEU:HA	1.92	0.50
23:Q:746:VAL:HG22	23:Q:1040:ILE:HD12	1.93	0.50
34:c:7:LEU:HB3	34:c:32:VAL:HG11	1.93	0.50
7:A:862:LEU:HD22	7:A:901:LEU:HG	1.94	0.50
7:A:1358:LEU:HD22	26:SR:21:MET:HE1	1.93	0.50
23:Q:399:LYS:HA	23:Q:402:LEU:HD12	1.93	0.50
4:35:28:THR:HG23	4:35:31:ARG:HH21	1.76	0.50
8:C:814:GLN:HA	8:C:817:ARG:HD3	1.93	0.50
19:O:237:PRO:HB2	19:O:255:LYS:HD3	1.93	0.50
39:s:114:VAL:HG23	39:s:117:ARG:HD2	1.94	0.50
4:35:423:LEU:HB3	4:35:429:LEU:HD13	1.94	0.50
10:E:319:HIS:HB2	10:E:324:ILE:HB	1.93	0.50
7:A:935:ASP:HB3	7:A:938:GLU:HG3	1.94	0.50
8:C:146:VAL:HG12	8:C:154:LYS:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:L:749:ASP:HA	15:L:752:ARG:HE	1.76	0.50
26:SR:68:LEU:HG	26:SR:127:LEU:HD22	1.93	0.50
32:a:6:LYS:HD2	32:a:90:PRO:HG2	1.93	0.50
5:5:38:U:H2'	5:5:39:G:H8	1.77	0.50
8:C:703:VAL:HG12	8:C:803:PHE:HA	1.93	0.50
23:Q:401:VAL:HG22	23:Q:446:LEU:HD11	1.94	0.50
39:r:347:LEU:HA	39:r:362:THR:H	1.77	0.50
23:Q:562:ILE:HA	23:Q:585:VAL:HG22	1.94	0.49
1:1:-1:U:H5'	1:1:0:G:H5''	1.94	0.49
7:A:1656:LEU:HA	7:A:1683:LYS:HD2	1.94	0.49
10:E:103:ARG:HD3	10:E:145:LYS:HA	1.93	0.49
12:I:286:THR:HG21	12:I:289:ASN:HB2	1.93	0.49
23:Q:369:ASP:H	23:Q:372:PHE:HB3	1.76	0.49
39:q:14:VAL:HG11	39:q:28:ILE:HG21	1.93	0.49
28:TF:505:HIS:HA	28:TF:508:ILE:HG22	1.94	0.49
7:A:405:ILE:HG22	8:C:346:ILE:HD13	1.93	0.49
23:Q:225:ILE:HA	23:Q:228:MET:HE2	1.94	0.49
27:T:384:ASN:HB3	27:T:400:TRP:HB3	1.93	0.49
28:TF:302:ARG:HG2	28:TF:348:PHE:HD2	1.77	0.49
23:Q:393:ILE:HD11	23:Q:435:ARG:HH21	1.78	0.49
27:T:16:LEU:HD21	39:q:105:LEU:HD21	1.94	0.49
9:CW:579:ARG:HA	9:CW:582:ARG:HE	1.76	0.49
10:E:46:MET:HB3	10:E:334:ILE:HG13	1.94	0.49
15:L:535:LEU:HB2	39:s:98:LYS:HE2	1.95	0.49
28:TF:317:SER:HA	28:TF:320:PHE:HB2	1.93	0.49
39:r:420:VAL:HG13	39:r:438:GLU:HB2	1.94	0.49
7:A:1669:LEU:HD13	7:A:1738:ALA:HB3	1.94	0.49
2:2:19:G:H22	6:6:50:A:H2	1.61	0.49
15:L:600:CYS:HB2	39:s:112:LEU:HD21	1.95	0.49
35:d:90:ILE:HG13	35:d:92:LYS:HZ1	1.78	0.49
7:A:48:GLU:HG2	7:A:49:LYS:HD3	1.95	0.48
8:C:227:VAL:HG11	8:C:254:ILE:HD12	1.93	0.48
8:C:490:MET:HG2	8:C:510:VAL:HA	1.95	0.48
23:Q:772:ASP:HB2	23:Q:974:ASN:HB2	1.94	0.48
4:35:80:ARG:HB2	4:35:83:VAL:HB	1.95	0.48
23:Q:1116:ALA:HB1	23:Q:1182:ILE:HD12	1.94	0.48
4:35:381:ASP:HA	4:35:384:ASN:HB2	1.95	0.48
7:A:1020:MET:HG2	7:A:1066:PHE:HZ	1.78	0.48
13:J:190:ALA:HA	13:J:193:ILE:HD12	1.94	0.48
28:TF:547:PHE:HA	28:TF:550:TRP:HD1	1.77	0.48
7:A:1542:LEU:HD23	7:A:1546:GLN:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:608:PRO:HD3	8:C:617:LEU:HD22	1.95	0.48
10:E:295:VAL:HB	10:E:304:TYR:HB2	1.95	0.48
7:A:398:GLU:HG3	36:e:6:GLN:HE22	1.78	0.48
7:A:1972:GLU:HG3	7:A:1975:LYS:HE2	1.94	0.48
9:CW:472:CYS:SG	9:CW:516:SER:HB3	2.53	0.48
20:O2:292:ASN:HD21	20:O2:293:ARG:HH11	1.62	0.48
7:A:969:GLU:HB2	7:A:973:LEU:HB3	1.95	0.48
12:I:227:VAL:HG21	12:I:259:TYR:HD1	1.79	0.48
7:A:1185:ARG:HE	21:P:229:VAL:HG11	1.79	0.48
10:E:245:ILE:HG23	10:E:258:LEU:HB2	1.96	0.48
25:S:17:LEU:HD22	25:S:26:CYS:HB2	1.94	0.48
7:A:229:GLU:HB2	7:A:232:ALA:HA	1.96	0.48
8:C:90:ASP:HB3	27:T:157:ARG:HG3	1.95	0.48
12:I:722:ARG:HD3	30:YB:196:ILE:HG23	1.95	0.48
24:R:127:LEU:HA	24:R:130:ARG:HG3	1.96	0.48
4:35:317:VAL:HB	4:35:362:VAL:HG22	1.96	0.48
8:C:724:PRO:HG2	8:C:727:ARG:HG3	1.96	0.48
13:J:70:MET:HE3	13:J:100:ASP:HB3	1.96	0.48
27:T:173:PRO:HG3	27:T:215:PRO:HA	1.95	0.48
7:A:1429:LEU:HD12	7:A:1430:GLU:H	1.79	0.47
28:TF:449:TRP:HE1	28:TF:457:ALA:HB2	1.77	0.47
14:K:134:LEU:HD22	15:L:700:ALA:HB1	1.95	0.47
7:A:1749:LEU:HD12	7:A:1752:GLN:HE21	1.78	0.47
17:M:145:ALA:HB3	17:M:148:ASP:HB2	1.96	0.47
23:Q:153:ASN:HB2	23:Q:178:TYR:HE2	1.79	0.47
34:c:32:VAL:HG23	34:c:38:THR:HG22	1.96	0.47
7:A:876:LYS:HG3	7:A:878:ARG:H	1.79	0.47
8:C:769:ASP:HB2	8:C:772:VAL:HB	1.97	0.47
8:C:852:ALA:HB1	8:C:856:SER:HB2	1.97	0.47
39:q:122:ARG:HH22	39:s:115:ILE:HD13	1.80	0.47
4:35:273:LEU:HD13	4:35:287:VAL:HA	1.96	0.47
7:A:111:GLY:HA3	24:R:214:PRO:HD3	1.97	0.47
10:E:85:ASN:HB3	33:b:97:GLY:HA3	1.96	0.47
33:b:12:HIS:NE2	33:b:84:PRO:HG3	2.30	0.47
4:35:621:GLU:HG2	4:35:626:ILE:HG13	1.97	0.47
24:R:66:PHE:HA	25:S:121:ARG:NH2	2.28	0.47
28:TF:534:LEU:HD13	28:TF:567:ILE:HD11	1.96	0.47
4:35:561:LEU:HD12	4:35:562:PRO:HD2	1.97	0.47
7:A:411:PHE:HB2	8:C:391:LYS:HD2	1.96	0.47
5:5:15:C:H2'	5:5:16:A:C8	2.47	0.47
7:A:1725:VAL:HA	7:A:1740:GLY:HA3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:84:A:H2'	6:6:85:G:C8	2.50	0.46
7:A:191:ASP:HB3	7:A:194:GLU:HG2	1.97	0.46
7:A:754:LEU:HD12	7:A:755:PRO:HD2	1.96	0.46
11:GP:127:ASP:H	11:GP:131:ARG:HH21	1.63	0.46
12:I:87:HIS:HB2	12:I:91:PHE:HE1	1.80	0.46
39:s:88:PHE:O	39:s:92:ARG:HG2	2.15	0.46
4:35:153:LEU:HD12	4:35:382:ILE:HG13	1.96	0.46
7:A:1423:GLN:HG3	7:A:1425:ARG:HG2	1.97	0.46
13:J:603:GLU:HG3	13:J:615:VAL:HG21	1.97	0.46
15:L:105:LEU:HD21	30:YB:164:ARG:HB3	1.97	0.46
23:Q:226:ILE:HG21	23:Q:270:MET:HG3	1.98	0.46
39:r:81:ASP:HB3	39:t:30:GLN:HE22	1.80	0.46
4:35:62:LEU:HB2	4:35:67:TRP:CD1	2.50	0.46
8:C:951:THR:HG22	8:C:955:LYS:HD2	1.97	0.46
8:C:938:ALA:HB3	8:C:943:LEU:HD23	1.97	0.46
13:J:294:LEU:HD23	13:J:298:SER:HB3	1.97	0.46
4:35:144:ILE:HG23	4:35:175:VAL:HB	1.97	0.46
7:A:1239:ASN:HB3	7:A:1248:ARG:HD3	1.96	0.46
14:K:30:GLU:HA	14:K:33:LEU:HD12	1.96	0.46
7:A:386:HIS:CE1	8:C:311:ARG:HG3	2.51	0.46
10:E:113:SER:HA	10:E:137:VAL:HG13	1.97	0.46
38:g:21:LEU:HD21	38:g:62:ILE:HD13	1.98	0.46
7:A:1917:PHE:HD1	7:A:1920:ILE:HD11	1.79	0.46
15:L:203:LYS:HB3	15:L:207:ILE:HD12	1.96	0.46
23:Q:560:ALA:HB2	23:Q:587:LEU:HD12	1.97	0.46
7:A:127:MET:HE1	7:A:605:PHE:HZ	1.79	0.46
7:A:1817:THR:HG22	7:A:1818:PHE:H	1.81	0.46
8:C:250:ASN:O	8:C:254:ILE:HG12	2.16	0.46
19:O:84:MET:HB2	20:O2:146:ALA:HB3	1.97	0.46
25:S:126:LEU:HG	25:S:130:LYS:HE3	1.97	0.46
23:Q:784:MET:HE3	23:Q:784:MET:HB2	1.74	0.46
7:A:1406:SER:HA	7:A:1439:GLY:HA2	1.98	0.46
7:A:196:PRO:HD3	7:A:543:TYR:CE2	2.51	0.45
23:Q:214:LYS:HE3	23:Q:259:LEU:HD12	1.98	0.45
6:6:47:A:H5''	6:6:47:A:H8	1.81	0.45
20:O2:118:LEU:HD11	20:O2:153:ARG:HH21	1.81	0.45
23:Q:1179:ASN:HA	23:Q:1208:SER:HB2	1.98	0.45
39:r:15:ILE:HD13	39:s:53:VAL:HG23	1.98	0.45
2:2:5:U:H3	6:6:87:G:H1	1.63	0.45
6:6:34:U:H2'	6:6:35:A:H8	1.81	0.45
13:J:83:GLN:HA	15:L:256:ILE:HG21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:L:682:LEU:HD13	39:t:64:PRO:HG3	1.97	0.45
20:O2:181:ILE:HG13	20:O2:183:PRO:HD3	1.98	0.45
27:T:405:LYS:HD3	27:T:408:GLU:HG2	1.98	0.45
7:A:1020:MET:HG2	7:A:1066:PHE:CZ	2.52	0.45
17:M:127:TYR:HE2	17:M:167:ARG:HH12	1.65	0.45
7:A:250:ASN:HB2	7:A:253:GLN:HG3	1.97	0.45
7:A:1602:ARG:HE	7:A:1770:ARG:NH2	2.14	0.45
20:O2:106:THR:HG23	20:O2:108:ALA:H	1.82	0.45
5:5:97:U:H1'	38:g:65:ASN:HB2	1.99	0.45
7:A:664:LEU:HA	7:A:667:ILE:HG22	1.99	0.45
7:A:1346:LEU:HD23	7:A:1508:ILE:HG21	1.99	0.45
7:A:1584:ILE:HD13	7:A:1597:LEU:HD13	1.99	0.45
8:C:922:PRO:HG2	8:C:943:LEU:HD12	1.99	0.45
23:Q:638:PHE:HE1	23:Q:990:THR:HG23	1.81	0.45
28:TF:441:LYS:HA	28:TF:441:LYS:HD3	1.76	0.45
14:K:150:ARG:HE	29:W:33:ALA:HA	1.81	0.45
23:Q:1143:VAL:HG13	23:Q:1166:VAL:HG12	1.98	0.45
33:b:76:VAL:HG21	34:c:21:ASN:HD21	1.82	0.45
8:C:206:LYS:HE3	32:a:9:HIS:CD2	2.51	0.45
19:O:46:ILE:HG23	19:O:113:ARG:HE	1.80	0.45
12:I:513:THR:H	12:I:544:PHE:HZ	1.64	0.45
39:s:87:GLN:HA	39:s:90:LEU:HD12	1.99	0.45
