



wwPDB EM Validation Summary Report ⓘ

Mar 24, 2026 – 03:21 PM UTC

PDB ID : 9ESH / pdb_00009esh
EMDB ID : EMD-19941
Title : Structure of a B-state intermediate committed to discard (Bd-I state)
Authors : Soni, K.; Wild, K.; Sinning, I.
Deposited on : 2024-03-26
Resolution : 3.20 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

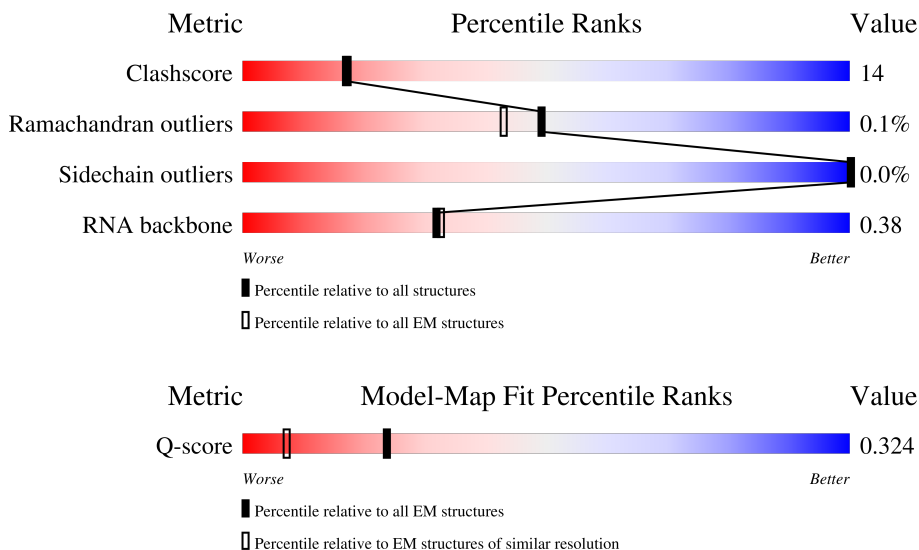
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.20 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	15020 (2.70 - 3.70)

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	29	
2	2	186	
3	5	120	

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Mol	Chain	Length	Quality of chain
4	6	99	
5	A	2363	
6	B	984	
7	C	340	
8	D	97	
9	E	147	
10	F	117	
11	G	115	
12	H	84	
13	I	78	
14	J	77	
15	K	473	
16	L	557	
17	M	354	
18	N	1284	
19	O	146	
20	P	388	
21	Q	265	
22	R	674	
23	S	488	
23	T	488	
23	U	488	
23	V	488	
24	W	757	
25	X	790	

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Mol	Chain	Length	Quality of chain
26	Y	229	
27	Z	187	
28	a	558	
29	b	293	
30	c	887	
31	d	155	
32	f	22	
33	m	797	
34	r	346	
35	y	534	
36	z	647	

2 Entry composition [i](#)

There are 41 unique types of molecules in this entry. The entry contains 90868 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
			Total	C	N	O	P		
1	1	29	605	272	91	213	29	0	0

- Molecule 2 is a RNA chain called U2snRNA.

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

- Molecule 3 is a RNA chain called U5snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	5	102	2149	963	358	726	102	0	0

- Molecule 4 is a RNA chain called U6snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	6	92	1970	882	365	631	92	0	0

- Molecule 5 is a protein called Pre-mRNA-splicing factor spp42.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	A	1737	14402	9229	2543	2565	65	0	0

- Molecule 6 is a protein called Pre-mRNA-splicing factor cwf10.

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

- Molecule 7 is a protein called Pre-mRNA-splicing factor cwf17.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	D	96	760	470	147	136	7	0	0

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

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

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

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

- Molecule 11 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	G	102	819	516	150	149	4	0	0

- Molecule 12 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	H	80	652	422	113	115	2	0	0

- Molecule 13 is a protein called Small nuclear ribonucleoprotein F.

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

- Molecule 14 is a protein called Small nuclear ribonucleoprotein G.

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

- Molecule 15 is a protein called Pre-mRNA-splicing factor prp5.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	391	Total	C	N	O	S	0	0
			3053	1925	551	563	14		

- Molecule 16 is a protein called Pre-mRNA-processing protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	234	Total	C	N	O	S	0	0
			1849	1154	345	345	5		

- Molecule 17 is a protein called Pre-mRNA-splicing factor cwf5.

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

- Molecule 18 is a protein called Pre-mRNA-splicing factor cwf11.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	1284	Total	C	N	O	S	0	0
			10461	6715	1732	1969	45		

- Molecule 19 is a protein called Pre-mRNA-splicing factor cwf14.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	O	144	Total	C	N	O	S	0	0
			1176	733	216	214	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	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
			Total	C	N	O	S		
21	Q	90	752	467	146	138	1	0	0

- Molecule 22 is a protein called Pre-mRNA-splicing factor cwf4.

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

- Molecule 23 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	S	132	1055	664	181	207	3	0	0
23	T	134	1069	671	183	212	3	0	0
23	U	430	2870	1806	492	563	9	0	0
23	V	131	1044	655	180	206	3	0	0

- Molecule 24 is a protein called Pre-mRNA-splicing factor cdc5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	W	526	4346	2710	792	832	12	0	0

- Molecule 25 is a protein called Pre-mRNA-splicing factor cwf3.

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

- Molecule 26 is a protein called Pre-mRNA-splicing factor syf2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
26	Y	120	1049	656	195	198	0	0

- Molecule 27 is a protein called Pre-mRNA-splicing factor cwf7.

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

- Molecule 28 is a protein called Pre-mRNA-processing factor 17.

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

- Molecule 29 is a protein called Pre-mRNA-splicing factor cwf21.

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

- Molecule 30 is a protein called Pre-mRNA-splicing factor cwf22.

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

- Molecule 31 is a protein called Peptidyl-prolyl cis-trans isomerase ppi1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	d	154	1179	750	202	223	4	0	0

- Molecule 32 is a protein called UNK1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
32	f	22	110	66	22	22	0	0

- Molecule 33 is a protein called G-patch domain-containing protein C1486.03.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	m	81	649	413	112	122	2	0	0

- Molecule 34 is a protein called UNK2.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	r	67	Total	C	N	O	0	0
			335	201	67	67		

- Molecule 35 is a protein called Uncharacterized protein C20H4.06c.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	y	185	Total	C	N	O	S	0	0
			1480	921	257	298	4		

- Molecule 36 is a protein called Putative pre-mRNA-splicing factor ATP-dependent RNA helicase C20H4.09.

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

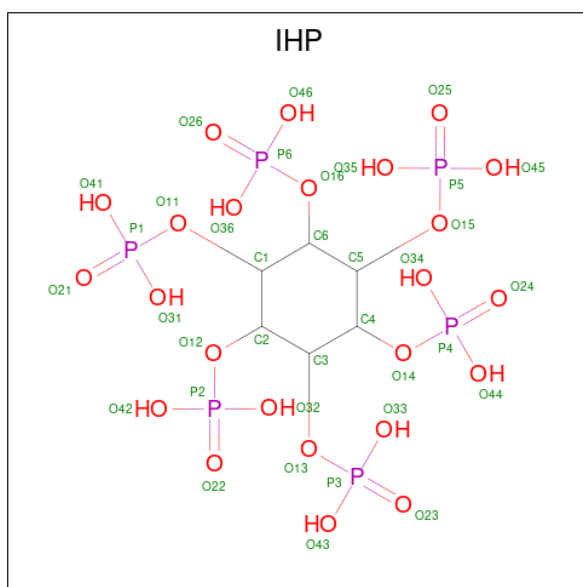
- Molecule 37 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
37	6	3	Total	Mg	0
			3	3	
37	B	1	Total	Mg	0
			1	1	

- Molecule 38 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

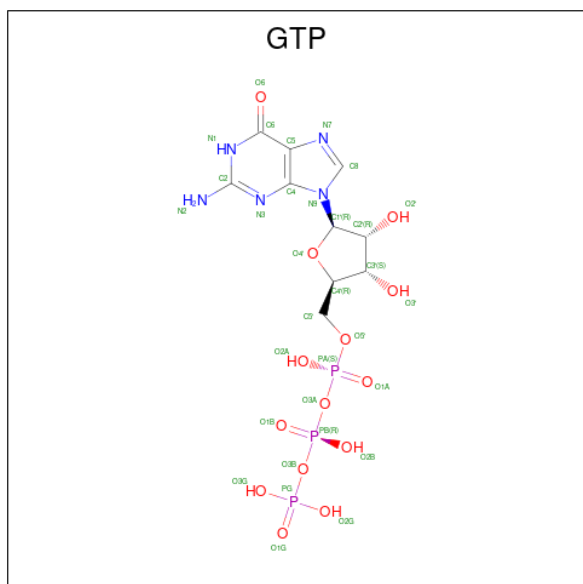
Mol	Chain	Residues	Atoms		AltConf
38	6	1	Total	K	0
			1	1	

- Molecule 39 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: C₆H₁₈O₂₄P₆) (labeled as "Ligand of Interest" by depositor).



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

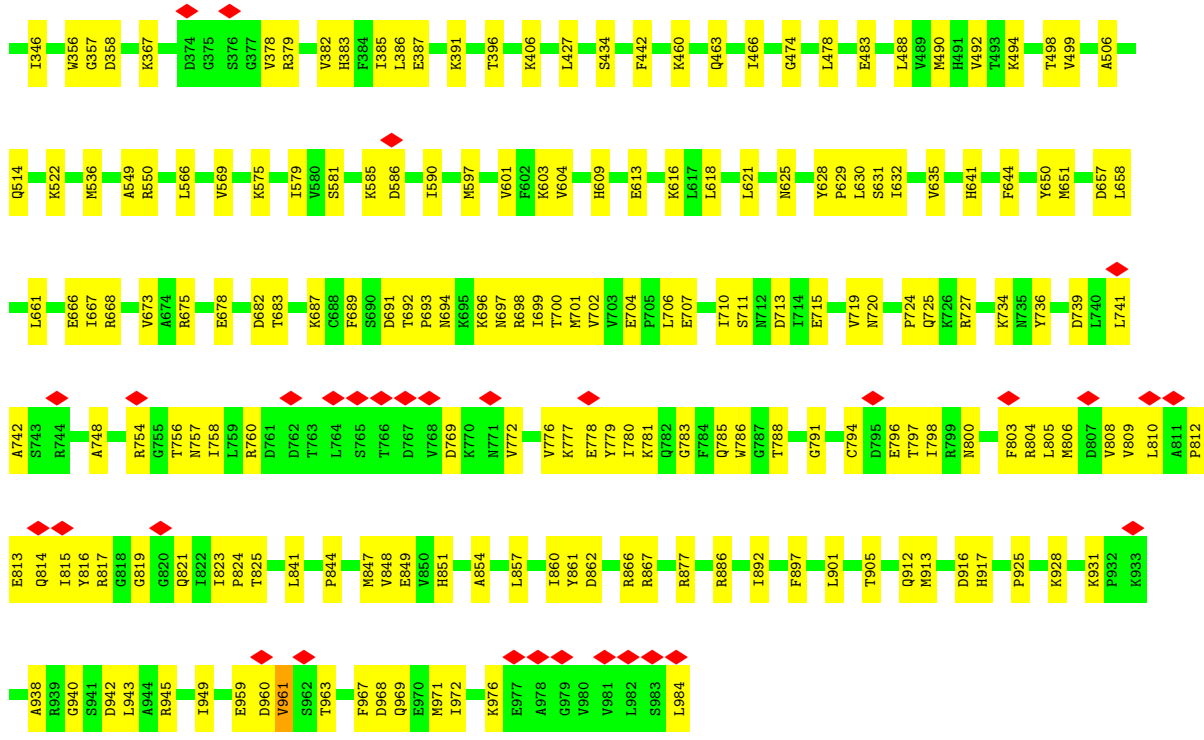
- Molecule 40 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