7:A:1429:LEU:C	7:A:1431:ASP:H	2.25	0.45
14:K:110:TYR:HD2	27:T:41:THR:HG21	1.82	0.45
19:O:35:MET:HE2	19:O:56:TRP:HB3	1.98	0.45
28:TF:592:PHE:HD1	28:TF:595:LEU:HD12	1.81	0.45
7:A:1034:ALA:HB2	15:L:78:THR:HB	1.99	0.44
7:A:1629:GLN:HA	7:A:1657:ALA:HA	1.97	0.44
33:b:14:LEU:HD13	33:b:28:LEU:HB2	1.99	0.44
8:C:930:ILE:HG22	8:C:932:PRO:HD3	1.98	0.44
34:c:61:ARG:HH21	34:c:63:ASN:ND2	2.16	0.44
39:q:29:GLU:HG3	39:q:33:ARG:HH21	1.82	0.44
7:A:101:LYS:HB2	7:A:101:LYS:HE3	1.83	0.44
23:Q:498:PRO:HG2	23:Q:589:PRO:HB3	1.99	0.44
24:R:140:LYS:HD3	27:T:344:PHE:HB2	1.98	0.44
34:c:47:VAL:HB	34:c:50:ARG:HB2	2.00	0.44
9:CW:519:TRP:HZ3	9:CW:560:LEU:HD22	1.83	0.44
7:A:783:ARG:HG2	7:A:788:ALA:HB3	1.99	0.44
7:A:1011:VAL:HG11	7:A:1053:LEU:HD12	2.00	0.44
7:A:1190:LEU:HD12	7:A:1191:THR:HG22	1.99	0.44
7:A:1296:THR:HG21	7:A:1489:TRP:CE3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1440:ILE:HD13	7:A:1440:ILE:HA	1.73	0.44
15:L:749:ASP:HA	15:L:752:ARG:HH21	1.83	0.44
20:O2:178:VAL:HG23	20:O2:243:VAL:HG22	1.99	0.44
27:T:472:ARG:HD2	27:T:472:ARG:HA	1.84	0.44
28:TF:322:VAL:HG12	28:TF:324:GLU:H	1.81	0.44
7:A:530:LEU:HD21	7:A:678:LEU:HD21	2.00	0.44
18:N:26:PHE:HE1	18:N:55:GLN:HG2	1.83	0.44
23:Q:778:SER:HB2	23:Q:979:MET:HE3	2.00	0.44
24:R:198:LYS:HB3	24:R:198:LYS:HE2	1.83	0.44
27:T:241:ARG:HG3	27:T:279:ARG:HD3	2.00	0.44
27:T:346:PHE:HB3	27:T:359:PHE:HE1	1.82	0.44
39:r:59:VAL:HG23	39:r:61:PRO:HD3	1.99	0.44
12:I:139:LEU:HD22	12:I:147:ILE:HG12	1.99	0.44
15:L:530:VAL:HG23	15:L:531:ILE:HG13	1.99	0.44
23:Q:318:LEU:HB2	23:Q:322:VAL:HG23	1.99	0.44
7:A:613:GLY:HA2	7:A:615:TYR:CE2	2.53	0.44
8:C:777:LYS:HA	8:C:780:ILE:HG22	1.99	0.44
9:CW:520:GLU:H	9:CW:520:GLU:HG2	1.56	0.44
12:I:202:LEU:HD11	23:Q:493:ILE:HD12	2.00	0.44
20:O2:160:ARG:HB3	20:O2:161:ASP:H	1.69	0.44
23:Q:1183:PHE:HB3	23:Q:1213:VAL:HG22	1.99	0.44
38:g:10:LYS:HE2	38:g:10:LYS:HB2	1.75	0.44
4:35:256:ILE:HG13	4:35:300:PHE:HZ	1.82	0.44
4:35:351:SER:HA	4:35:362:VAL:HG21	2.00	0.44
4:35:392:LEU:HD11	4:35:450:ALA:HB2	1.99	0.44
9:CW:486:PHE:CD2	9:CW:521:VAL:HB	2.53	0.44
10:E:283:PHE:CD1	10:E:297:SER:HA	2.53	0.44
11:GP:42:GLU:HG2	11:GP:43:ALA:H	1.82	0.44
11:GP:125:ILE:HG13	11:GP:131:ARG:HD3	2.00	0.44
12:I:108:MET:HG3	12:I:110:VAL:HG12	1.98	0.44
25:S:93:ALA:HB2	29:W:67:LEU:HA	1.98	0.44
12:I:398:ARG:HD3	12:I:398:ARG:HA	1.81	0.43
23:Q:155:LEU:HD22	23:Q:160:LYS:HD3	1.99	0.43
23:Q:741:PRO:HA	23:Q:1004:ARG:HG2	2.00	0.43
25:S:23:PRO:O	25:S:27:GLN:HG3	2.17	0.43
7:A:921:PHE:HD2	7:A:928:LEU:HB3	1.81	0.43
7:A:1567:ASN:HB2	7:A:1593:LEU:HD21	2.01	0.43
12:I:252:GLN:HB2	12:I:255:LYS:HZ3	1.82	0.43
14:K:101:TYR:HB3	39:t:69:LEU:HB3	1.99	0.43
15:L:159:GLU:HA	15:L:162:MET:HG2	1.98	0.43
15:L:663:ARG:HH11	27:T:31:GLU:HB3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:182:ASP:HB2	24:R:239:ARG:HH21	1.82	0.43
7:A:1460:TRP:H	7:A:1460:TRP:CD1	2.36	0.43
28:TF:547:PHE:HA	28:TF:550:TRP:CD1	2.52	0.43
39:q:100:GLU:HA	39:q:103:THR:HG22	2.00	0.43
6:6:85:G:H2'	6:6:86:A:C8	2.53	0.43
7:A:873:TYR:HE1	7:A:883:GLN:HG2	1.84	0.43
7:A:949:LEU:HD23	7:A:949:LEU:HA	1.87	0.43
7:A:1663:VAL:HG11	7:A:1741:ASN:HB3	2.01	0.43
12:I:724:LYS:HE2	12:I:724:LYS:HB3	1.89	0.43
15:L:536:ILE:HD12	15:L:536:ILE:HG23	1.82	0.43
19:O:178:ALA:HA	19:O:182:ALA:HB3	1.99	0.43
23:Q:773:ARG:HB2	23:Q:973:PHE:HA	2.00	0.43
27:T:109:GLN:HA	27:T:133:GLN:NE2	2.33	0.43
1:1:-10:A:C2	26:SR:3:TYR:HB3	2.54	0.43
6:6:54:C:H4'	24:R:221:LYS:HE3	1.99	0.43
10:E:157:ASP:OD1	10:E:159:THR:HG22	2.18	0.43
35:d:34:GLN:HG2	35:d:60:PHE:HZ	1.83	0.43
7:A:1642:LYS:HG3	7:A:1650:CYS:SG	2.59	0.43
7:A:1660:LYS:HZ1	7:A:1680:THR:C	2.26	0.43
25:S:46:VAL:HG22	25:S:52:ILE:HG23	2.00	0.43
8:C:149:HIS:CG	8:C:150:LEU:H	2.36	0.43
8:C:331:THR:H	8:C:334:SER:HB2	1.82	0.43
10:E:154:VAL:HB	10:E:180:LEU:HB2	2.01	0.43
10:E:306:LEU:HA	10:E:307:PRO:HD3	1.92	0.43
20:O:2:85:ASP:HB2	20:O:2:88:LYS:HB2	2.00	0.43
29:W:71:ASN:HA	29:W:72:PRO:HD3	1.92	0.43
7:A:1182:ILE:HD13	7:A:1185:ARG:HH11	1.84	0.43
8:C:501:ALA:HB2	8:C:661:LEU:HD12	2.01	0.43
12:I:448:ARG:HH12	12:I:498:THR:HG21	1.84	0.43
23:Q:202:LEU:HD23	23:Q:228:MET:HE1	1.99	0.43
39:q:122:ARG:NH1	39:s:118:LEU:HD22	2.34	0.43
39:r:24:GLU:HB3	39:r:27:LEU:HD12	2.00	0.43
6:6:34:U:H2'	6:6:35:A:C8	2.53	0.43
7:A:1378:ARG:HD2	26:SR:8:LEU:HD22	2.00	0.43
8:C:701:MET:HE2	8:C:805:LEU:HD13	2.01	0.43
8:C:706:LEU:HD23	8:C:710:ILE:HB	2.01	0.43
13:J:588:LEU:HB3	13:J:591:GLU:HB2	2.01	0.43
23:Q:686:VAL:HG13	23:Q:690:LEU:HD13	2.01	0.43
23:Q:1240:LEU:HB3	23:Q:1263:ILE:HB	2.00	0.43
7:A:1641:ARG:HB3	7:A:1645:LYS:HE3	2.00	0.43
7:A:1689:GLN:HE21	7:A:1707:LYS:HG2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:396:THR:HG23	8:C:427:LEU:HG	2.00	0.43
14:K:153:LYS:HA	14:K:153:LYS:HD3	1.82	0.43
19:O:69:ILE:HG23	19:O:84:MET:HE1	2.01	0.43
19:O:93:ILE:HD12	19:O:93:ILE:HA	1.93	0.43
34:c:68:TYR:HB2	35:d:100:PHE:HB3	2.01	0.43
7:A:1295:MET:SD	7:A:1354:MET:HE2	2.59	0.42
12:I:503:TYR:HA	12:I:506:VAL:HG12	2.01	0.42
15:L:67:GLU:HB3	30:YB:169:PHE:CZ	2.54	0.42
18:N:125:LYS:HB3	18:N:125:LYS:HE3	1.81	0.42
27:T:259:LEU:HB2	27:T:261:VAL:HG12	2.01	0.42
32:a:89:VAL:HG12	32:a:91:LEU:HG	2.01	0.42
34:c:8:MET:HE1	34:c:34:MET:HE2	2.01	0.42
39:r:40:VAL:HG12	39:r:41:THR:HG23	2.01	0.42
7:A:1654:LEU:HD12	7:A:1720:PRO:HG2	2.01	0.42
12:I:278:TYR:HE1	12:I:332:ILE:HD13	1.84	0.42
23:Q:502:LYS:HE3	23:Q:584:ASN:HB3	2.01	0.42
31:Z:105:LEU:HA	31:Z:105:LEU:HD23	1.82	0.42
36:e:81:ILE:HB	38:g:61:ALA:HB3	2.00	0.42
7:A:329:THR:HG23	26:SR:4:ASN:H	1.84	0.42
10:E:261:PHE:HE1	10:E:300:GLY:HA2	1.83	0.42
10:E:283:PHE:HD1	10:E:297:SER:HA	1.83	0.42
12:I:682:LEU:HD23	12:I:682:LEU:HA	1.82	0.42
14:K:83:LEU:HD23	14:K:94:GLN:HE22	1.84	0.42
18:N:106:ILE:HD13	18:N:106:ILE:HG21	1.82	0.42
4:35:131:ILE:HG21	4:35:161:VAL:HG11	2.01	0.42
8:C:242:ASP:CG	8:C:271:LYS:HD2	2.44	0.42
8:C:386:LEU:HD23	8:C:386:LEU:HA	1.90	0.42
15:L:596:GLU:HB3	39:s:112:LEU:HD13	2.02	0.42
29:W:62:MET:HA	29:W:64:GLN:NE2	2.34	0.42
39:r:121:GLU:HB3	39:t:122:ARG:HH22	1.83	0.42
3:3:180:GLU:HB3	3:3:181:LYS:H	1.67	0.42
15:L:257:ILE:O	15:L:261:ILE:HG12	2.19	0.42
23:Q:52:LEU:HD22	23:Q:57:LEU:HD13	2.02	0.42
33:b:81:GLN:HE21	33:b:81:GLN:HB2	1.63	0.42
35:d:72:LYS:HD3	35:d:72:LYS:HA	1.93	0.42
39:r:356:GLU:HA	39:r:372:GLY:HA2	2.02	0.42
6:6:55:C:H2'	6:6:56:C:O4'	2.19	0.42
7:A:88:ARG:HG2	7:A:92:LYS:NZ	2.34	0.42
13:J:259:ARG:NH1	27:T:87:ASP:HA	2.34	0.42
13:J:514:GLU:HB2	13:J:523:ALA:HB2	2.02	0.42
39:s:10:PRO:HG2	39:s:13:PRO:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:123:LYS:HB2	3:3:123:LYS:HE2	1.81	0.42
8:C:492:VAL:HG22	8:C:508:ALA:HB2	2.00	0.42
23:Q:674:VAL:HG13	23:Q:686:VAL:HG11	2.01	0.42
7:A:348:LEU:HA	7:A:348:LEU:HD23	1.86	0.42
7:A:959:PHE:HB3	7:A:963:VAL:HG21	2.00	0.42
7:A:1585:MET:HB3	7:A:1585:MET:HE3	1.84	0.42
10:E:85:ASN:HD22	33:b:99:GLY:H	1.66	0.42
12:I:628:TYR:HE2	12:I:655:LEU:HD22	1.84	0.42
25:S:45:ARG:NH1	29:W:68:GLY:HA3	2.35	0.42
34:c:74:LEU:HA	34:c:75:PRO:HD3	1.93	0.42
39:q:90:LEU:HB2	39:s:90:LEU:HD11	2.01	0.42
15:L:266:MET:HA	15:L:269:GLU:HG2	2.02	0.42
29:W:126:ASP:O	29:W:130:LYS:HG3	2.20	0.42
34:c:70:LEU:HB3	34:c:74:LEU:HD21	2.02	0.42
39:t:14:VAL:HG11	39:t:50:LEU:HD13	2.01	0.42
39:t:14:VAL:HB	39:t:50:LEU:HB2	2.01	0.42
7:A:661:LEU:HD23	7:A:661:LEU:HA	1.85	0.42