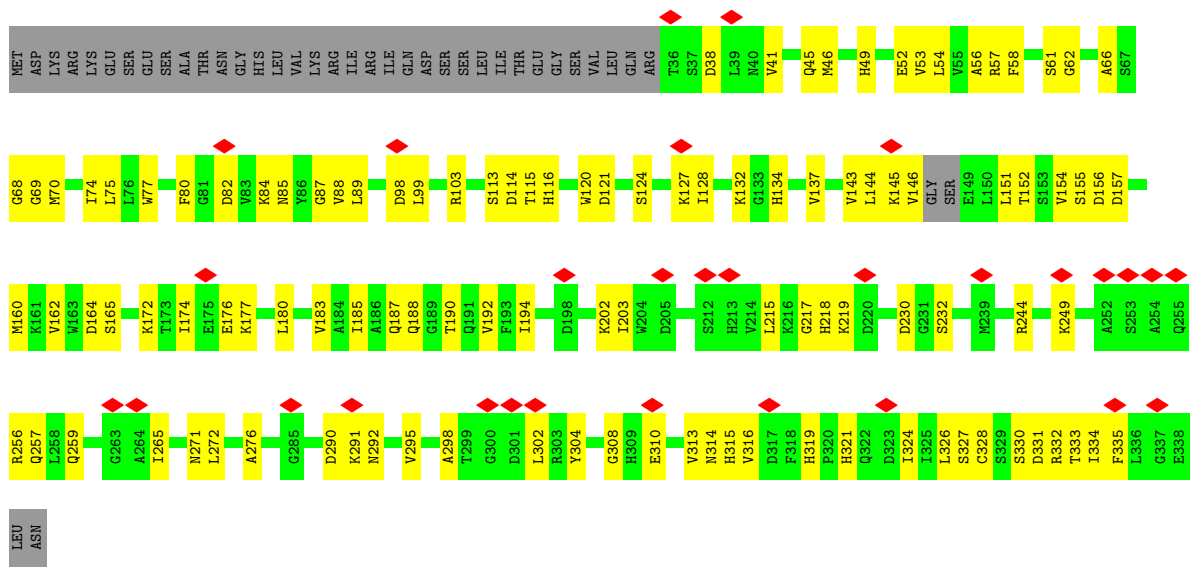
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
40	B	1	32	10	5	14	3	0

- Molecule 41 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

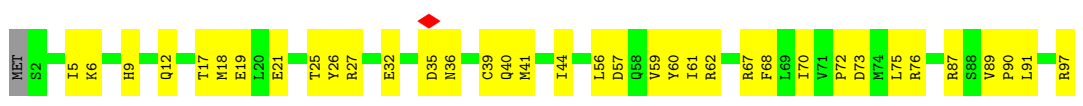
Mol	Chain	Residues	Atoms		AltConf
41	M	2	Total 2	Zn 2	0
41	O	3	Total 3	Zn 3	0
41	P	1	Total 1	Zn 1	0



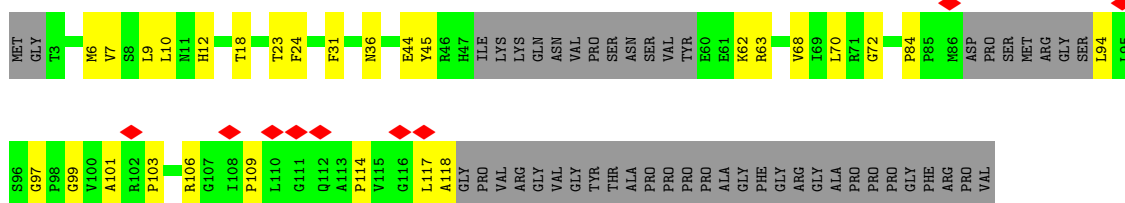
• Molecule 7: Pre-mRNA-splicing factor cwf17



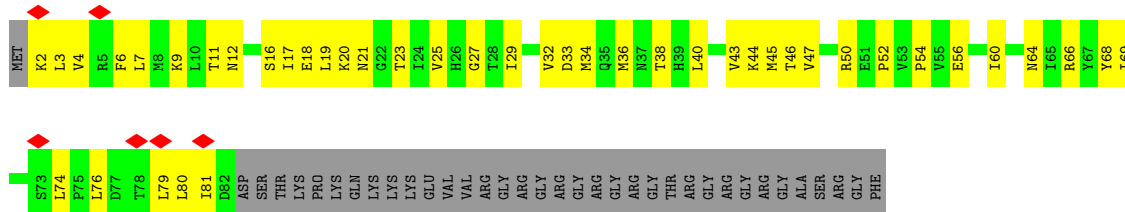
• Molecule 8: Small nuclear ribonucleoprotein Sm D3



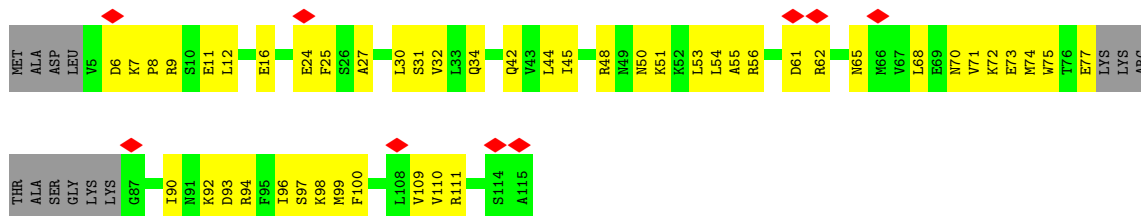
• Molecule 9: Small nuclear ribonucleoprotein-associated protein B



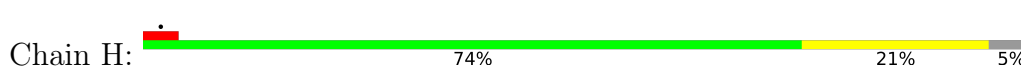
• Molecule 10: Small nuclear ribonucleoprotein Sm D1



• Molecule 11: Small nuclear ribonucleoprotein Sm D2



• Molecule 12: Small nuclear ribonucleoprotein E

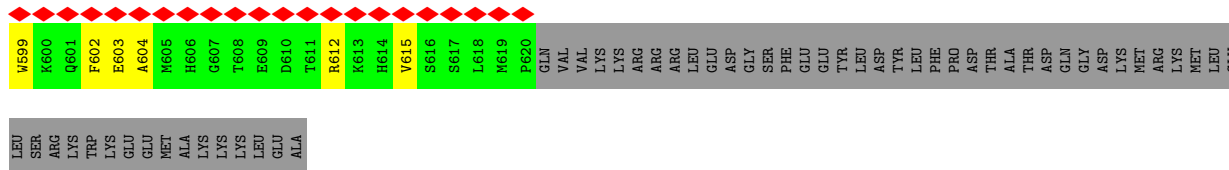
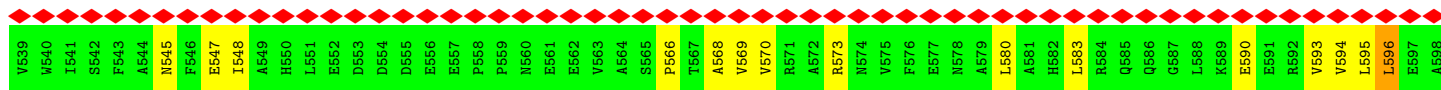


• Molecule 13: Small nuclear ribonucleoprotein F

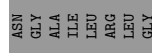
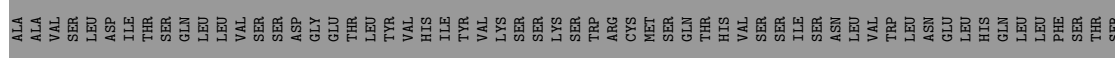
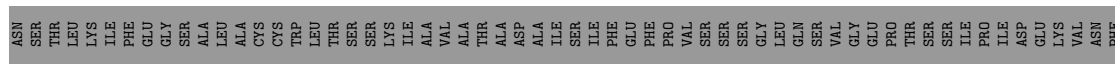
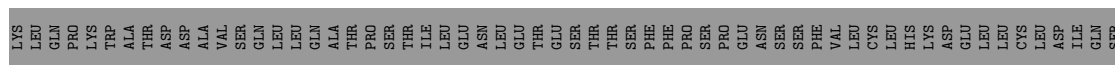
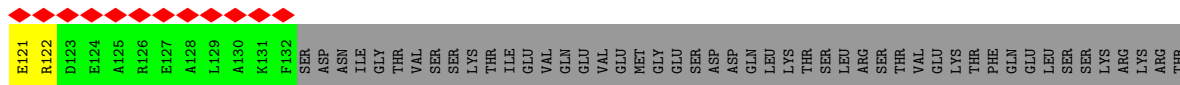
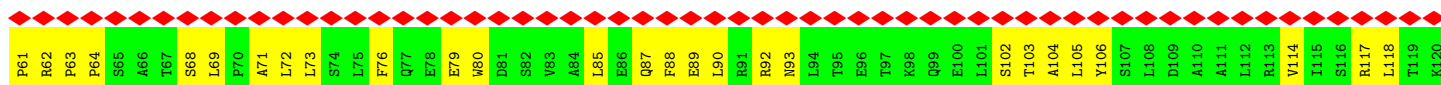
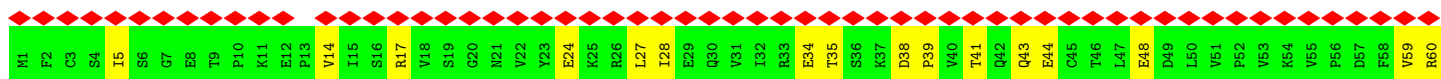