7:A:1272:LEU:HD23	7:A:1272:LEU:HA	1.79	0.42
7:A:1825:LYS:HE2	7:A:1848:THR:HG21	2.01	0.42
13:J:460:TRP:CE2	13:J:470:PRO:HG3	2.55	0.42
23:Q:445:LEU:HB2	23:Q:621:TYR:HB3	2.01	0.42
23:Q:745:MET:HE1	23:Q:1007:LEU:HD12	2.01	0.42
27:T:354:ILE:HB	27:T:368:PHE:HB2	2.02	0.42
39:r:94:LEU:HA	39:r:97:THR:HG22	2.01	0.42
8:C:760:ARG:HH21	8:C:804:ARG:HD3	1.83	0.41
15:L:600:CYS:SG	39:s:108:LEU:HB2	2.59	0.41
39:r:71:ALA:HB1	39:s:63:PRO:HD3	2.02	0.41
7:A:177:ARG:HD3	7:A:643:PRO:HB2	2.01	0.41
8:C:371:GLN:HE22	8:C:373:LEU:HB2	1.85	0.41
8:C:933:LYS:HZ1	8:C:935:LEU:HB2	1.86	0.41
13:J:302:ASP:HA	13:J:305:ARG:HG2	2.02	0.41
18:N:11:ARG:HG2	18:N:12:PRO:HD2	2.01	0.41
18:N:103:LEU:HD23	18:N:103:LEU:HA	1.87	0.41
23:Q:628:LEU:HD11	23:Q:987:SER:HB2	2.02	0.41
28:TF:619:LEU:HD23	28:TF:622:LEU:HD12	2.02	0.41
4:35:561:LEU:HD12	4:35:561:LEU:HA	1.92	0.41
15:L:242:ASP:HA	15:L:249:LYS:HZ3	1.85	0.41
25:S:21:HIS:HB3	25:S:77:HIS:HE1	1.85	0.41
6:6:44:A:H2'	6:6:45:U:C6	2.55	0.41
7:A:1360:PRO:HB2	7:A:1374:ILE:HD12	2.03	0.41
8:C:271:LYS:HG2	43:C:1001:GTP:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:E:44:LEU:HD23	10:E:336:LEU:HD12	2.02	0.41
23:Q:480:LEU:HD21	23:Q:483:PHE:HB2	2.01	0.41
35:d:88:LYS:HE3	35:d:88:LYS:HB3	1.87	0.41
7:A:1261:ILE:HG12	7:A:1308:LEU:HG	2.03	0.41
12:I:455:VAL:HA	12:I:476:LEU:HD21	2.02	0.41
13:J:369:CYS:HA	13:J:372:GLU:HG2	2.02	0.41
19:O:147:VAL:HG21	20:O2:267:ALA:HB2	2.03	0.41
20:O2:120:PHE:HB2	20:O2:135:HIS:CD2	2.55	0.41
23:Q:1049:ARG:HG2	23:Q:1075:LEU:HD22	2.03	0.41
27:T:172:GLU:HG2	27:T:177:TRP:CE2	2.56	0.41
27:T:314:ARG:HG2	27:T:326:THR:HG23	2.03	0.41
39:q:25:LYS:HA	39:q:25:LYS:HD2	1.94	0.41
7:A:624:GLN:HG2	7:A:663:PHE:HB2	2.03	0.41
7:A:1689:GLN:NE2	7:A:1707:LYS:HG2	2.36	0.41
8:C:132:PHE:HZ	8:C:553:LEU:HB3	1.84	0.41
8:C:728:ILE:H	8:C:728:ILE:HG13	1.75	0.41
10:E:218:HIS:CE1	10:E:244:ARG:HG3	2.55	0.41
23:Q:164:LEU:HD13	23:Q:244:PRO:HB3	2.02	0.41
8:C:935:LEU:HD23	8:C:935:LEU:HA	1.92	0.41
12:I:463:ILE:HG23	12:I:470:LEU:HD22	2.03	0.41
12:I:585:PRO:HB3	12:I:619:VAL:HA	2.03	0.41
13:J:268:ILE:HD13	13:J:268:ILE:HA	1.89	0.41
39:t:11:LYS:HD3	39:t:60:ARG:HH22	1.85	0.41
7:A:821:GLY:HA3	24:R:285:ASN:HD22	1.84	0.41
7:A:1268:ILE:HD13	7:A:1268:ILE:HA	1.85	0.41
7:A:1742:TRP:CG	7:A:1747:LYS:HD2	2.56	0.41
7:A:1957:PHE:HB3	11:GP:129:LEU:HD22	2.02	0.41
8:C:520:LYS:HE3	8:C:520:LYS:HB2	1.83	0.41
8:C:721:ILE:HD13	8:C:721:ILE:HA	1.90	0.41
8:C:872:LEU:HD21	8:C:888:LEU:HD13	2.03	0.41
9:CW:509:ALA:HB2	9:CW:543:MET:HG3	2.02	0.41
21:P:50:LYS:HA	21:P:50:LYS:HD3	1.91	0.41
2:2:19:G:N1	6:6:50:A:C2	2.73	0.41
4:35:497:SER:HA	4:35:500:PHE:CD1	2.56	0.41
7:A:97:MET:HE3	7:A:97:MET:HB3	1.95	0.41
7:A:1595:ILE:HG12	11:GP:55:ALA:HB2	2.03	0.41
7:A:1685:TRP:HE3	7:A:1721:SER:HB2	1.86	0.41
13:J:84:LYS:NZ	13:J:87:ALA:HB3	2.35	0.41
15:L:157:GLU:HA	15:L:160:LYS:HE3	2.03	0.41
15:L:537:ARG:HD2	15:L:577:PHE:CG	2.56	0.41
19:O:232:PHE:HD1	19:O:235:TYR:HD2	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:O2:98:VAL:HG12	20:O2:101:ARG:NH1	2.35	0.41
23:Q:81:LEU:HD23	23:Q:81:LEU:HA	1.86	0.41
24:R:295:LEU:HD23	24:R:295:LEU:HA	1.91	0.41
27:T:272:ARG:HE	27:T:281:ASN:ND2	2.19	0.41
28:TF:287:LYS:HB2	28:TF:287:LYS:HE2	1.93	0.41
28:TF:771:LYS:HB3	28:TF:771:LYS:HE2	1.74	0.41
39:q:17:ARG:NH1	39:t:17:ARG:HA	2.36	0.41
39:q:80:TRP:CZ2	39:r:69:LEU:HB3	2.56	0.41
39:r:205:GLU:HA	39:r:217:PRO:HA	2.03	0.41
3:3:196:LEU:HD13	7:A:767:LYS:HD2	2.03	0.41
7:A:247:TRP:HD1	7:A:441:THR:HG23	1.85	0.41
7:A:1629:GLN:HB3	7:A:1655:LEU:HD12	2.03	0.41
8:C:601:VAL:HB	8:C:844:PRO:HG3	2.02	0.41
9:CW:588:PHE:CD2	9:CW:596:LEU:HD11	2.55	0.41
13:J:199:VAL:HG13	27:T:133:GLN:OE1	2.20	0.41
13:J:303:LYS:HA	13:J:303:LYS:HD2	1.83	0.41
32:a:17:THR:HA	32:a:26:TYR:O	2.21	0.41
38:g:40:ILE:HD11	38:g:62:ILE:HD12	2.01	0.41
3:3:258:LEU:HD12	3:3:258:LEU:HA	1.90	0.40
6:6:43:G:H5'	15:L:176:LYS:HD3	2.03	0.40
13:J:189:ARG:HE	13:J:189:ARG:HB3	1.53	0.40
39:q:13:PRO:HG2	39:q:53:VAL:HG11	2.02	0.40
39:r:90:LEU:HD22	39:t:90:LEU:HD13	2.03	0.40
4:35:143:VAL:HB	4:35:172:PHE:HZ	1.86	0.40
4:35:582:ALA:HB1	4:35:590:TYR:HB3	2.02	0.40
5:5:40:U:H2'	5:5:41:U:H6	1.85	0.40
12:I:722:ARG:HH12	30:YB:199:PRO:HD3	1.85	0.40
24:R:237:PRO:HA	24:R:238:PRO:HD3	1.94	0.40
34:c:5:ARG:HE	34:c:5:ARG:HB3	1.66	0.40
7:A:1185:ARG:NE	21:P:229:VAL:HG11	2.36	0.40
27:T:291:THR:H	27:T:291:THR:HG23	1.69	0.40
35:d:12:LEU:HD23	35:d:16:GLU:HB2	2.03	0.40
35:d:38:LYS:HB3	35:d:38:LYS:HE3	1.87	0.40
39:s:111:ALA:O	39:s:115:ILE:HG12	2.21	0.40
5:5:49:U:H2'	5:5:50:U:C6	2.57	0.40
7:A:1523:GLU:HB3	16:LG:104:LEU:HD12	2.03	0.40
8:C:406:LYS:HE3	8:C:406:LYS:HB3	1.83	0.40
8:C:933:LYS:HA	8:C:934:PRO:HD3	1.91	0.40
15:L:701:TRP:HD1	39:q:60:ARG:CZ	2.34	0.40
23:Q:737:ARG:HD3	23:Q:1040:ILE:HD11	2.02	0.40
39:r:120:LYS:HD3	39:r:120:LYS:HA	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:35:35:LEU:HD23	4:35:35:LEU:HA	1.89	0.40
7:A:133:GLU:H	7:A:133:GLU:HG3	1.66	0.40
7:A:1979:ARG:HA	7:A:1979:ARG:HD3	1.92	0.40
9:CW:541:LYS:O	9:CW:545:GLN:HG3	2.22	0.40
13:J:466:GLU:HB3	13:J:501:GLU:HG3	2.03	0.40
23:Q:360:PHE:HB3	23:Q:366:ILE:HD12	2.03	0.40
23:Q:966:LEU:HD23	23:Q:966:LEU:HA	1.94	0.40
32:a:19:GLU:HB3	32:a:25:THR:HG22	2.02	0.40
33:b:23:THR:HB	33:b:45:TYR:HB2	2.03	0.40
35:d:29:PRO:HG3	37:f:36:SER:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	3	156/384 (41%)	146 (94%)	10 (6%)	0	100	100
4	35	624/647 (96%)	605 (97%)	17 (3%)	2 (0%)	36	67
7	A	1984/2363 (84%)	1880 (95%)	103 (5%)	1 (0%)	48	78
8	C	916/984 (93%)	872 (95%)	44 (5%)	0	100	100
9	CW	202/887 (23%)	193 (96%)	9 (4%)	0	100	100
10	E	297/340 (87%)	275 (93%)	22 (7%)	0	100	100
11	GP	216/534 (40%)	179 (83%)	32 (15%)	5 (2%)	5	23
12	I	642/790 (81%)	603 (94%)	38 (6%)	1 (0%)	43	73
13	J	597/674 (89%)	583 (98%)	13 (2%)	1 (0%)	43	73
14	K	151/187 (81%)	145 (96%)	5 (3%)	1 (1%)	18	49
15	L	507/757 (67%)	473 (93%)	30 (6%)	4 (1%)	16	47
16	LG	55/198 (28%)	53 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	M	94/229 (41%)	87 (93%)	6 (6%)	1 (1%)	11	39
18	N	142/146 (97%)	135 (95%)	7 (5%)	0	100	100
19	O	222/354 (63%)	215 (97%)	7 (3%)	0	100	100
20	O2	265/388 (68%)	244 (92%)	20 (8%)	1 (0%)	30	61
21	P	86/265 (32%)	80 (93%)	5 (6%)	1 (1%)	10	37
22	PX	28/361 (8%)	27 (96%)	1 (4%)	0	100	100
23	Q	1282/1284 (100%)	1263 (98%)	19 (2%)	0	100	100
24	R	282/557 (51%)	261 (93%)	19 (7%)	2 (1%)	18	49
25	S	152/155 (98%)	140 (92%)	12 (8%)	0	100	100
26	SR	98/293 (33%)	92 (94%)	6 (6%)	0	100	100
27	T	425/473 (90%)	382 (90%)	40 (9%)	3 (1%)	18	49
28	TF	455/797 (57%)	446 (98%)	8 (2%)	1 (0%)	43	73
29	W	150/558 (27%)	137 (91%)	13 (9%)	0	100	100
30	YB	58/299 (19%)	55 (95%)	3 (5%)	0	100	100
31	Z	40/142 (28%)	40 (100%)	0	0	100	100
32	a	94/97 (97%)	93 (99%)	1 (1%)	0	100	100
33	b	91/147 (62%)	89 (98%)	2 (2%)	0	100	100
34	c	79/117 (68%)	74 (94%)	5 (6%)	0	100	100
35	d	98/115 (85%)	91 (93%)	7 (7%)	0	100	100
36	e	78/84 (93%)	76 (97%)	2 (3%)	0	100	100
37	f	71/78 (91%)	67 (94%)	4 (6%)	0	100	100
38	g	71/77 (92%)	70 (99%)	1 (1%)	0	100	100
39	q	130/488 (27%)	121 (93%)	9 (7%)	0	100	100
39	r	414/488 (85%)	394 (95%)	20 (5%)	0	100	100
39	s	129/488 (26%)	118 (92%)	11 (8%)	0	100	100
39	t	132/488 (27%)	125 (95%)	6 (4%)	1 (1%)	16	47
All	All	11513/17713 (65%)	10929 (95%)	559 (5%)	25 (0%)	44	73