• Molecule 14: Small nuclear ribonucleoprotein G

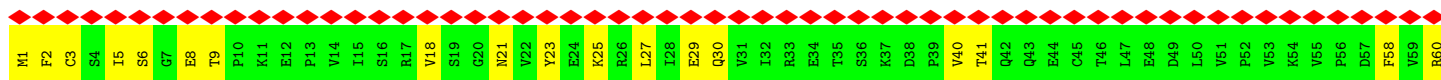
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T961	R962	L963	G964	T965	L966	K967	E968	K969	G970	F971	C972	F973	N974	N975	L976	I977	V978	M979	N980	S981	Q982	N983	I984	S985	E986	S987	S988	R989	T990	S991	I992	L993	L994	R995	N996	C997	E998	P999	T1000	G1001	F1002	D1003	R1004	L1005	V1006	L1007	L1008	G1009	S9949	N1010	Q1011	I1012	G953	L1013	T1014	S995	G996	R997	Q1018	D1019	S960
I841	Q842	A843	P844	B845	S846	H847	D848	A849	S850	P851	D852	T853	A854	L855	Y856	F857	R858	D859	A860	Y861	I862	K863	R864	L865	W866	E867	K868	Y869	L870	R871	T872	W873	L874	D875	K876	D877	W878	F879	D880	A881	F882	W883	R884	F885	P886	F887	H888	S889	F891	G892	D893	K894	S895	K896	R897	L898	E900				
M781	F782	S783	M784	W785	T786	L787	F788	T789	L790	L791	E792	K793	A794	R795	C796	F797	H798	Q799	G800	H801	L802	L803	Y804	L805	S806	D807	E808	G809	K810	D811	E812	T813	L814	E815	R816	Y817	G818	T819	L820	S821	S822	W823	T824	S825	K826	L827	P828	G829	L831	R832	E833	T834	G835	R836	L837	A839	S840				
S721	N722	R723	L724	Y725	T726	Y727	N728	D729	K730	Q731	L732	E733	S734	I735	L736	R737	G738	S739	Q740	P741	G742	L743	T744	W745	V746	W747	G748	P749	T750	R751	C752	G753	K754	H755	V756	L757	W758	C759	K760	L761	L762	E763	V764	L765	W766	D767	T768	S769	P770	W771	D772	R773	T774	V775	V776	L777	D778	D779	S780		
G661	L662	M663	S664	Q665	L666	A667	R668	M669	L670	A671	M672	T673	V674	E675	Q676	L677	Q678	S679	V680	L681	P682	M683	C684	H685	V686	P687	S688	M689	L690	S691	T692	E693	S694	L695	L696	I697	K698	F699	Y700	T701	N702	Q703	N704	W705	L706	S707	A708	D709	W710	T711	A712	S713	D714	R715	H716	F717	L718	L719	P720		
Y601	R602	P603	K604	Q605	L606	K607	F608	N609	F610	A611	L612	G613	L614	S615	P616	E617	A618	M619	K620	Y621	L622	L623	D624	L625	N626	I627	L628	V629	S630	L631	L632	M633	R634	A635	K636	E637	F638	P639	K640	W641	F642	E643	D644	L645	F646	L647	G648	F649	G650	L651	P652	D653	I654	C655	A656	F657	P658	M659	A660		
M481	M482	F483	K484	V485	T486	S487	V488	A489	P490	P491	Q492	F493	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	K526	P527	F528	L529	C530	L531	I532	Y533	I534	S535	K536	D537	M538	E539	Y540		
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	Q570	Q571	S572	D573	N574	Q575	S576	D577	S578	D579	N580	K581	S582	I583	N584	V585	S586	L587	S588	P589	F590	Y591	Y592	H593	S594	L595	A596	G597	L598	G599	E600		
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	I337	T338	T339	S340	F341	L342	S343	F344	N345	S346	L347	K348	S349	L350	C351	S352	K353	C354	Y355	L356	R357	L358	S359	F360		
P361	E362	K363	Y364	A365	L366	K367	V368	D369	F370	E371	F372	L373	K374	N375	V376	F377	I378	N379	T380	Y381	D382	R383	T384	L385	L386	V387	N388	D389	Y390	D391	E392	I393	L394	N395	F396	T397	I398	K399	D400	V401	L402	G403	E404	R405	S406	V407	M408	D409	Q410	E411	N412	S413	L414	T415	N416	Y417	F418	L419	L420		
Q421	N422	T423	A424	I425	Q426	Q427	L428	S429	I430	S431	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	L462	L463	S464	L465	K466	N467	A468	T469	K470	E471	N472	K473	L474	T475	N476	F477	F478	S479	L480		

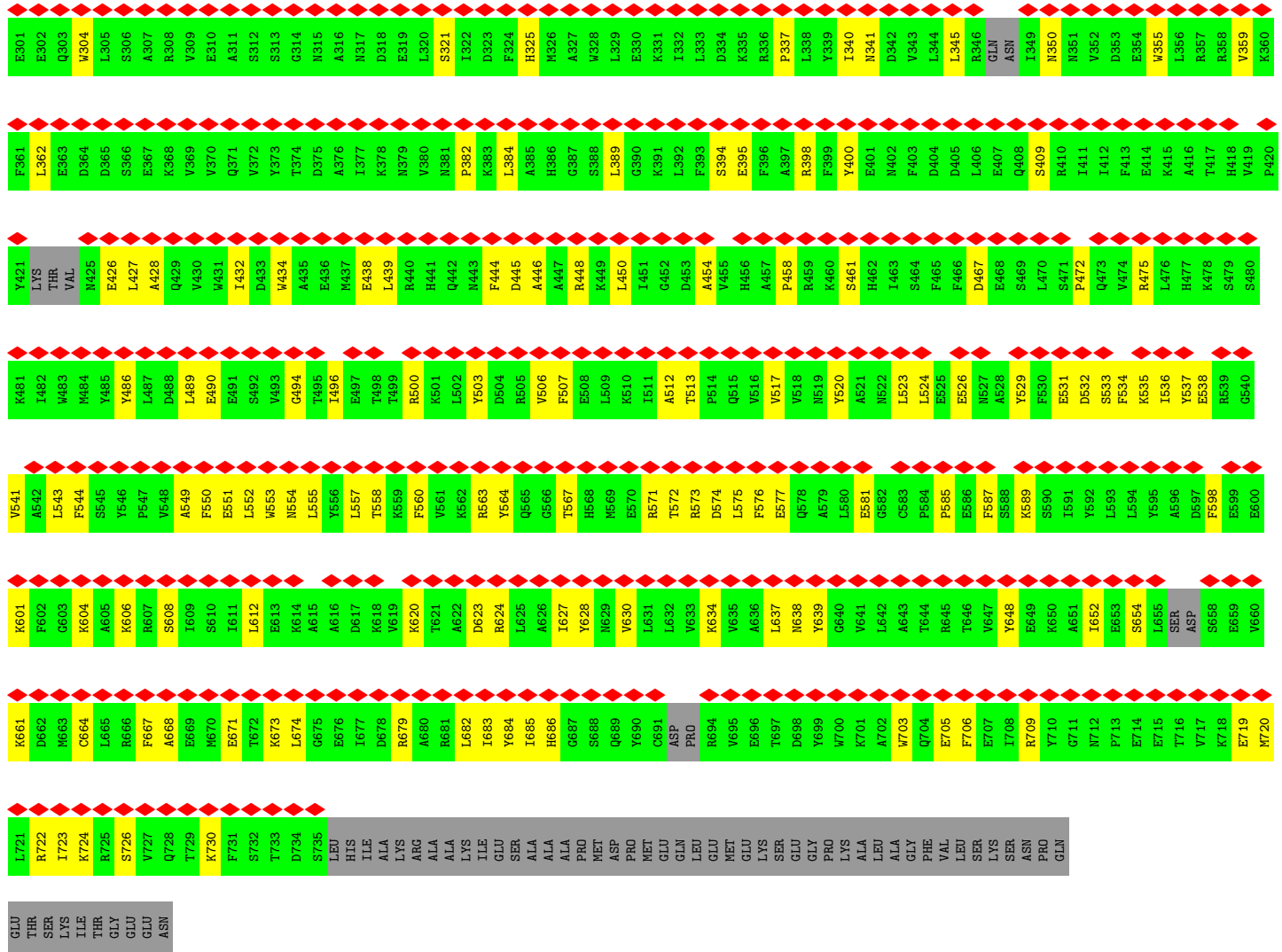


• Molecule 23: Pre-mRNA-processing factor 19

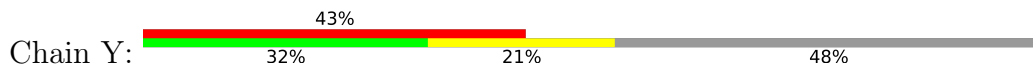


• Molecule 23: Pre-mRNA-processing factor 19

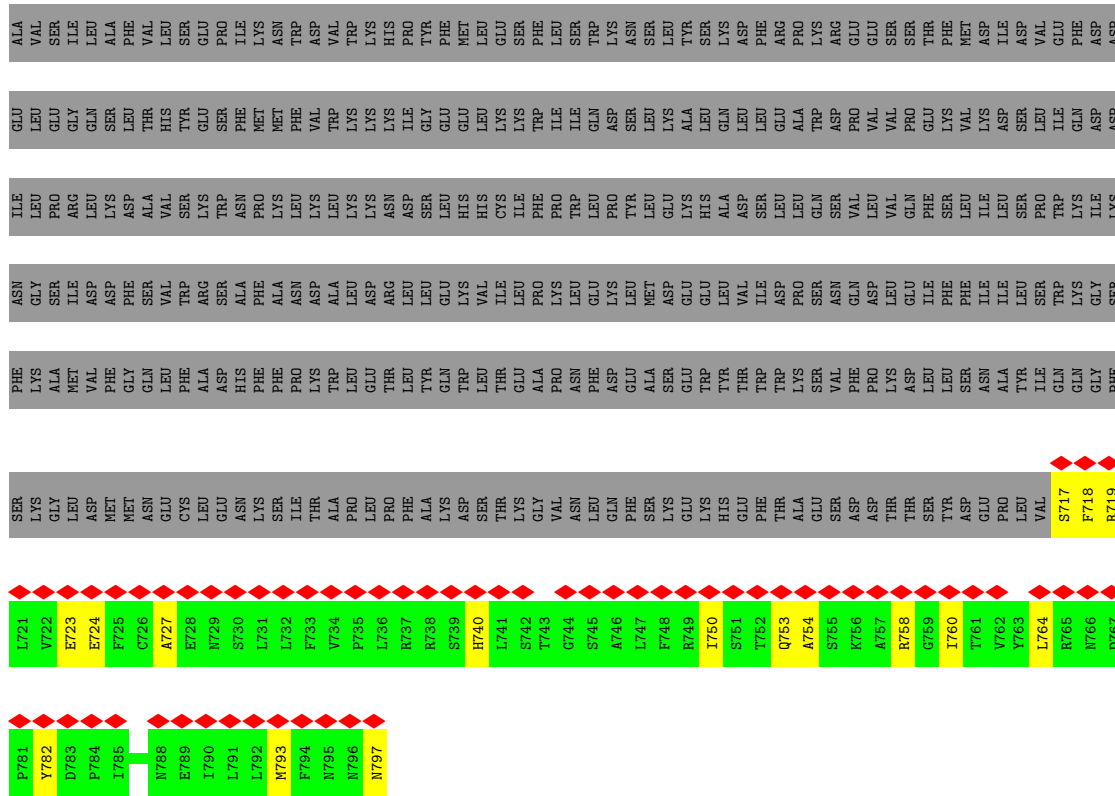




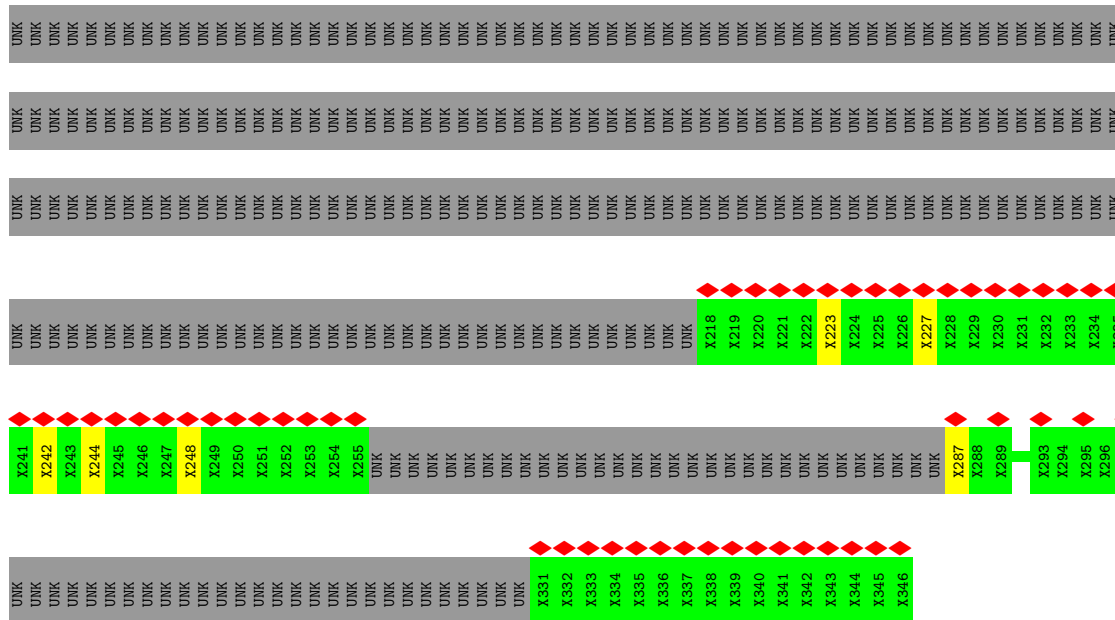
• Molecule 26: Pre-mRNA-splicing factor syf2



• Molecule 27: Pre-mRNA-splicing factor cwf7



• Molecule 34: UNK2



• Molecule 35: Uncharacterized protein C20H4.06c



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	61423	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49.4	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	37.729	Depositor
Minimum map value	-20.085	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.902	Depositor
Recommended contour level	3.55	Depositor
Map size (\AA)	460.32, 460.32, 460.32	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.822, 0.822, 0.822	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	0.17	0/673	0.40	0/1043
2	2	0.12	0/554	0.24	0/856
3	5	0.18	0/2397	0.25	0/3727
4	6	0.14	0/2207	0.35	0/3438
5	A	0.24	0/14793	0.43	5/20040 (0.0%)
6	B	0.22	0/7459	0.43	0/10117
7	C	0.18	0/2376	0.48	0/3216
8	D	0.21	0/772	0.43	0/1038
9	E	0.17	0/737	0.43	0/993
10	F	0.22	0/646	0.57	0/875
11	G	0.23	0/829	0.66	0/1111
12	H	0.16	0/662	0.44	0/894
13	I	0.16	0/585	0.48	0/794
14	J	0.19	0/578	0.48	0/774
15	K	0.23	0/3130	0.47	0/4251
16	L	0.19	0/1885	0.43	0/2545
17	M	0.19	0/1841	0.47	0/2468
18	N	0.12	0/10690	0.33	0/14463
19	O	0.24	0/1199	0.49	0/1609
20	P	0.28	0/2222	0.58	3/2991 (0.1%)
21	Q	0.16	0/767	0.35	0/1028
22	R	0.19	0/5235	0.48	1/7067 (0.0%)
23	S	0.21	0/1072	0.47	0/1453
23	T	0.23	0/1086	0.61	0/1472
23	U	0.14	0/2897	0.42	1/3914 (0.0%)
23	V	0.19	0/1060	0.48	0/1437
24	W	0.20	0/4407	0.50	3/5907 (0.1%)
25	X	0.16	0/5599	0.40	0/7566
26	Y	0.17	0/1065	0.50	0/1413
27	Z	0.17	0/1244	0.43	0/1667
28	a	0.18	0/1055	0.45	0/1443
29	b	0.17	0/829	0.38	0/1111

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
30	c	0.20	0/1711	0.46	0/2312
31	d	0.20	0/1206	0.50	0/1636
33	m	0.14	0/663	0.38	0/895
35	y	0.18	0/1511	0.52	0/2032
36	z	0.16	0/5079	0.41	0/6875
All	All	0.19	0/92721	0.44	13/126471 (0.0%)

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	531	ILE	N-CA-C	-6.22	105.65	112.80
24	W	626	THR	CA-C-N	-5.86	112.92	120.65
24	W	626	THR	C-N-CA	-5.86	112.92	120.65
5	A	533	ARG	N-CA-C	-5.85	106.38	112.93
23	U	118	LEU	CA-CB-CG	5.68	136.19	116.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	605	0	302	12	0
2	2	500	0	257	14	0
3	5	2149	0	1085	23	0
4	6	1970	0	994	53	0
5	A	14402	0	14306	361	0
6	B	7298	0	7336	189	0
7	C	2328	0	2276	89	0
8	D	760	0	776	28	0
9	E	726	0	750	24	0
10	F	638	0	682	37	0
11	G	819	0	845	49	0
12	H	652	0	680	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	I	574	0	591	28	0
14	J	573	0	602	14	0
15	K	3053	0	3011	92	0
16	L	1849	0	1879	55	0
17	M	1818	0	1822	74	0
18	N	10461	0	10412	198	0
19	O	1176	0	1167	37	0
20	P	2178	0	2101	108	0
21	Q	752	0	729	15	0
22	R	5108	0	5024	185	0
23	S	1055	0	1075	61	0
23	T	1069	0	1084	74	0
23	U	2870	0	2403	85	0
23	V	1044	0	1066	47	0
24	W	4346	0	4375	184	0
25	X	5467	0	5372	163	0
26	Y	1049	0	1052	54	0
27	Z	1232	0	1242	59	0
28	a	1035	0	837	40	0
29	b	822	0	820	28	0
30	c	1678	0	1659	63	0
31	d	1179	0	1169	60	0
32	f	110	0	29	0	0
33	m	649	0	641	16	0
34	r	335	0	77	8	0
35	y	1480	0	1379	62	0
36	z	4980	0	5047	153	0
37	6	3	0	0	0	0
37	B	1	0	0	0	0
38	6	1	0	0	0	0
39	A	36	0	6	0	0
40	B	32	0	12	3	0
41	M	2	0	0	0	0
41	O	3	0	0	0	0
41	P	1	0	0	0	0
All	All	90868	0	86972	2460	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.

The worst 5 of 2460 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)
5:A:1642:LYS:HD3	5:A:1650:CYS:SG	1.36	1.62
5:A:1642:LYS:CD	5:A:1650:CYS:SG	2.14	1.34
5:A:1638:ILE:CD1	5:A:1642:LYS:HE3	1.73	1.18
4:6:32:G:N2	20:P:82:MET:HG2	1.57	1.17
4:6:32:G:N2	20:P:82:MET:CG	2.07	1.16

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	
5	A	1735/2363 (73%)	1635 (94%)	99 (6%)	1 (0%)	48	79
6	B	916/984 (93%)	866 (94%)	49 (5%)	1 (0%)	48	79
7	C	297/340 (87%)	274 (92%)	23 (8%)	0	100	100
8	D	94/97 (97%)	92 (98%)	2 (2%)	0	100	100
9	E	91/147 (62%)	85 (93%)	6 (7%)	0	100	100
10	F	79/117 (68%)	73 (92%)	6 (8%)	0	100	100
11	G	98/115 (85%)	93 (95%)	5 (5%)	0	100	100
12	H	78/84 (93%)	77 (99%)	1 (1%)	0	100	100
13	I	71/78 (91%)	70 (99%)	1 (1%)	0	100	100
14	J	71/77 (92%)	66 (93%)	5 (7%)	0	100	100
15	K	389/473 (82%)	357 (92%)	32 (8%)	0	100	100
16	L	230/557 (41%)	211 (92%)	19 (8%)	0	100	100
17	M	222/354 (63%)	214 (96%)	8 (4%)	0	100	100
18	N	1282/1284 (100%)	1260 (98%)	22 (2%)	0	100	100
19	O	142/146 (97%)	135 (95%)	7 (5%)	0	100	100
20	P	265/388 (68%)	244 (92%)	19 (7%)	2 (1%)	16	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	Q	86/265 (32%)	77 (90%)	9 (10%)	0	100	100
22	R	597/674 (89%)	588 (98%)	9 (2%)	0	100	100
23	S	130/488 (27%)	122 (94%)	8 (6%)	0	100	100
23	T	132/488 (27%)	123 (93%)	9 (7%)	0	100	100
23	U	414/488 (85%)	394 (95%)	20 (5%)	0	100	100
23	V	129/488 (26%)	118 (92%)	11 (8%)	0	100	100
24	W	514/757 (68%)	479 (93%)	32 (6%)	3 (1%)	21	56
25	X	642/790 (81%)	610 (95%)	31 (5%)	1 (0%)	43	73
26	Y	114/229 (50%)	108 (95%)	5 (4%)	1 (1%)	14	47
27	Z	151/187 (81%)	144 (95%)	7 (5%)	0	100	100
28	a	150/558 (27%)	140 (93%)	10 (7%)	0	100	100
29	b	98/293 (33%)	94 (96%)	4 (4%)	0	100	100
30	c	202/887 (23%)	192 (95%)	10 (5%)	0	100	100
31	d	152/155 (98%)	137 (90%)	15 (10%)	0	100	100
33	m	79/797 (10%)	78 (99%)	1 (1%)	0	100	100
35	y	179/534 (34%)	154 (86%)	23 (13%)	2 (1%)	11	43
36	z	624/647 (96%)	611 (98%)	12 (2%)	1 (0%)	43	73
All	All	10453/16329 (64%)	9921 (95%)	520 (5%)	12 (0%)	49	79

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
20	P	90	GLN
24	W	536	ILE
35	y	115	LYS
5	A	1115	ILE
26	Y	144	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	A	1570/2138 (73%)	1569 (100%)	1 (0%)	88	91
6	B	821/881 (93%)	821 (100%)	0	100	100
7	C	257/292 (88%)	257 (100%)	0	100	100
8	D	85/86 (99%)	85 (100%)	0	100	100
9	E	80/118 (68%)	80 (100%)	0	100	100
10	F	76/102 (74%)	76 (100%)	0	100	100
11	G	91/101 (90%)	91 (100%)	0	100	100
12	H	73/76 (96%)	73 (100%)	0	100	100
13	I	64/69 (93%)	64 (100%)	0	100	100
14	J	63/67 (94%)	63 (100%)	0	100	100
15	K	333/405 (82%)	333 (100%)	0	100	100
16	L	200/477 (42%)	200 (100%)	0	100	100
17	M	198/306 (65%)	198 (100%)	0	100	100
18	N	1188/1188 (100%)	1188 (100%)	0	100	100
19	O	130/132 (98%)	130 (100%)	0	100	100
20	P	231/340 (68%)	231 (100%)	0	100	100
21	Q	79/240 (33%)	79 (100%)	0	100	100
22	R	532/597 (89%)	532 (100%)	0	100	100
23	S	121/443 (27%)	121 (100%)	0	100	100
23	T	123/443 (28%)	123 (100%)	0	100	100
23	U	223/443 (50%)	223 (100%)	0	100	100
23	V	120/443 (27%)	120 (100%)	0	100	100
24	W	469/656 (72%)	469 (100%)	0	100	100
25	X	586/707 (83%)	586 (100%)	0	100	100
26	Y	116/214 (54%)	116 (100%)	0	100	100
27	Z	132/163 (81%)	132 (100%)	0	100	100
28	a	79/496 (16%)	79 (100%)	0	100	100
29	b	95/275 (34%)	95 (100%)	0	100	100
30	c	188/816 (23%)	188 (100%)	0	100	100
31	d	128/129 (99%)	128 (100%)	0	100	100
33	m	72/719 (10%)	72 (100%)	0	100	100
35	y	158/478 (33%)	158 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	z	564/585 (96%)	564 (100%)	0	100	100
All	All	9245/14625 (63%)	9244 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	A	1209	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 100 such sidechains are listed below:

Mol	Chain	Res	Type
20	P	324	GLN
24	W	387	ASN
36	z	384	ASN
22	R	119	ASN
23	T	42	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	28/29 (96%)	19 (67%)	2 (7%)
2	2	22/186 (11%)	4 (18%)	0
3	5	101/120 (84%)	23 (22%)	2 (1%)
4	6	91/99 (91%)	44 (48%)	7 (7%)
All	All	242/434 (55%)	90 (37%)	11 (4%)

5 of 90 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

5 of 11 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	6	30	A

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Mol	Chain	Res	Type
4	6	37	A
4	6	74	U
4	6	52	G
4	6	13	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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$
40	GTP	B	1001	37	33,34,34	0.87	1 (3%)	50,54,54	1.58	9 (18%)
39	IHP	A	2401	-	36,36,36	1.43	13 (36%)	60,60,60	1.50	10 (16%)

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
40	GTP	B	1001	37	-	0/22/38/38	0/3/3/3
39	IHP	A	2401	-	-	3/30/54/54	0/1/1/1

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	A	2401	IHP	P6-O46	-2.50	1.45	1.54
39	A	2401	IHP	P1-O31	-2.26	1.46	1.54
39	A	2401	IHP	P1-O11	2.23	1.63	1.59
39	A	2401	IHP	P5-O45	-2.17	1.46	1.54
39	A	2401	IHP	P6-O36	-2.17	1.46	1.54

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	B	1001	GTP	C5-C4-N3	-5.04	120.36	128.39
40	B	1001	GTP	C2-N3-C4	4.60	120.22	112.30
39	A	2401	IHP	O11-P1-O21	-3.42	97.15	109.33
40	B	1001	GTP	N9-C4-N3	3.24	132.43	125.95
39	A	2401	IHP	C5-C6-C1	3.13	117.30	110.43

There are no chirality outliers.