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	GP	174	TYR
15	L	536	ILE

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Mol	Chain	Res	Type
17	M	144	VAL
4	35	308	SER
11	GP	122	SER
27	T	30	ALA
27	T	36	THR
39	t	69	LEU
7	A	1115	ILE
11	GP	121	THR
11	GP	172	GLN
20	O2	90	GLN
27	T	35	VAL
4	35	437	ASP
13	J	87	ALA
14	K	71	LYS
21	P	224	ARG
24	R	112	GLU
24	R	131	LEU
28	TF	321	THR
15	L	537	ARG
12	I	83	ASN
15	L	538	PRO
11	GP	127	ASP
15	L	530	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	3	149/346 (43%)	149 (100%)	0	100	100
4	35	564/585 (96%)	561 (100%)	3 (0%)	81	85
7	A	1798/2138 (84%)	1794 (100%)	4 (0%)	87	89
8	C	821/881 (93%)	821 (100%)	0	100	100
9	CW	188/816 (23%)	188 (100%)	0	100	100
10	E	257/292 (88%)	257 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	GP	193/478 (40%)	190 (98%)	3 (2%)	55	75
12	I	586/707 (83%)	586 (100%)	0	100	100
13	J	532/597 (89%)	532 (100%)	0	100	100
14	K	132/163 (81%)	132 (100%)	0	100	100
15	L	462/656 (70%)	461 (100%)	1 (0%)	87	89
16	LG	54/187 (29%)	54 (100%)	0	100	100
17	M	94/214 (44%)	94 (100%)	0	100	100
18	N	130/132 (98%)	130 (100%)	0	100	100
19	O	198/306 (65%)	198 (100%)	0	100	100
20	O2	231/340 (68%)	231 (100%)	0	100	100
21	P	79/240 (33%)	79 (100%)	0	100	100
22	PX	28/335 (8%)	28 (100%)	0	100	100
23	Q	1188/1188 (100%)	1188 (100%)	0	100	100
24	R	243/477 (51%)	242 (100%)	1 (0%)	84	86
25	S	128/129 (99%)	125 (98%)	3 (2%)	44	70
26	SR	95/275 (34%)	95 (100%)	0	100	100
27	T	367/405 (91%)	367 (100%)	0	100	100
28	TF	425/719 (59%)	425 (100%)	0	100	100
29	W	79/496 (16%)	79 (100%)	0	100	100
30	YB	56/274 (20%)	56 (100%)	0	100	100
31	Z	38/133 (29%)	37 (97%)	1 (3%)	40	68
32	a	85/86 (99%)	85 (100%)	0	100	100
33	b	80/118 (68%)	80 (100%)	0	100	100
34	c	76/102 (74%)	76 (100%)	0	100	100
35	d	91/101 (90%)	91 (100%)	0	100	100
36	e	73/76 (96%)	73 (100%)	0	100	100
37	f	64/69 (93%)	64 (100%)	0	100	100
38	g	63/67 (94%)	63 (100%)	0	100	100
39	q	121/443 (27%)	121 (100%)	0	100	100
39	r	221/443 (50%)	219 (99%)	2 (1%)	70	80
39	s	120/443 (27%)	120 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	t	123/443 (28%)	123 (100%)	0	100	100
All	All	10232/15900 (64%)	10214 (100%)	18 (0%)	85	89

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	35	266	ASP
4	35	294	ASP
4	35	593	ILE
7	A	896	ASN
7	A	899	GLU
7	A	1490	GLN
7	A	1769	GLU
11	GP	107	GLU
11	GP	115	LYS
11	GP	273	LEU
15	L	467	LEU
24	R	322	GLN
25	S	10	LEU
25	S	105	THR
25	S	121	ARG
31	Z	139	THR
39	r	184	PRO
39	r	415	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (100) such sidechains are listed below:

Mol	Chain	Res	Type
3	3	147	HIS
4	35	57	GLN
4	35	262	HIS
4	35	289	ASN
4	35	451	ASN
7	A	52	ASN
7	A	62	GLN
7	A	352	HIS
7	A	402	ASN
7	A	694	GLN
7	A	726	GLN
7	A	816	ASN
7	A	857	HIS

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Mol	Chain	Res	Type
7	A	896	ASN
7	A	1027	ASN
7	A	1037	ASN
7	A	1049	ASN
7	A	1065	GLN
7	A	1387	HIS
7	A	1397	GLN
7	A	1452	HIS
7	A	1490	GLN
7	A	1492	ASN
7	A	1511	HIS
7	A	1544	ASN
7	A	1761	ASN
7	A	1799	GLN
8	C	72	HIS
8	C	111	HIS
8	C	343	HIS
8	C	371	GLN
8	C	412	GLN
8	C	497	ASN
8	C	503	ASN
8	C	583	ASN
8	C	596	HIS
8	C	609	HIS
8	C	735	ASN
8	C	904	HIS
9	CW	442	GLN
9	CW	484	GLN
9	CW	510	ASN
9	CW	570	HIS
10	E	40	ASN
10	E	191	GLN
10	E	259	GLN
10	E	292	ASN
11	GP	66	ASN
12	I	117	GLN
12	I	203	ASN
12	I	289	ASN
12	I	473	GLN
12	I	477	HIS
12	I	527	ASN
12	I	704	GLN

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Mol	Chain	Res	Type
13	J	22	GLN
13	J	225	GLN
13	J	307	GLN
13	J	497	GLN
13	J	529	GLN
14	K	61	ASN
15	L	43	GLN
15	L	172	ASN
15	L	222	ASN
15	L	532	GLN
15	L	632	ASN
15	L	720	GLN
17	M	98	GLN
19	O	118	GLN
19	O	120	GLN
19	O	121	GLN
20	O2	72	ASN
20	O2	111	ASN
20	O2	156	HIS
20	O2	208	ASN
21	P	64	HIS
21	P	68	GLN
23	Q	53	HIS
23	Q	580	ASN
23	Q	584	ASN
23	Q	659	ASN
23	Q	672	ASN
23	Q	747	ASN
23	Q	1084	HIS
24	R	113	HIS
24	R	235	HIS
25	S	77	HIS
27	T	19	ASN
27	T	281	ASN
27	T	392	ASN
28	TF	381	HIS
28	TF	766	ASN
33	b	11	ASN
34	c	21	ASN
34	c	35	GLN
34	c	37	ASN
35	d	40	HIS

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Mol	Chain	Res	Type
35	d	50	ASN
36	e	33	GLN
39	s	77	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	29/30 (96%)	15 (51%)	2 (6%)
2	2	22/186 (11%)	5 (22%)	0
5	5	101/120 (84%)	22 (21%)	2 (1%)
6	6	91/99 (91%)	44 (48%)	6 (6%)
All	All	243/435 (55%)	86 (35%)	10 (4%)

All (86) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	-14	U
1	1	-13	U
1	1	-12	U
1	1	-8	U
1	1	-4	A
1	1	0	G
1	1	1	G
1	1	2	U
1	1	3	A
1	1	5	G
1	1	9	U
1	1	10	U
1	1	12	U
1	1	13	U
1	1	14	U
2	2	11	U
2	2	12	G
2	2	13	C
2	2	24	A
2	2	29	A
5	5	13	A
5	5	14	G
5	5	27	G
5	5	28	C
5	5	30	A

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Mol	Chain	Res	Type
5	5	31	A
5	5	33	G
5	5	37	C
5	5	50	U
5	5	54	C
5	5	79	G
5	5	82	A
5	5	83	A
5	5	90	U
5	5	91	G
5	5	92	U
5	5	98	U
5	5	99	U
5	5	102	G
5	5	103	U
5	5	105	A
5	5	108	U
6	6	4	C
6	6	7	C
6	6	8	G
6	6	9	G
6	6	10	A
6	6	11	U
6	6	12	C
6	6	14	C
6	6	18	G
6	6	19	G
6	6	20	U
6	6	21	C
6	6	22	A
6	6	23	A
6	6	24	A
6	6	27	G
6	6	28	A
6	6	29	A
6	6	30	A
6	6	31	C
6	6	38	G
6	6	39	A
6	6	40	G
6	6	43	G
6	6	44	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	6	46	U
6	6	48	G
6	6	52	G
6	6	53	G
6	6	61	A
6	6	62	C
6	6	63	A
6	6	68	U
6	6	74	U
6	6	75	G
6	6	76	C
6	6	78	A
6	6	79	C
6	6	80	A
6	6	81	U
6	6	82	U
6	6	83	G
6	6	91	A
6	6	92	C

All (10) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	0	G
1	1	1	G
5	5	27	G
5	5	49	U
6	6	13	A
6	6	17	U
6	6	30	A
6	6	38	G
6	6	52	G
6	6	74	U

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 13 ligands modelled in this entry, 11 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
43	GTP	C	1001	40	30,34,34	1.33	3 (10%)	46,54,54	2.04	12 (26%)
42	IHP	A	2401	-	36,36,36	2.25	12 (33%)	54,60,60	1.24	7 (12%)

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
43	GTP	C	1001	40	-	0/22/38/38	0/3/3/3
42	IHP	A	2401	-	-	4/30/54/54	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	A	2401	IHP	P3-O13	4.48	1.67	1.59
42	A	2401	IHP	P2-O12	4.33	1.67	1.59
42	A	2401	IHP	P5-O15	4.31	1.67	1.59
42	A	2401	IHP	P1-O11	4.25	1.67	1.59
42	A	2401	IHP	C3-C2	-4.16	1.43	1.52
42	A	2401	IHP	P6-O16	3.77	1.66	1.59
42	A	2401	IHP	P4-O14	3.70	1.66	1.59
42	A	2401	IHP	C2-C1	-3.50	1.45	1.52
42	A	2401	IHP	O15-C5	-3.15	1.32	1.44
42	A	2401	IHP	O13-C3	-2.88	1.33	1.44
43	C	1001	GTP	C5-N7	-2.80	1.33	1.39
42	A	2401	IHP	O12-C2	-2.75	1.34	1.44
42	A	2401	IHP	O11-C1	-2.66	1.34	1.44
43	C	1001	GTP	O4'-C4'	-2.26	1.39	1.45
43	C	1001	GTP	C5-C6	-2.16	1.36	1.44

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	C	1001	GTP	PB-O3B-PG	-6.49	110.57	132.83
43	C	1001	GTP	C5-C4-N3	-4.82	120.64	128.46
43	C	1001	GTP	C2-N3-C4	4.40	120.14	112.30
42	A	2401	IHP	C6-C1-C2	3.76	118.64	110.41
43	C	1001	GTP	PA-O3A-PB	-3.52	120.73	132.83
43	C	1001	GTP	C2-N1-C6	-3.25	119.17	125.10
43	C	1001	GTP	N9-C8-N7	-3.13	107.50	113.39
43	C	1001	GTP	C5-C6-N1	3.02	120.87	113.19
42	A	2401	IHP	O11-C1-C2	3.00	115.76	108.69
43	C	1001	GTP	N9-C4-N3	2.93	131.82	125.94
43	C	1001	GTP	O3G-PG-O3B	2.67	113.59	104.64
43	C	1001	GTP	O6-C6-C5	-2.60	119.71	126.60
43	C	1001	GTP	C8-N7-C5	2.55	108.86	104.24
42	A	2401	IHP	C6-C5-C4	2.46	115.80	110.41
42	A	2401	IHP	C3-C2-C1	2.25	115.34	110.41
42	A	2401	IHP	C5-C6-C1	2.11	115.03	110.41
42	A	2401	IHP	O15-C5-C6	2.11	113.65	108.69
43	C	1001	GTP	C3'-C2'-C1'	-2.06	97.50	101.43
42	A	2401	IHP	O15-C5-C4	2.06	113.53	108.69