All (3) torsion outliers are listed below:

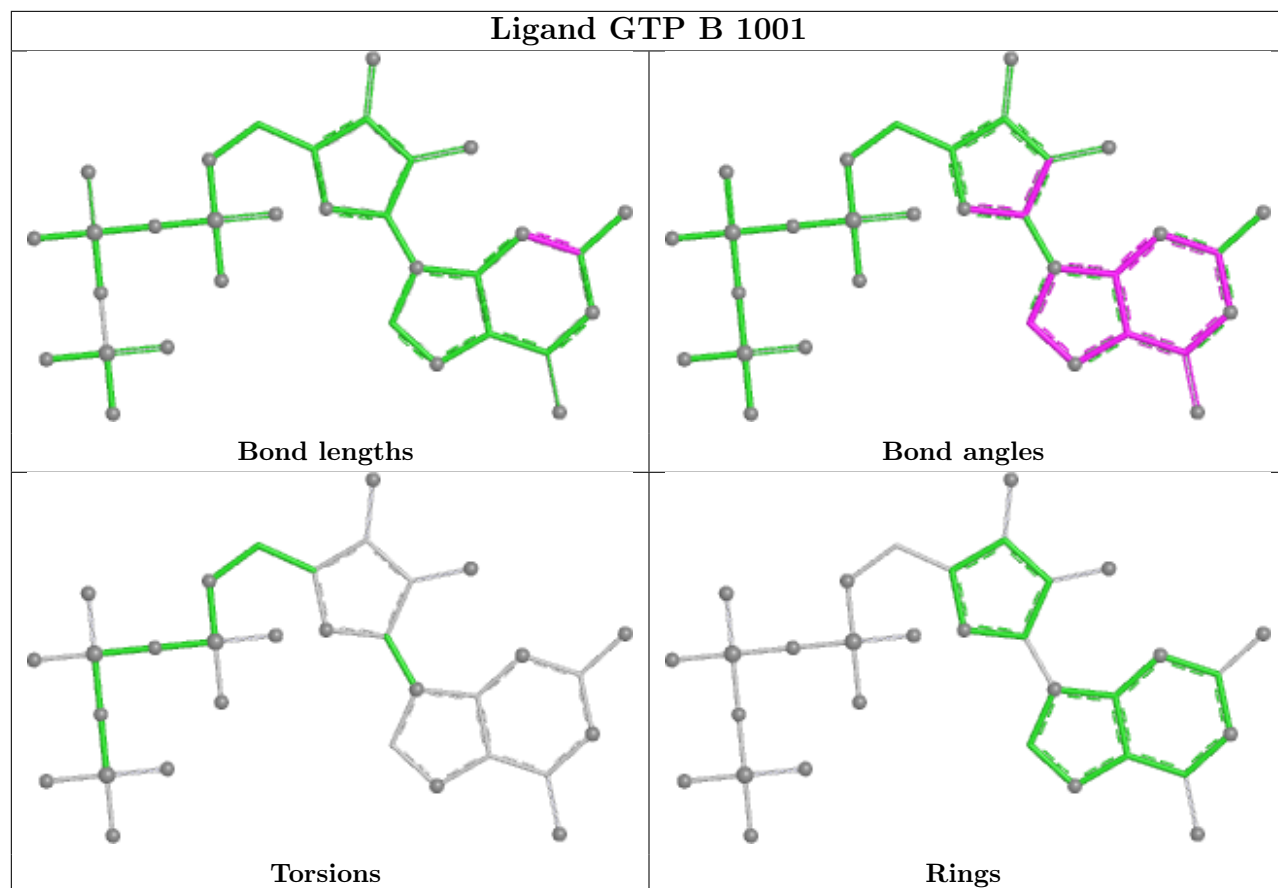
Mol	Chain	Res	Type	Atoms
39	A	2401	IHP	C6-O16-P6-O36
39	A	2401	IHP	C6-O16-P6-O26
39	A	2401	IHP	C1-O11-P1-O41

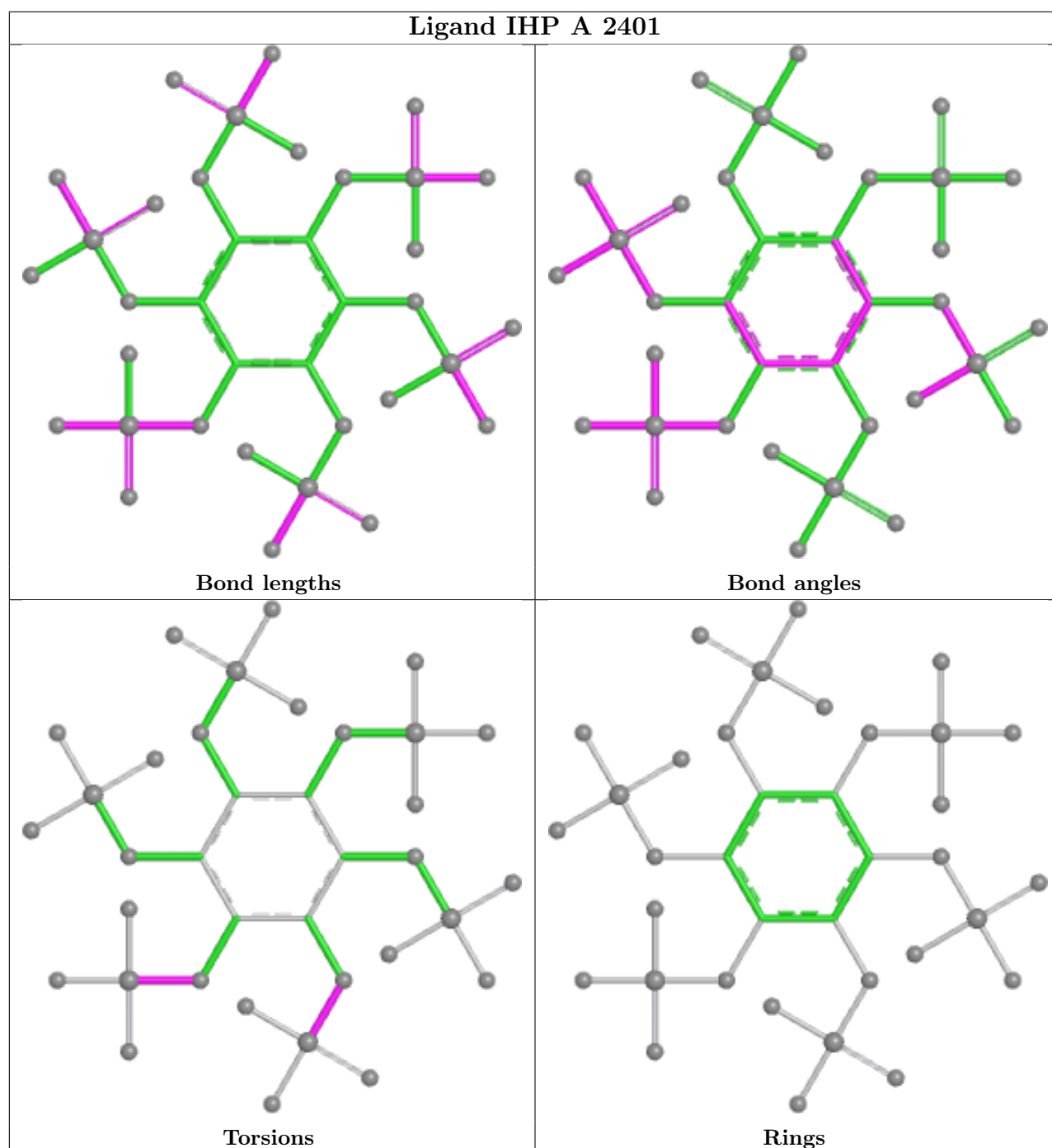
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	B	1001	GTP	3	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.

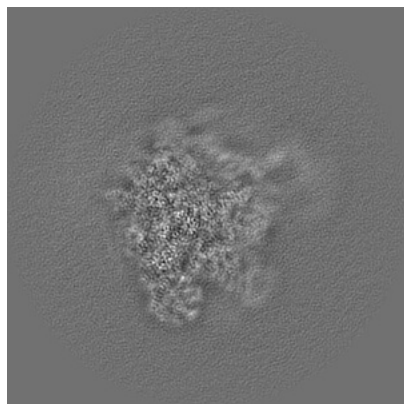
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19941. These allow visual inspection of the internal detail of the map and identification of artifacts.

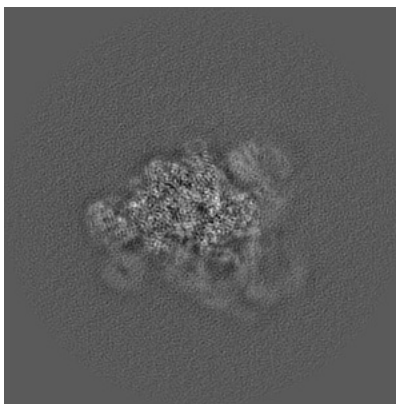
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

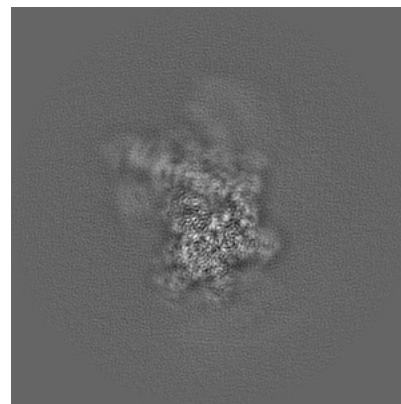
6.1.1 Primary map



X

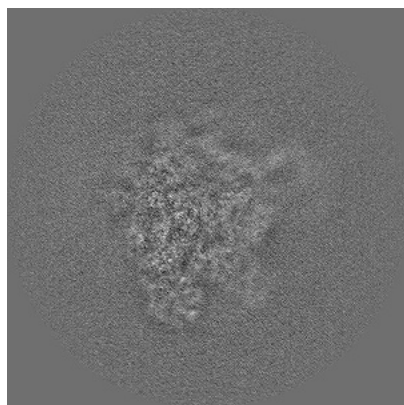


Y

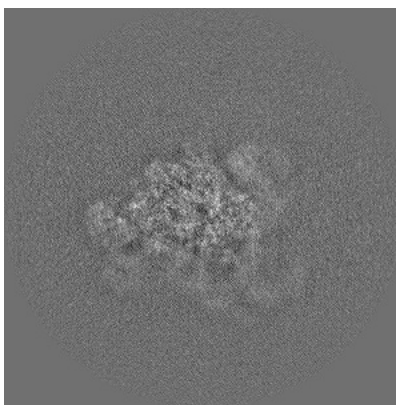


Z

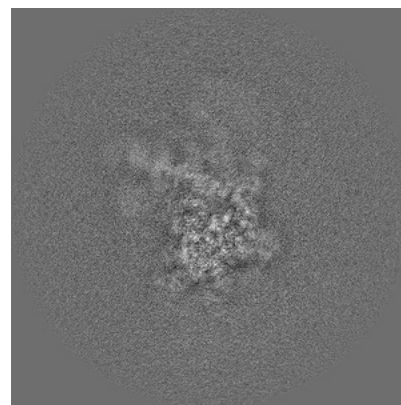
6.1.2 Raw map



X



Y

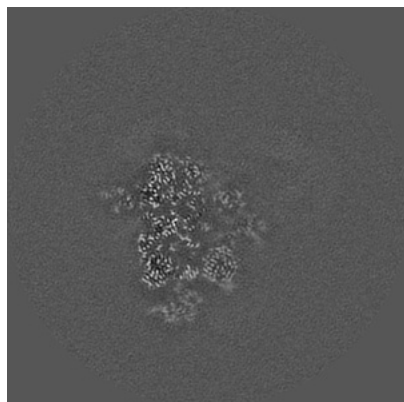


Z

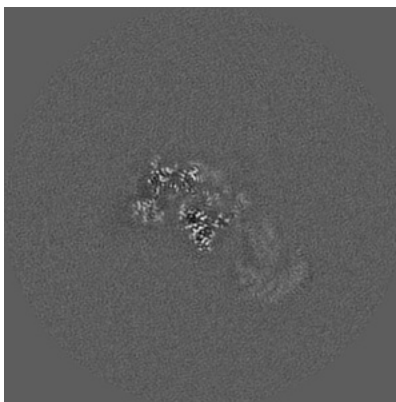
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

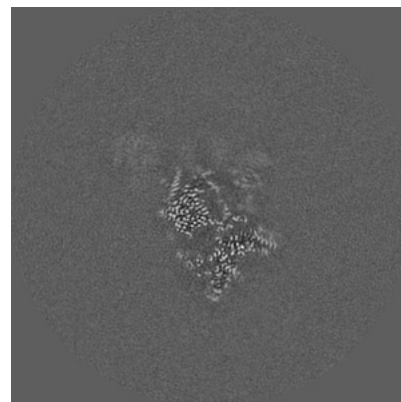
6.2.1 Primary map



X Index: 280

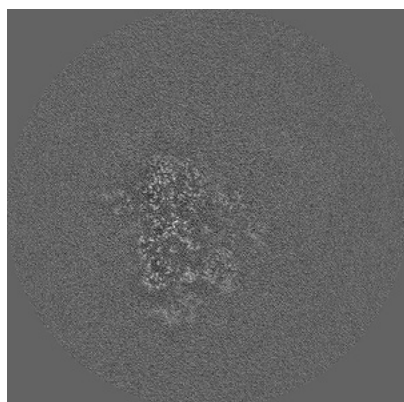


Y Index: 280

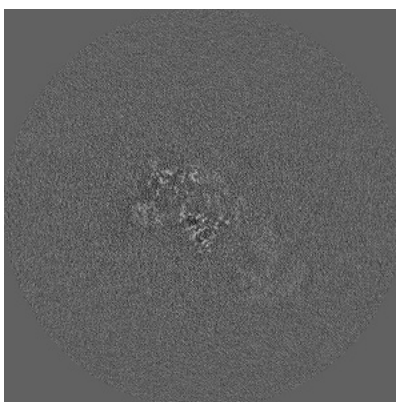


Z Index: 280

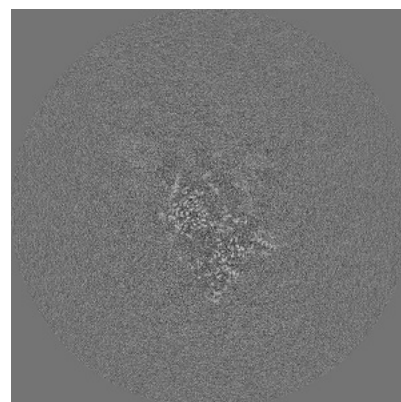
6.2.2 Raw map



X Index: 280



Y Index: 280

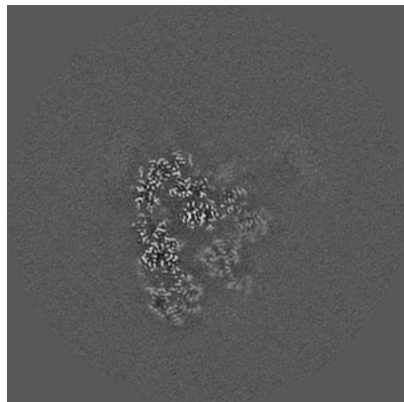


Z Index: 280

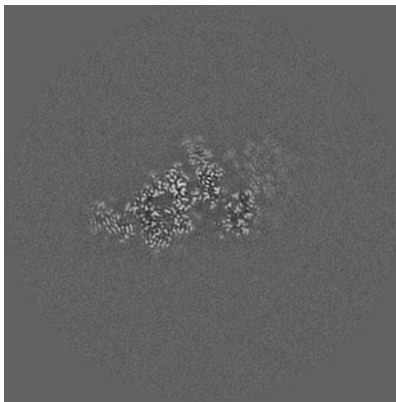
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

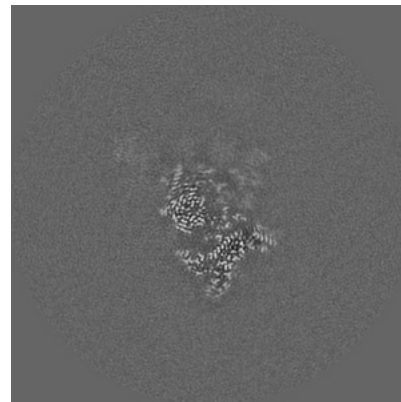
6.3.1 Primary map



X Index: 263

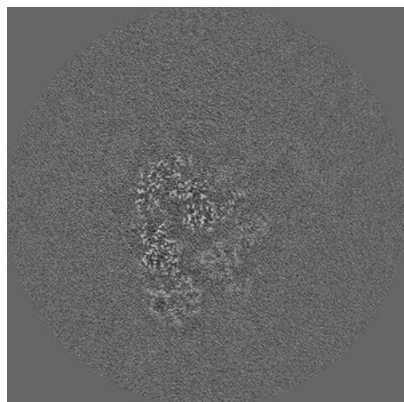


Y Index: 220

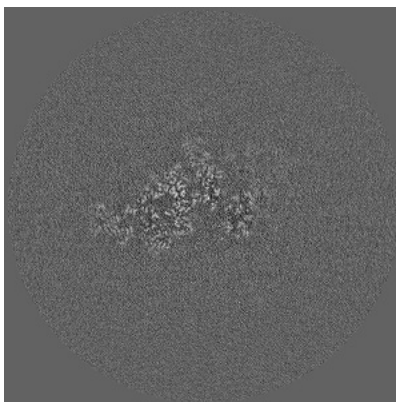


Z Index: 282

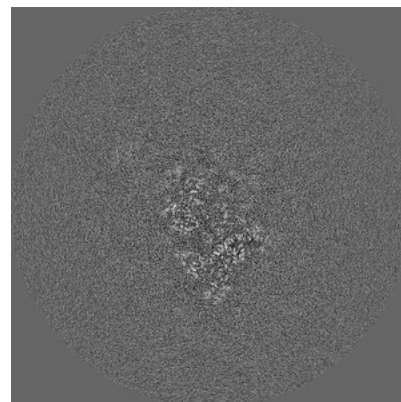
6.3.2 Raw map



X Index: 263



Y Index: 220

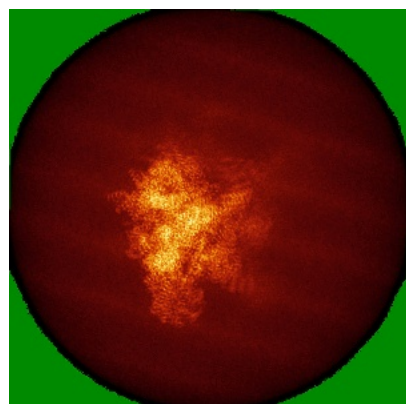


Z Index: 284

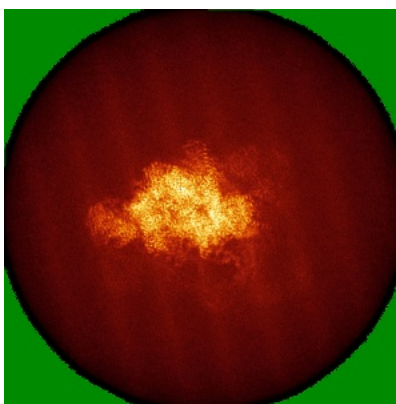
The images above show the largest variance slices of the map in three orthogonal directions.

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

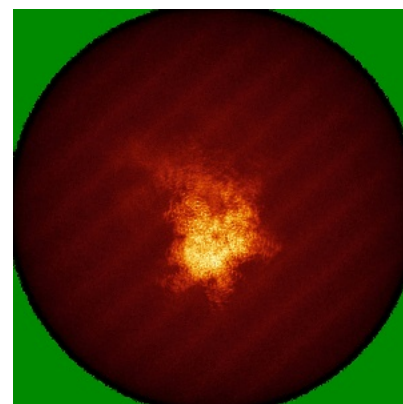
6.4.1 Primary map



X

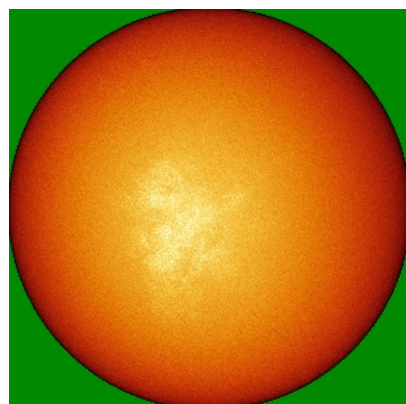


Y

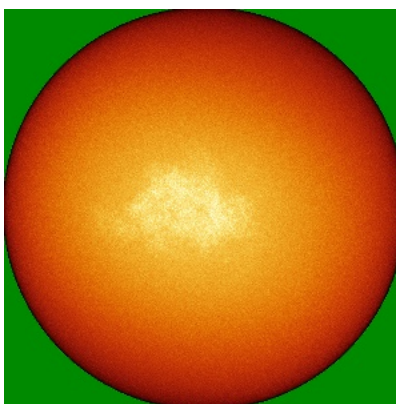


Z

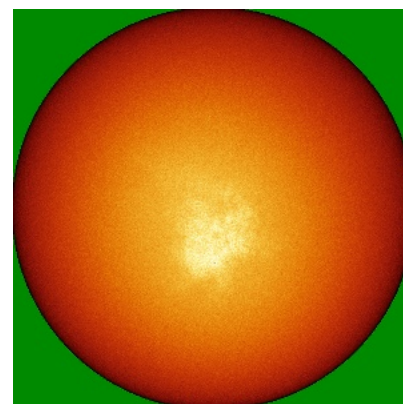
6.4.2 Raw map



X



Y

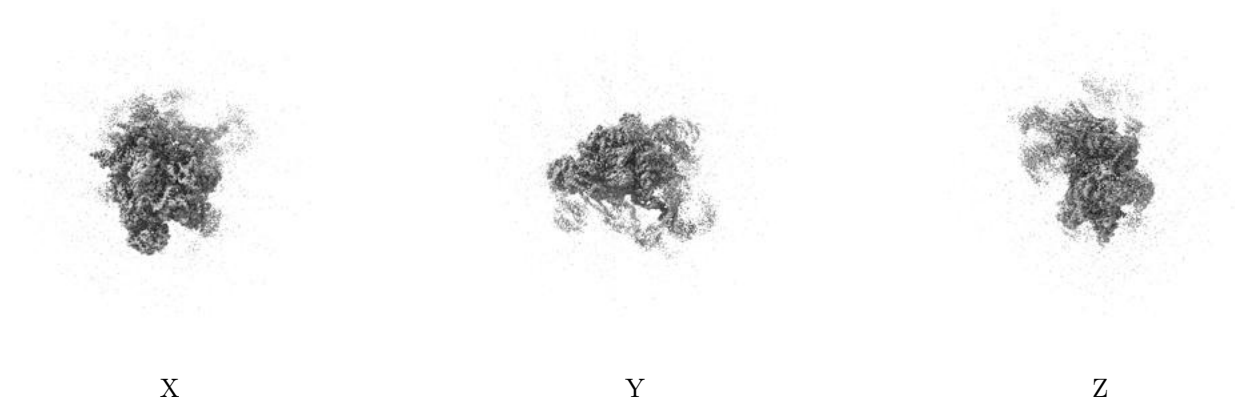


Z

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.