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
42	A	2401	IHP	C6-O16-P6-O26
42	A	2401	IHP	C1-O11-P1-O41
42	A	2401	IHP	C5-O15-P5-O35
42	A	2401	IHP	C6-O16-P6-O36

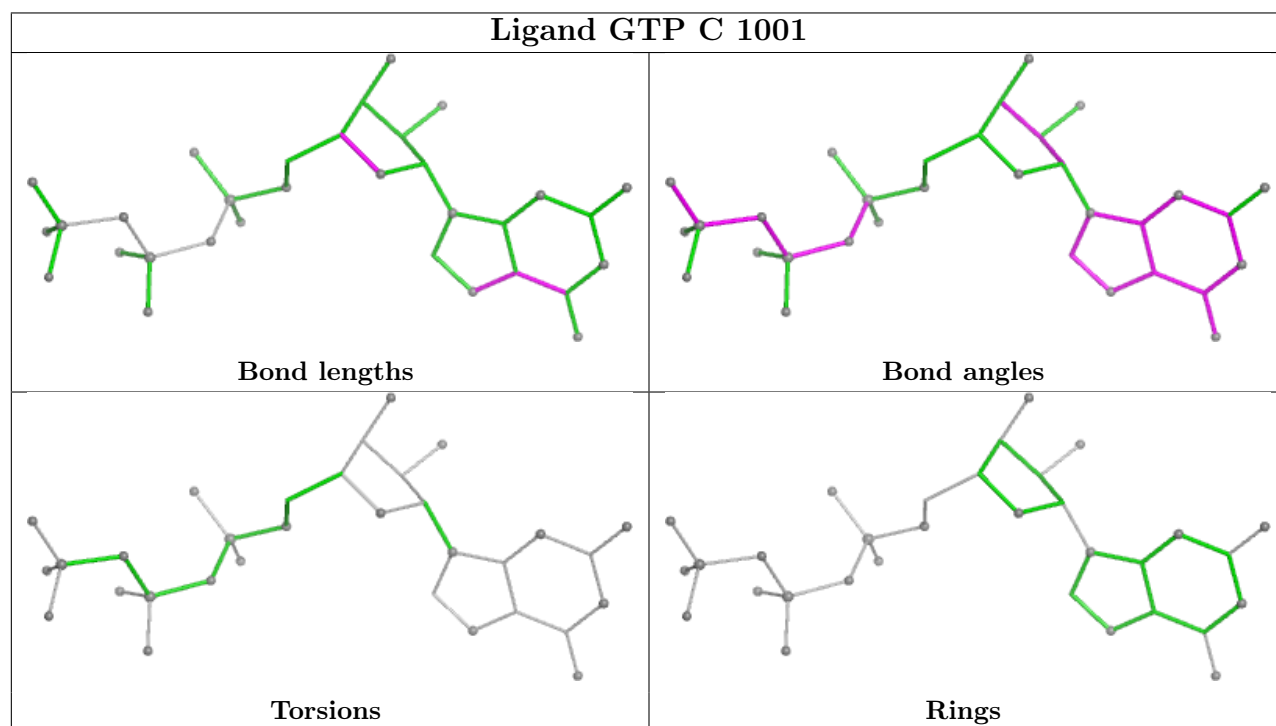
There are no ring outliers.

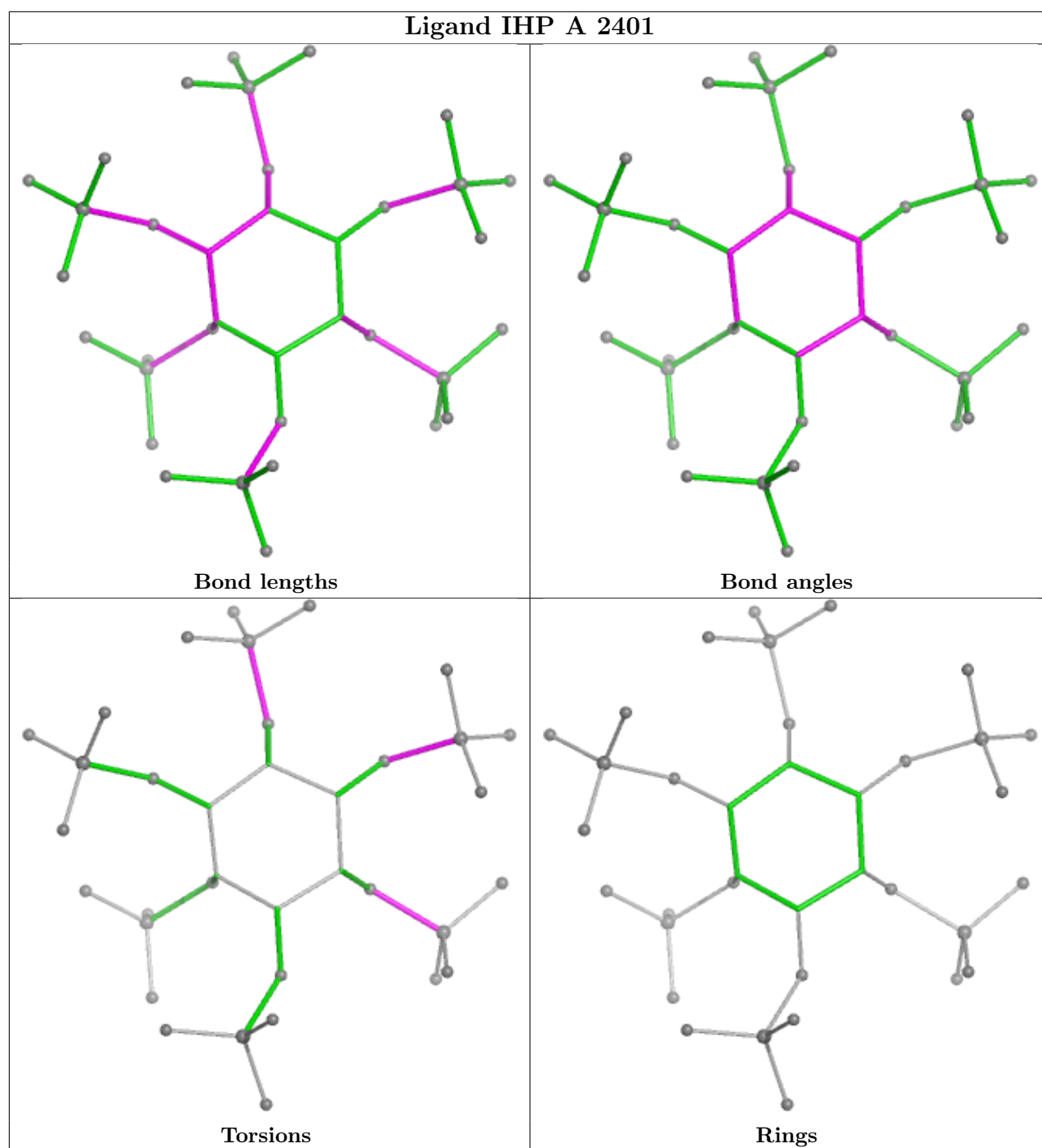
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	C	1001	GTP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

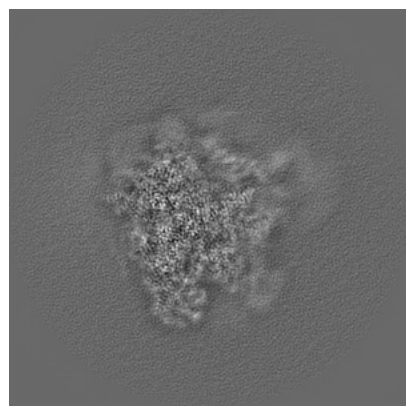
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19942. These allow visual inspection of the internal detail of the map and identification of artifacts.

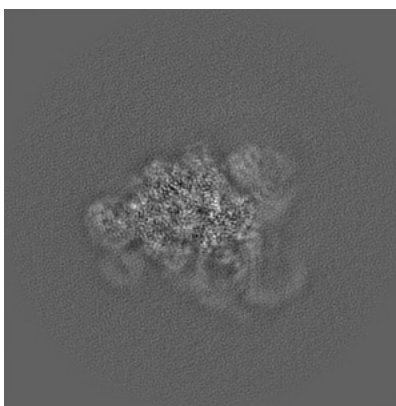
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

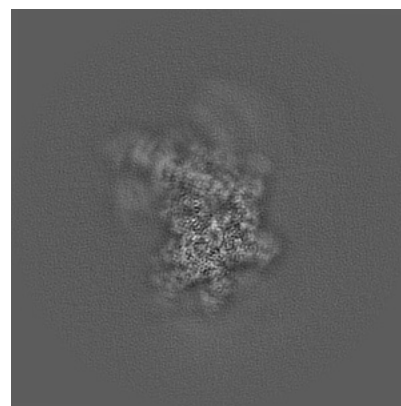
6.1.1 Primary map



X

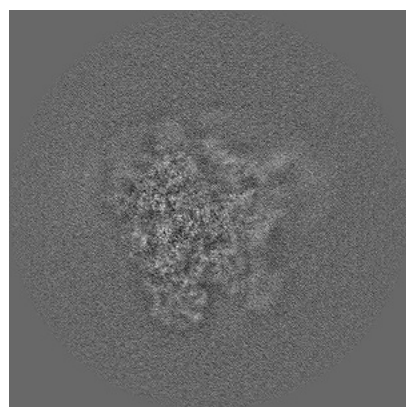


Y

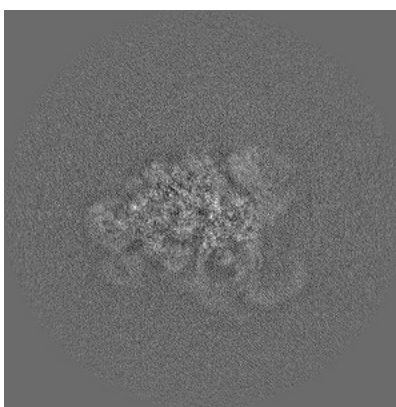


Z

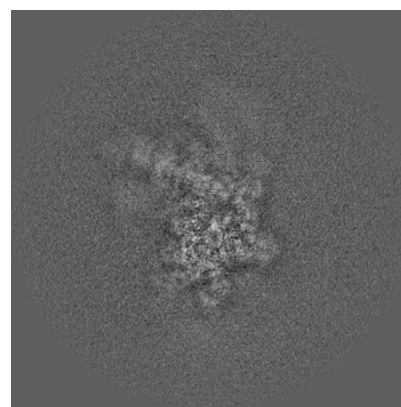
6.1.2 Raw map



X



Y

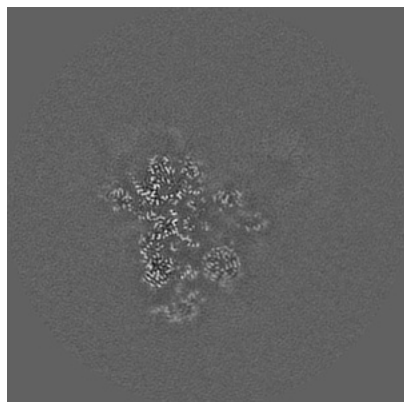


Z

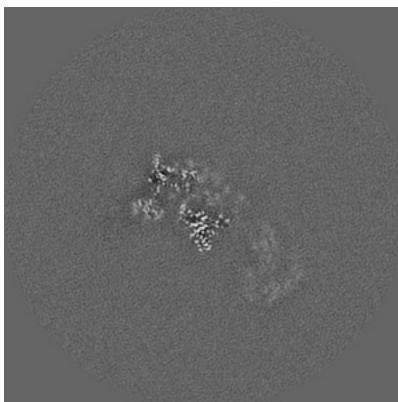
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

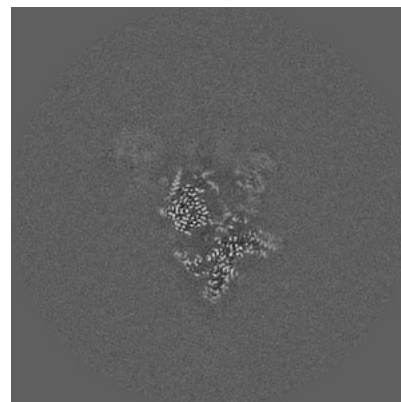
6.2.1 Primary map



X Index: 280

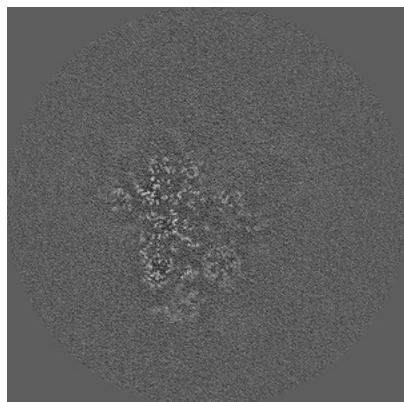


Y Index: 280

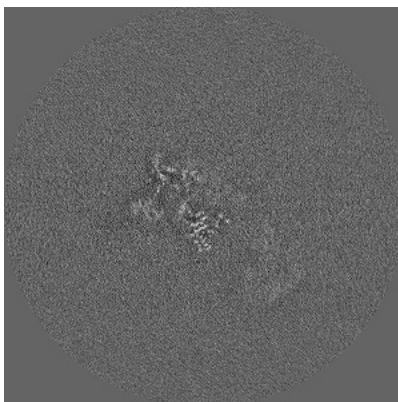


Z Index: 280

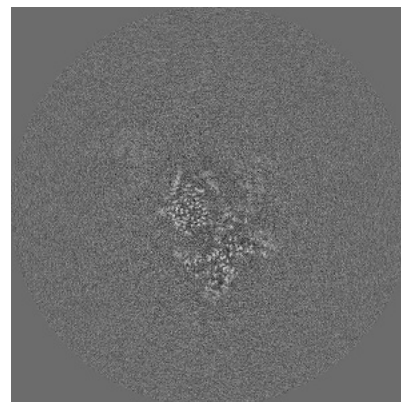
6.2.2 Raw map



X Index: 280



Y Index: 280

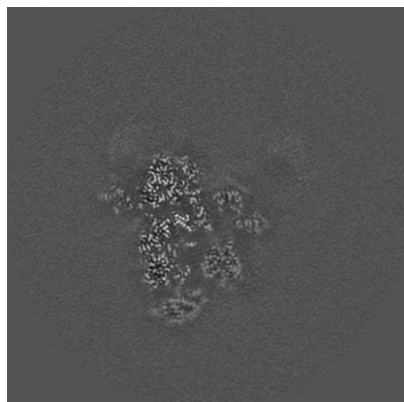


Z Index: 280

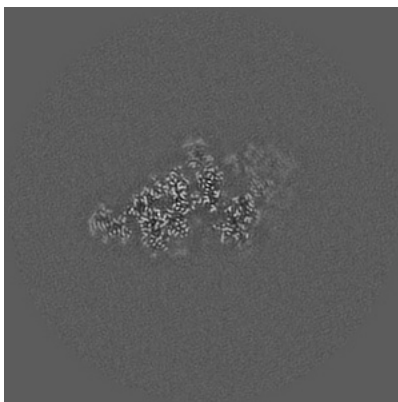
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

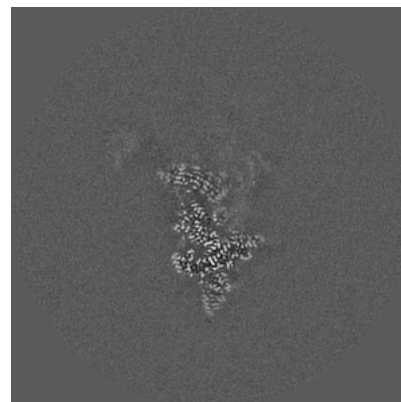
6.3.1 Primary map



X Index: 276

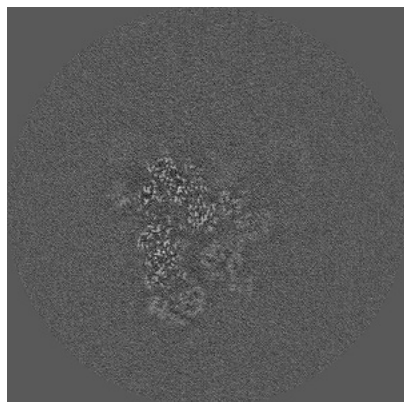


Y Index: 219

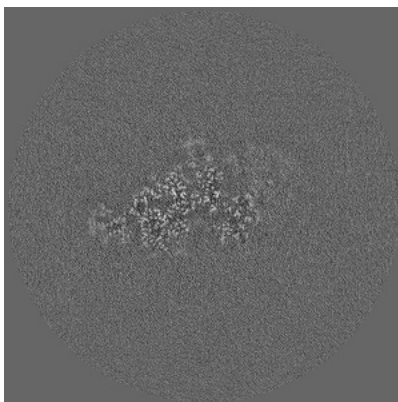


Z Index: 295

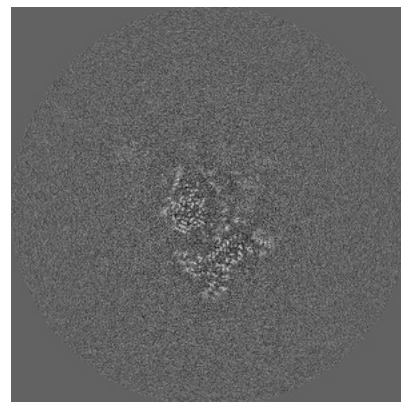
6.3.2 Raw map



X Index: 269



Y Index: 219

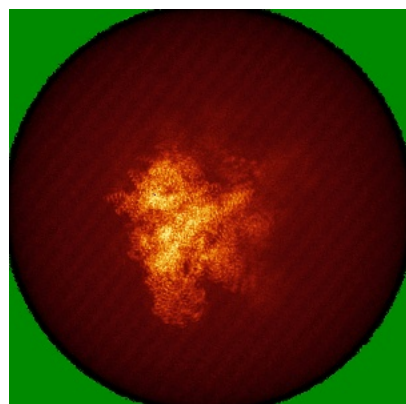


Z Index: 282

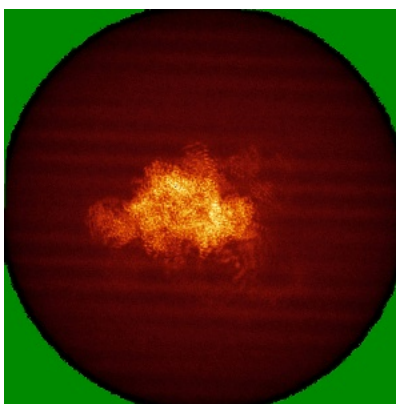
The images above show the largest variance slices of the map in three orthogonal directions.

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

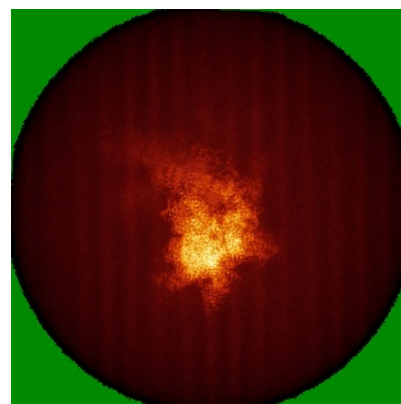
6.4.1 Primary map



X

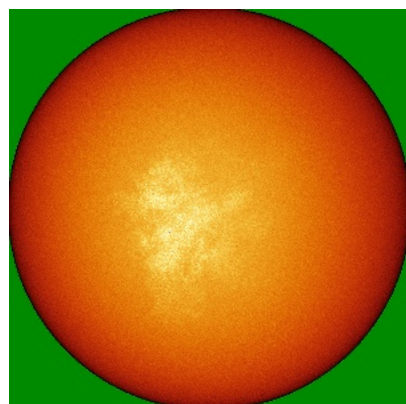


Y

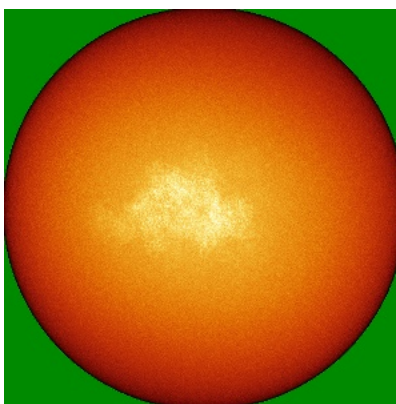


Z

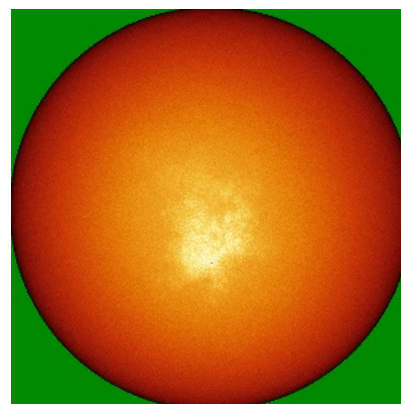
6.4.2 Raw map



X



Y

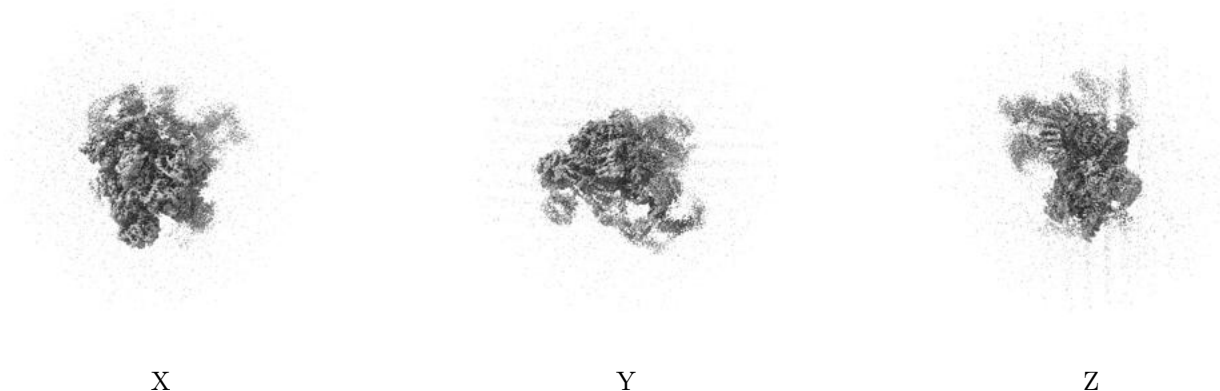


Z

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

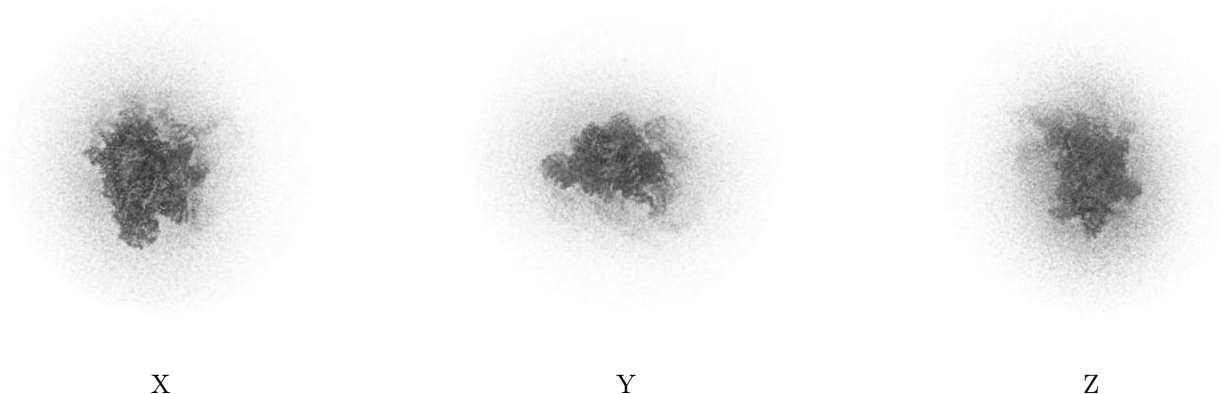
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

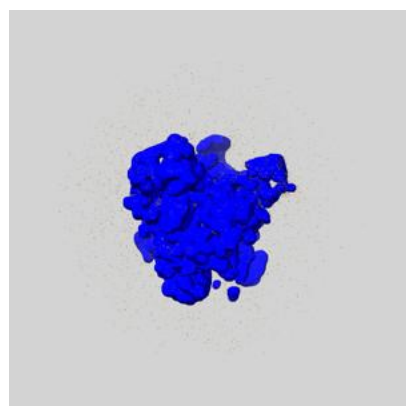
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

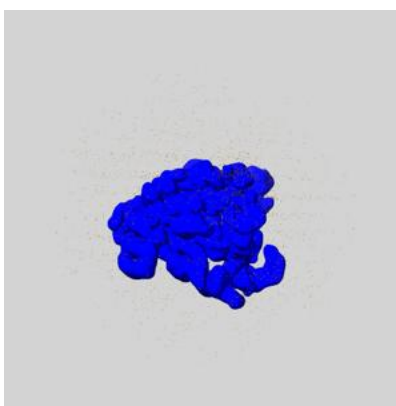
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

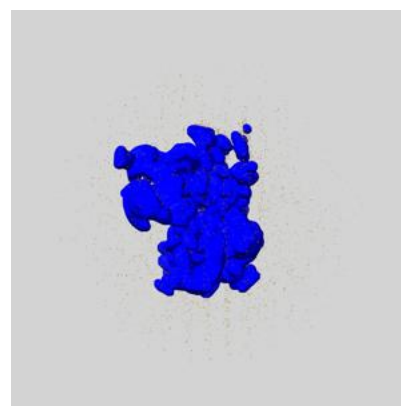
6.6.1 emd_19942_msk_1.map [i](#)