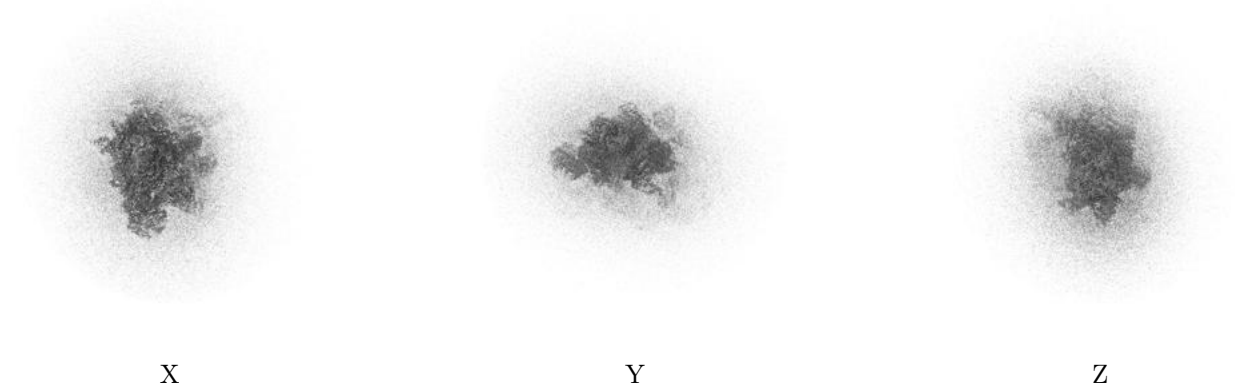
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.55. 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.

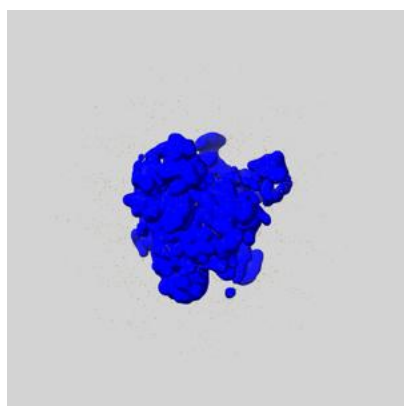
6.6 Mask visualisation [i](#)

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

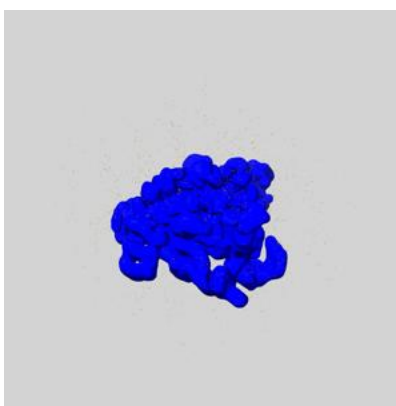
A mask typically either:

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

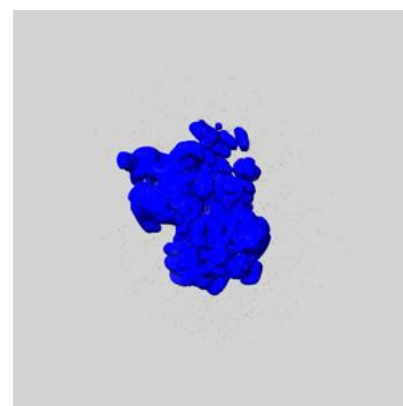
6.6.1 emd_19941_msk_1.map [i](#)



X



Y

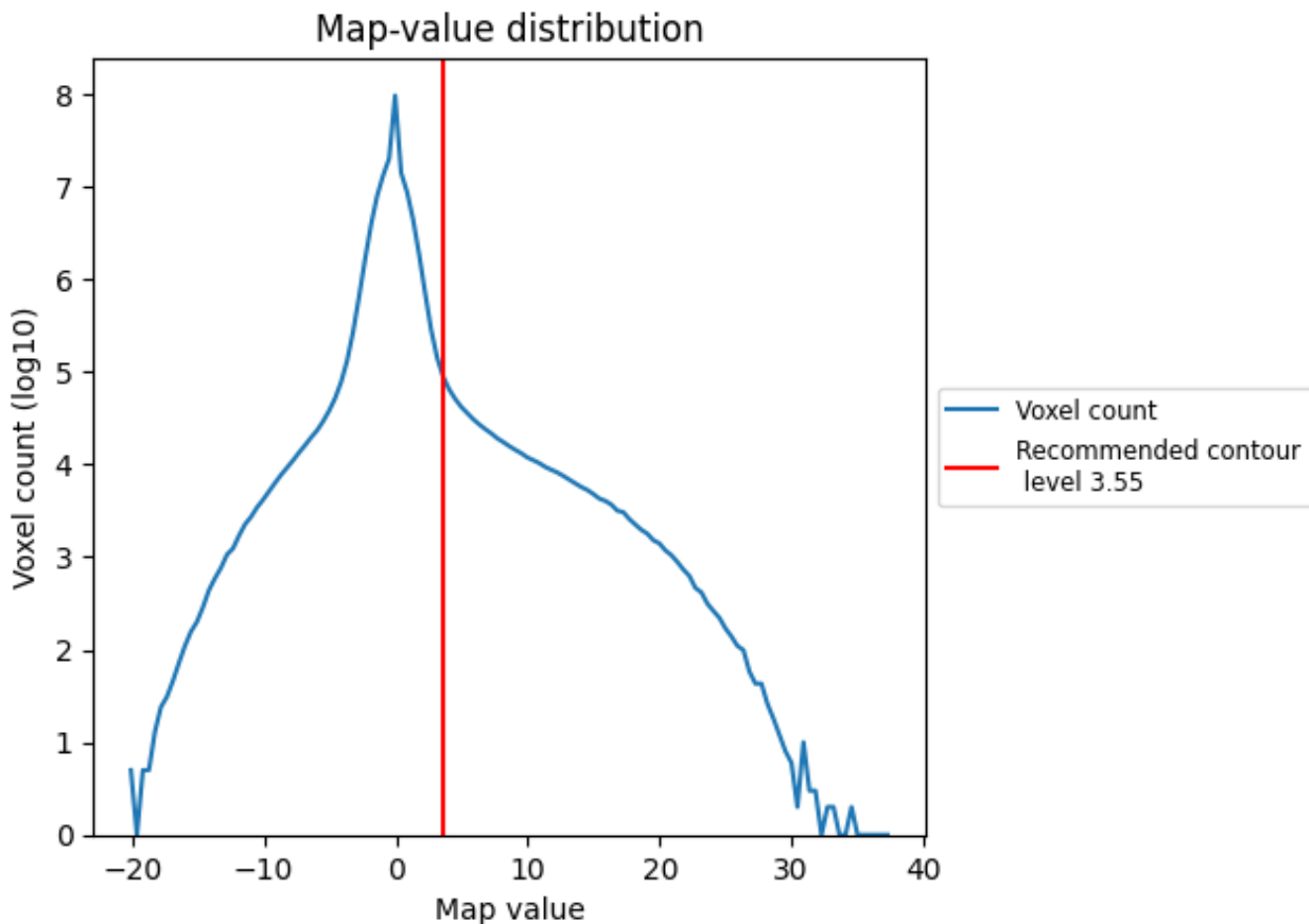


Z

7 Map analysis [i](#)

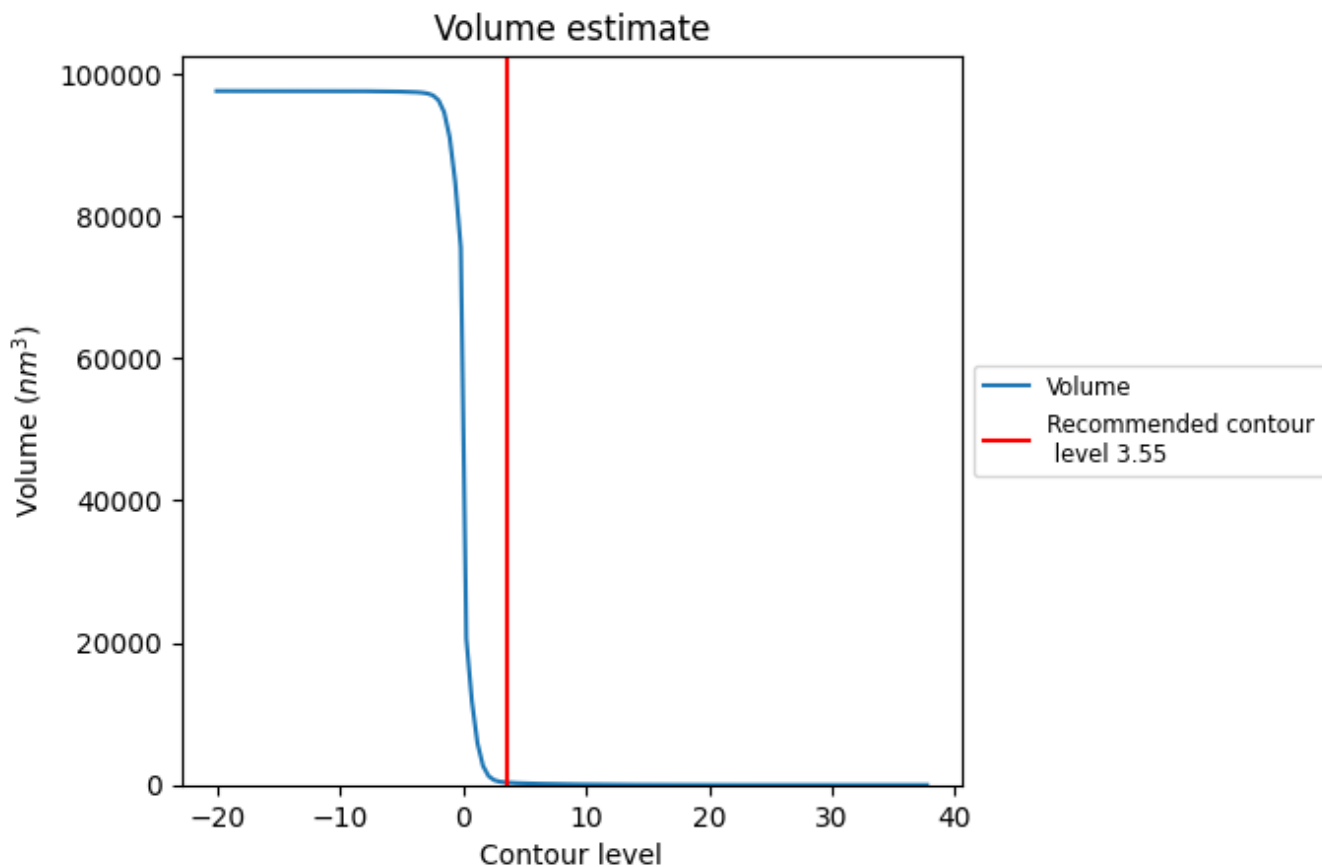
This section contains the results of statistical analysis of the map.