X



Y

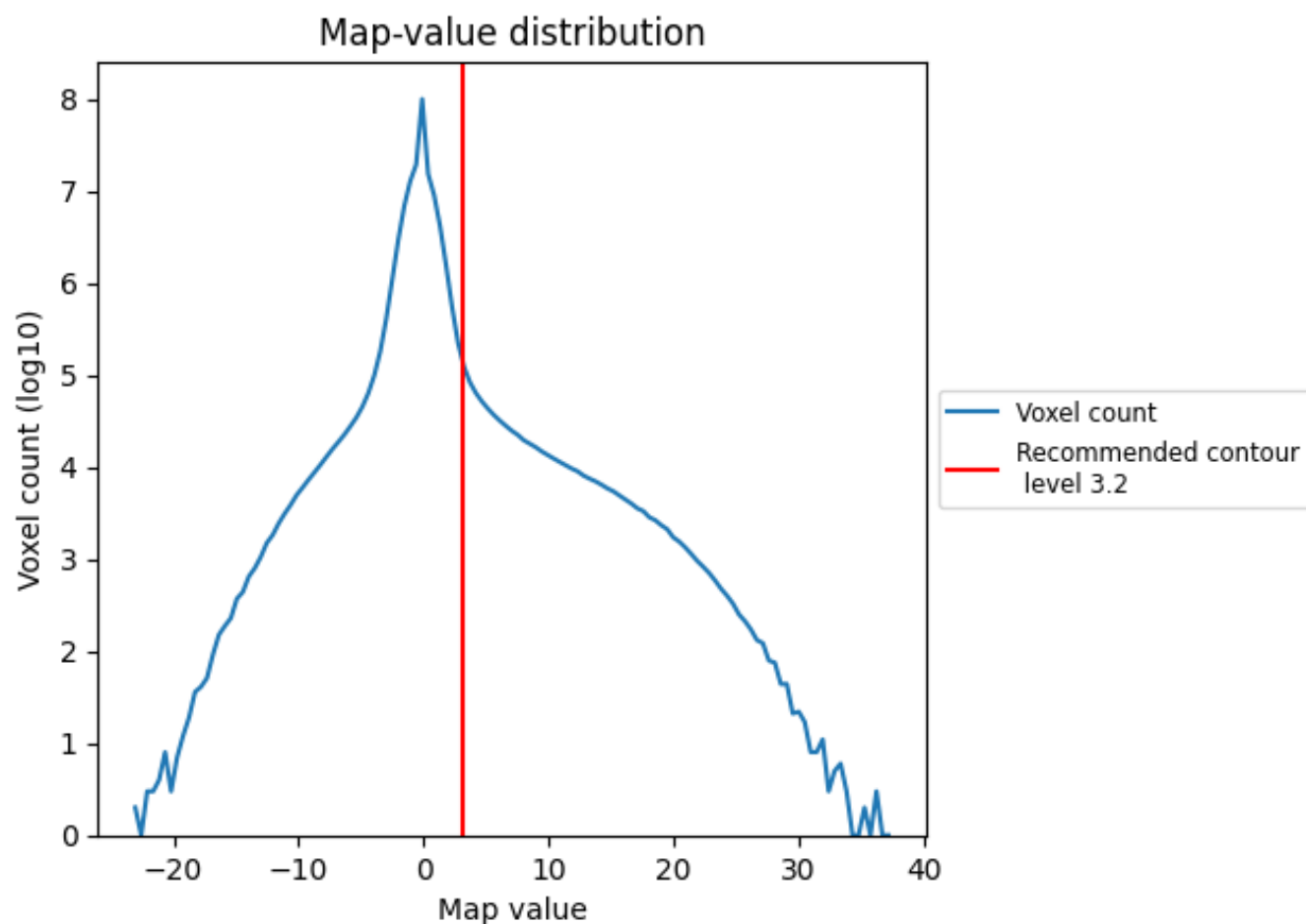


Z

7 Map analysis [i](#)

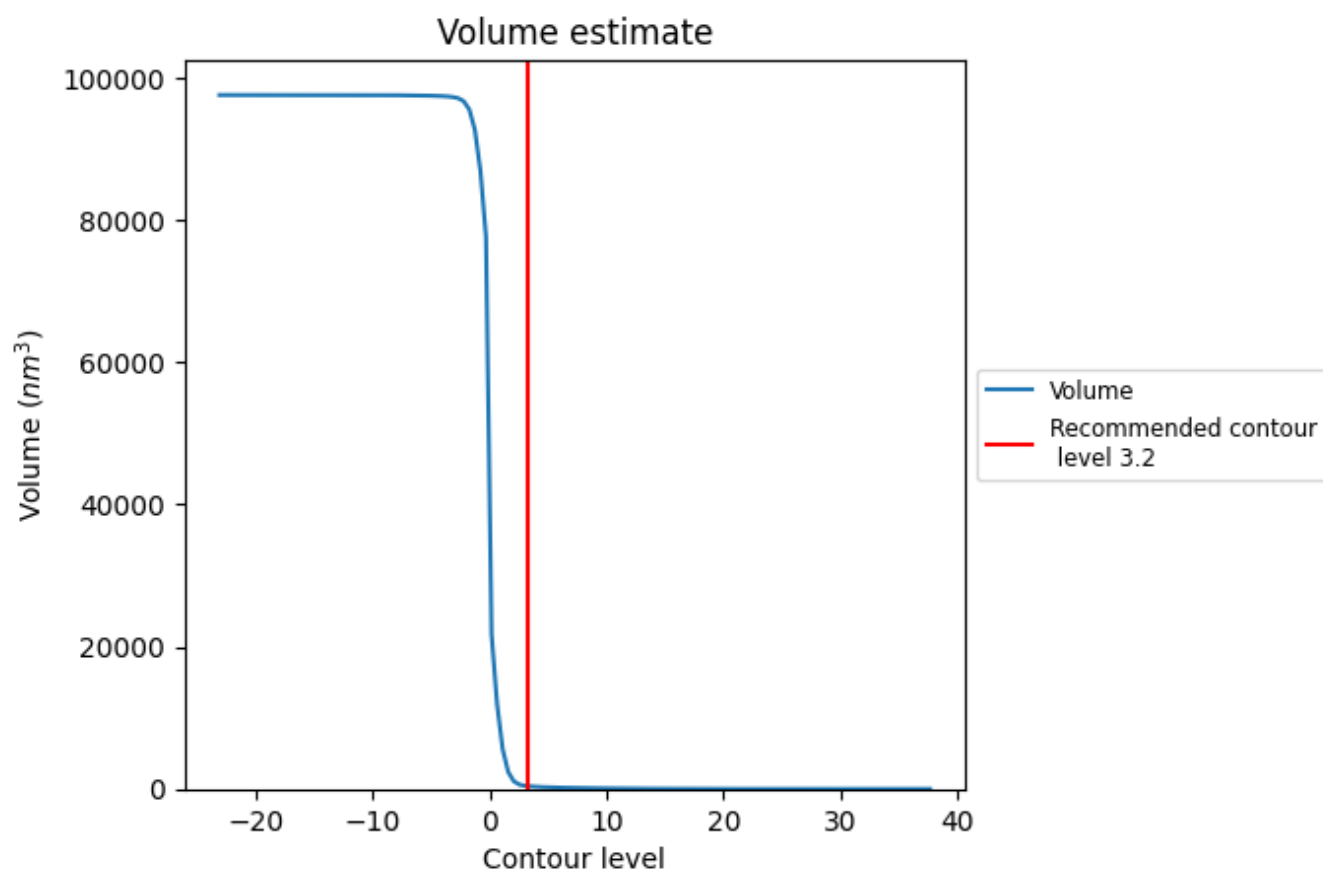
This section contains the results of statistical analysis of the map.

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.

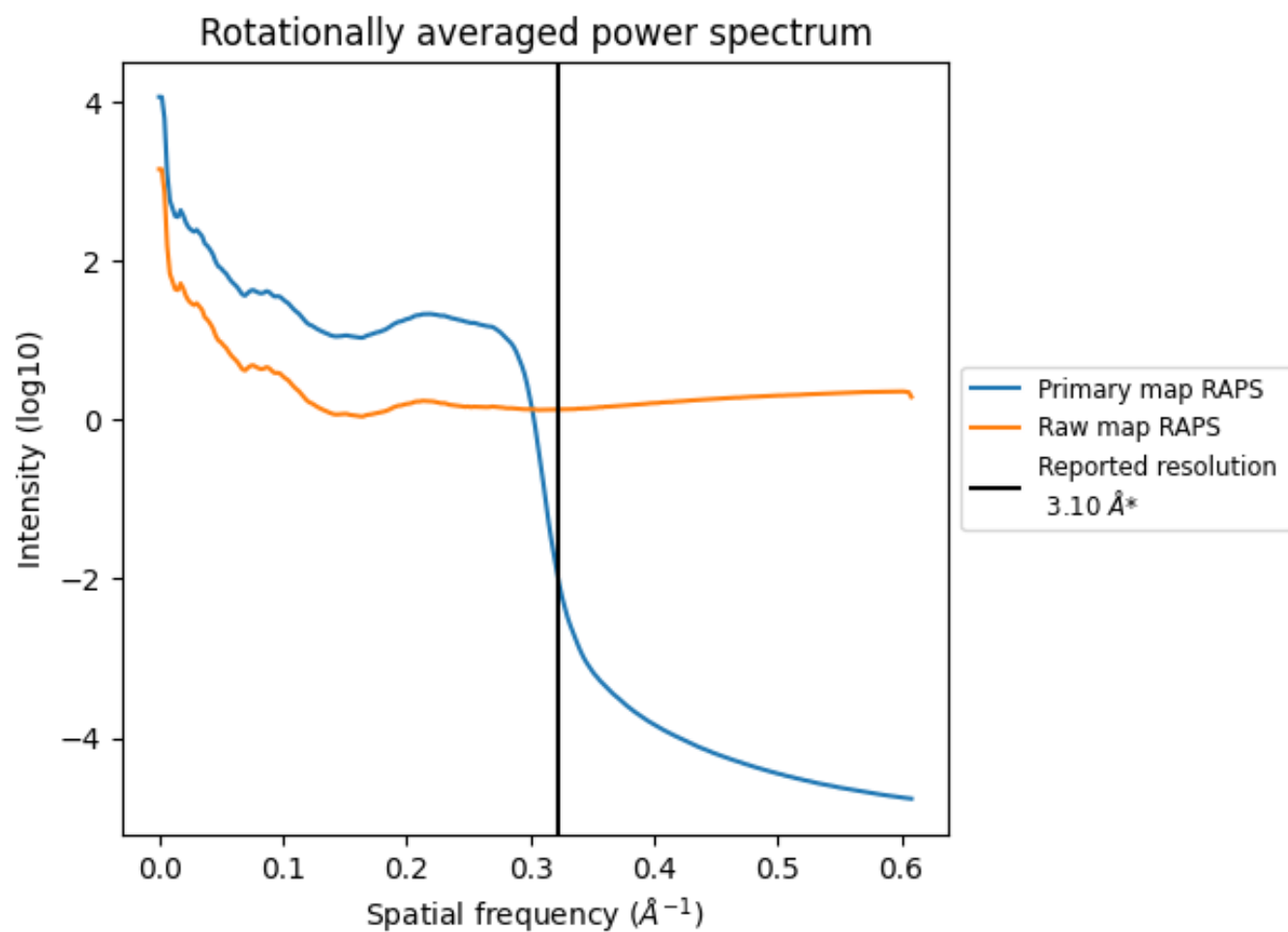
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 415 nm³; this corresponds to an approximate mass of 375 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 ⓘ

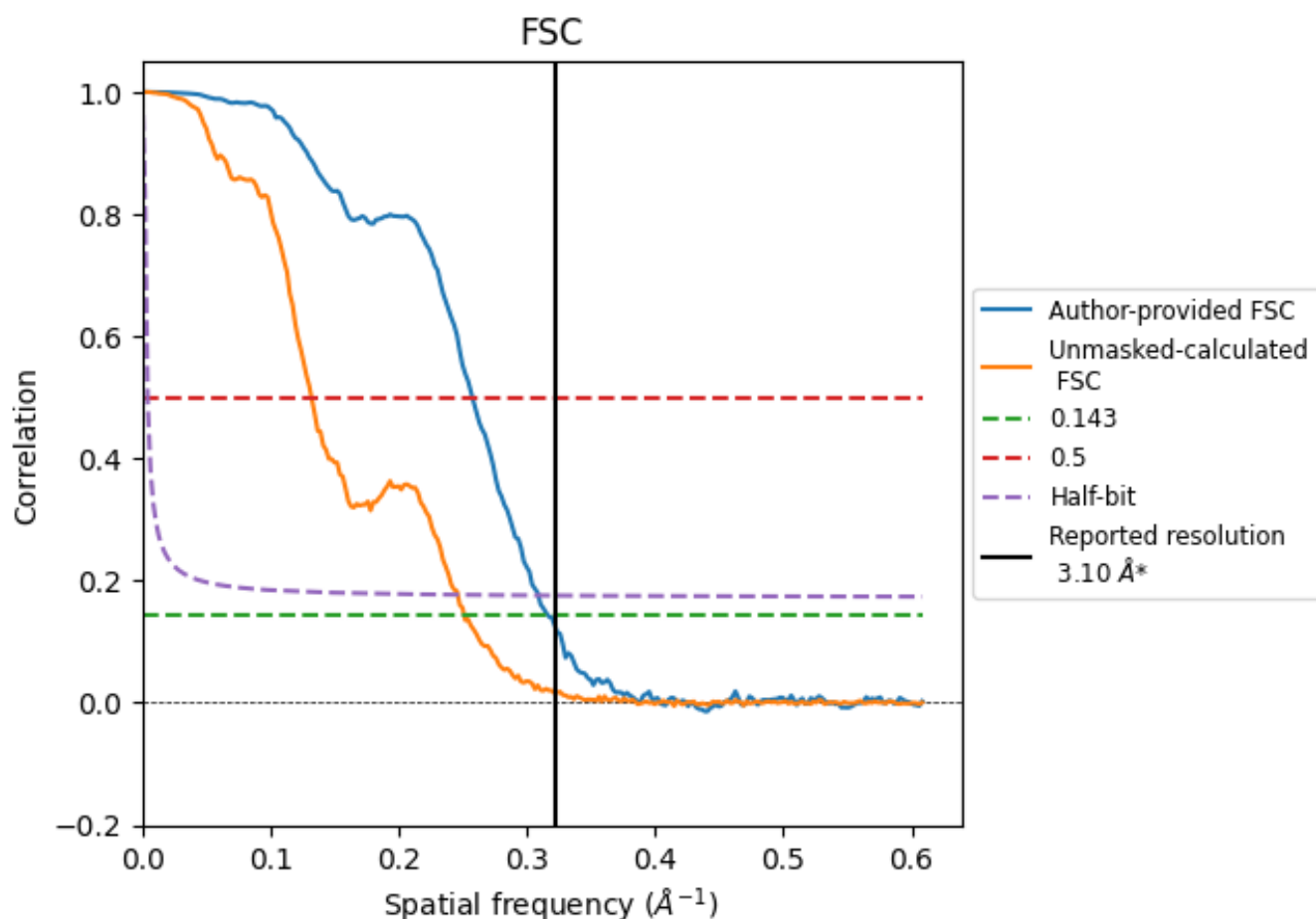


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

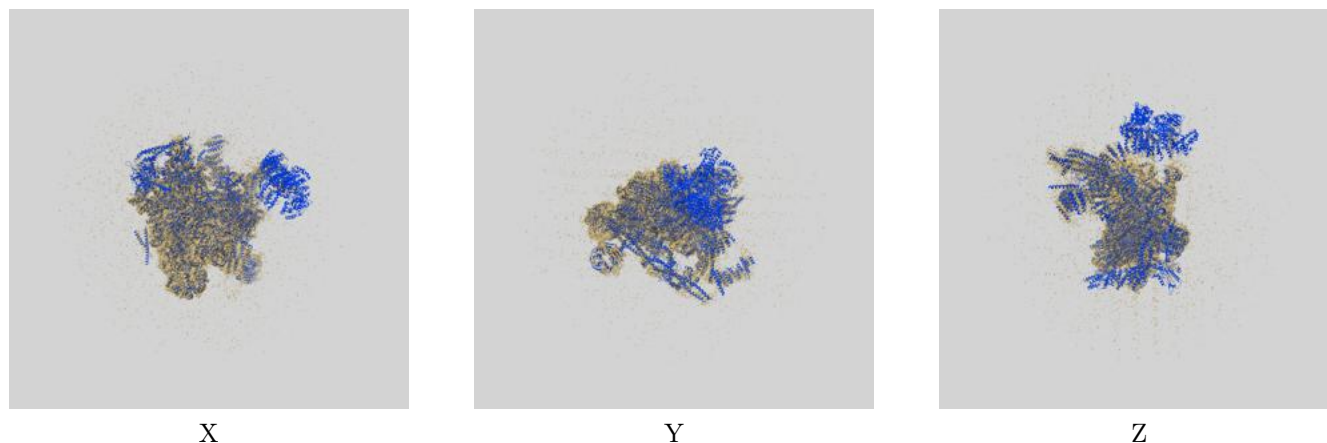
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.16	3.88	3.24
Unmasked-calculated*	3.98	7.58	4.06

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.98 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

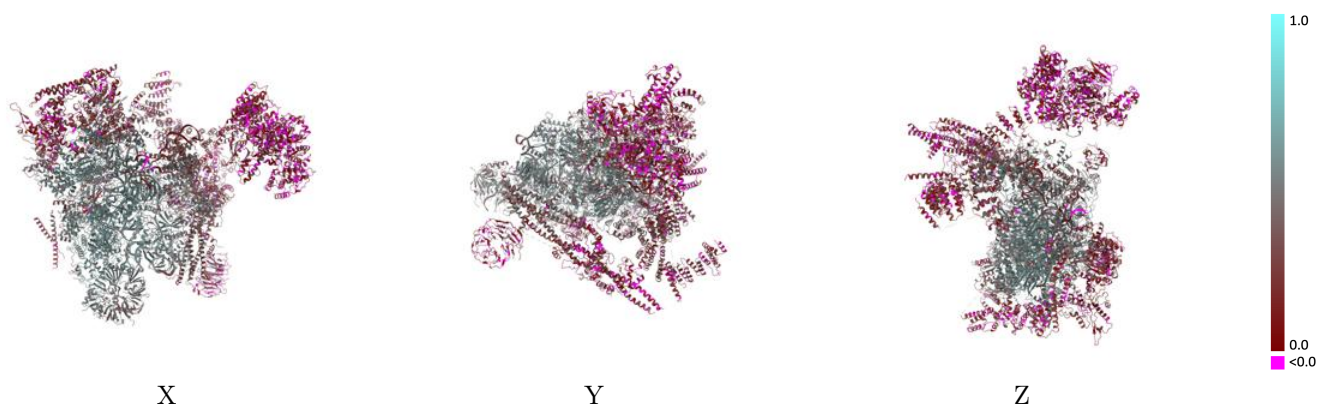
This section contains information regarding the fit between EMDB map EMD-19942 and PDB model 9S2G. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



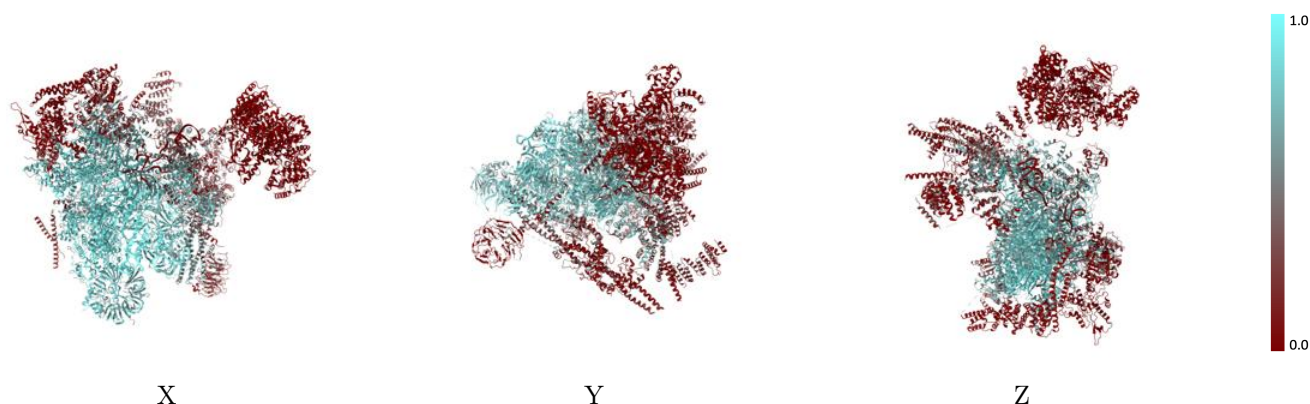
The images above show the 3D surface view of the map at the recommended contour level 3.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



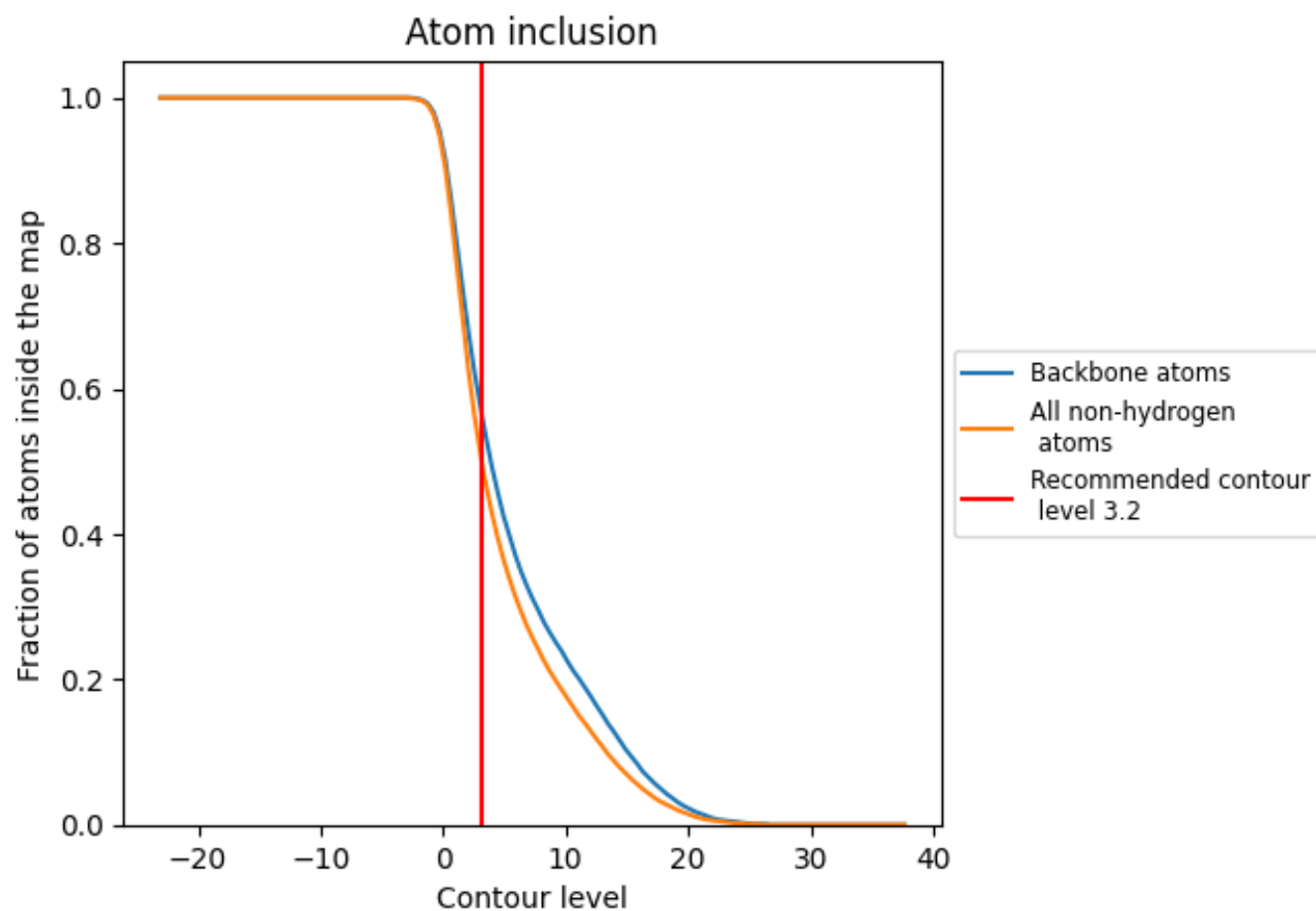
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 56% of all backbone atoms, 49% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (3.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4940	 0.3640
1	 0.5060	 0.3980
2	 0.4220	 0.3160
3	 0.4710	 0.4550
35	 0.2830	 0.2730
5	 0.9320	 0.5310
6	 0.5000	 0.3780
A	 0.7640	 0.5000
C	 0.8490	 0.5330
CW	 0.8170	 0.5060
E	 0.7930	 0.5000
GP	 0.4260	 0.3340
I	 0.1740	 0.2050
J	 0.4360	 0.3260
K	 0.3810	 0.2720
L	 0.4420	 0.3100
LG	 0.2410	 0.3630
M	 0.1790	 0.3140
N	 0.8630	 0.5430
O	 0.4720	 0.3840
O2	 0.6630	 0.4380
P	 0.7760	 0.5300
PX	 0.0330	 0.1670
Q	 0.0060	 0.1150
R	 0.6960	 0.4550
S	 0.7010	 0.4620
SR	 0.2990	 0.3300
T	 0.8140	 0.5150
TF	 0.0800	 0.1890
W	 0.6370	 0.4410
YB	 0.3420	 0.3540
Z	 0.1490	 0.1580
a	 0.8790	 0.5510
b	 0.7780	 0.5060
c	 0.7130	 0.4650



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Chain	Atom inclusion	Q-score
d	 0.6950	 0.4160
e	 0.7890	 0.5010
f	 0.7140	 0.4440
g	 0.8350	 0.5370
q	 0.0640	 0.1360
r	 0.1290	 0.1730
s	 0.0800	 0.1370
t	 0.1960	 0.2160