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.

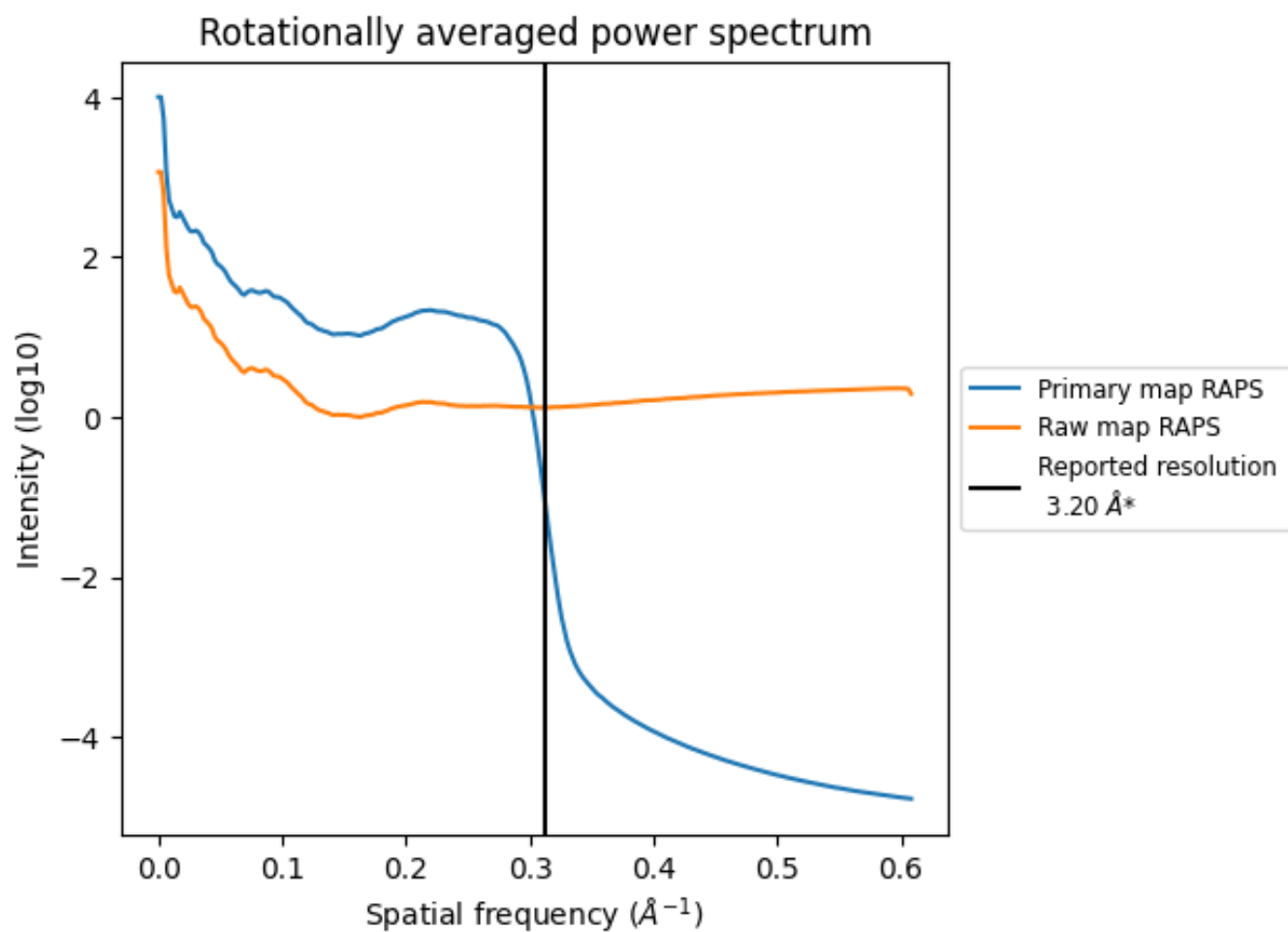
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 341 nm^3 ; this corresponds to an approximate mass of 308 kDa.

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

7.3 Rotationally averaged power spectrum i

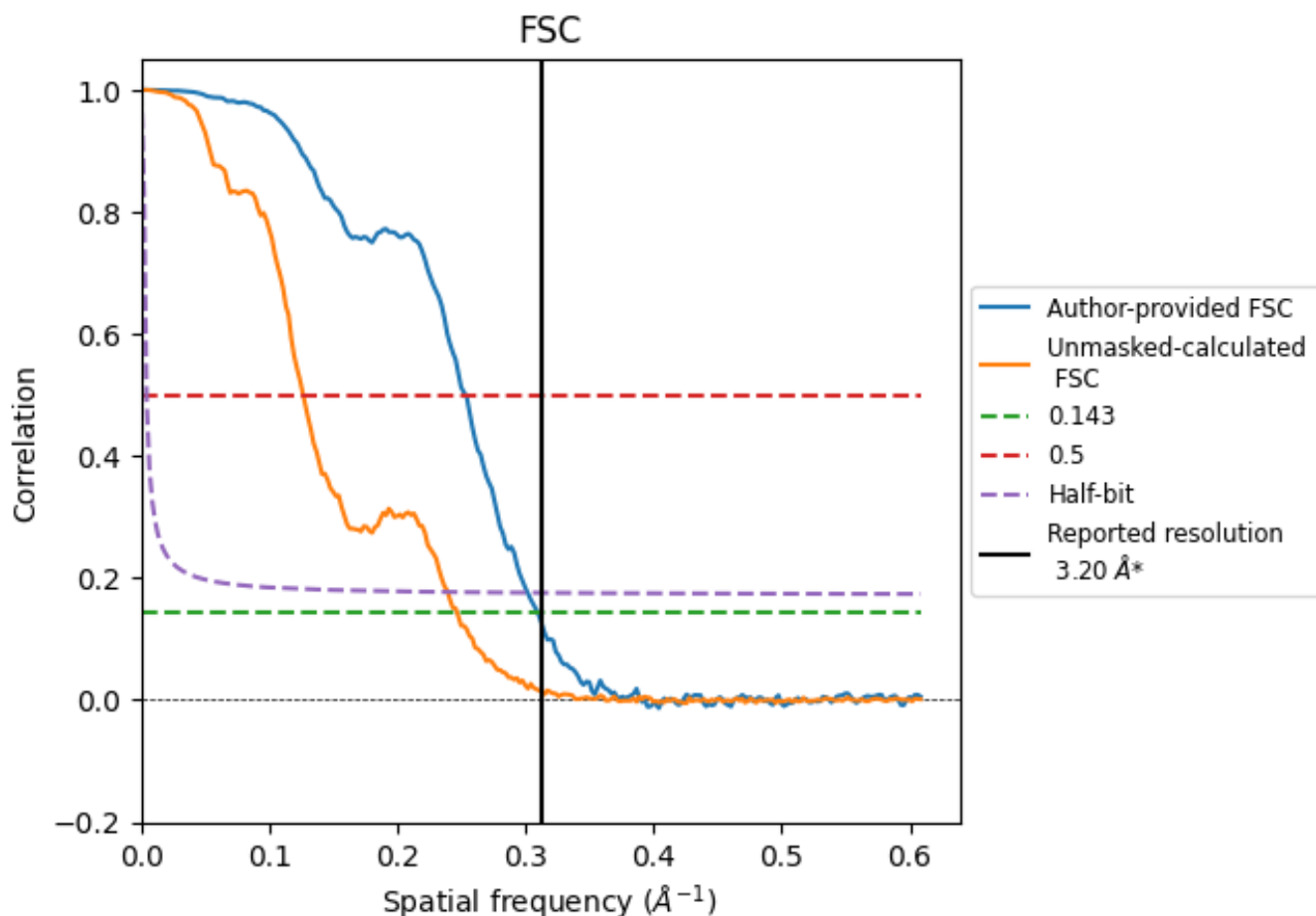


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

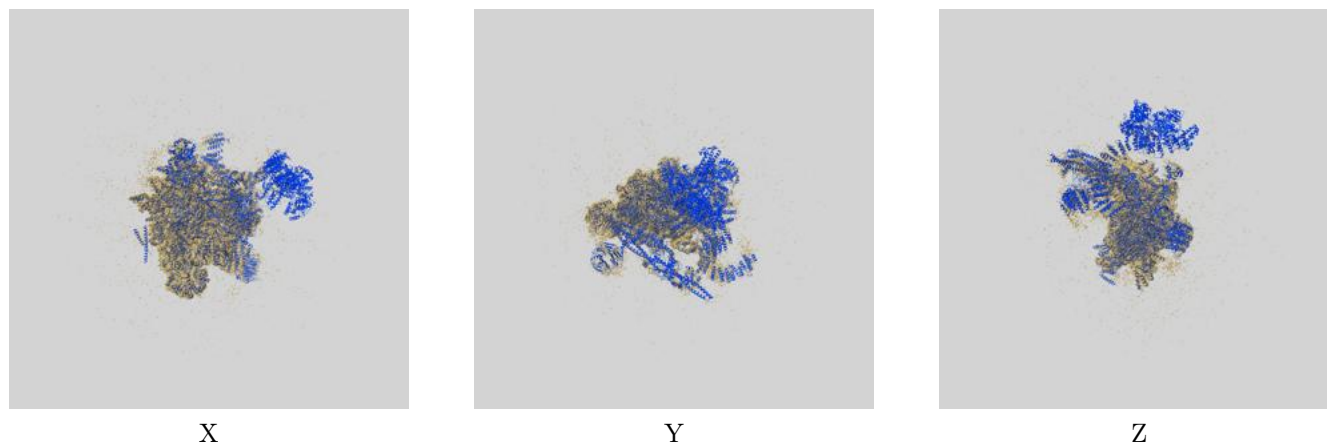
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.23	3.95	3.31
Unmasked-calculated*	4.06	7.91	4.18

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.06 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

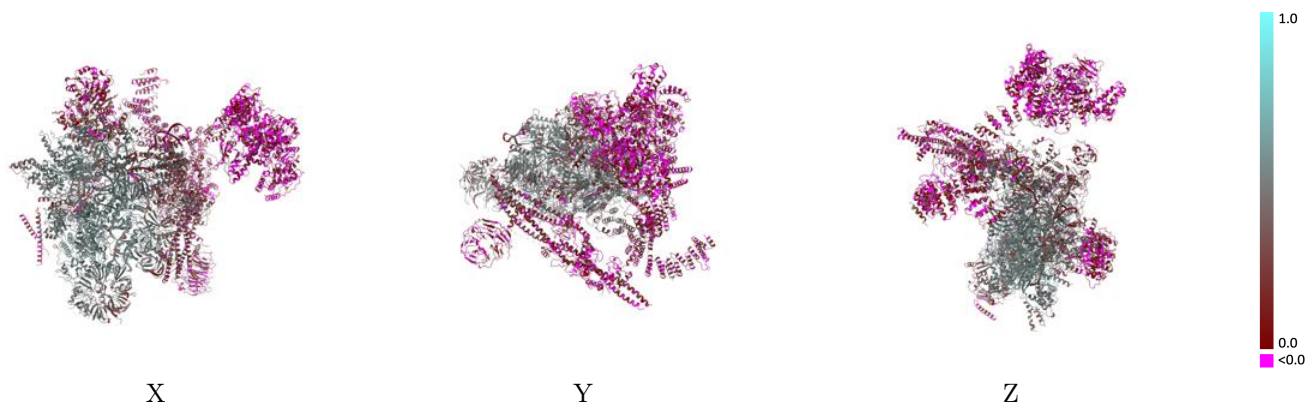
This section contains information regarding the fit between EMDB map EMD-19941 and PDB model 9ESH. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



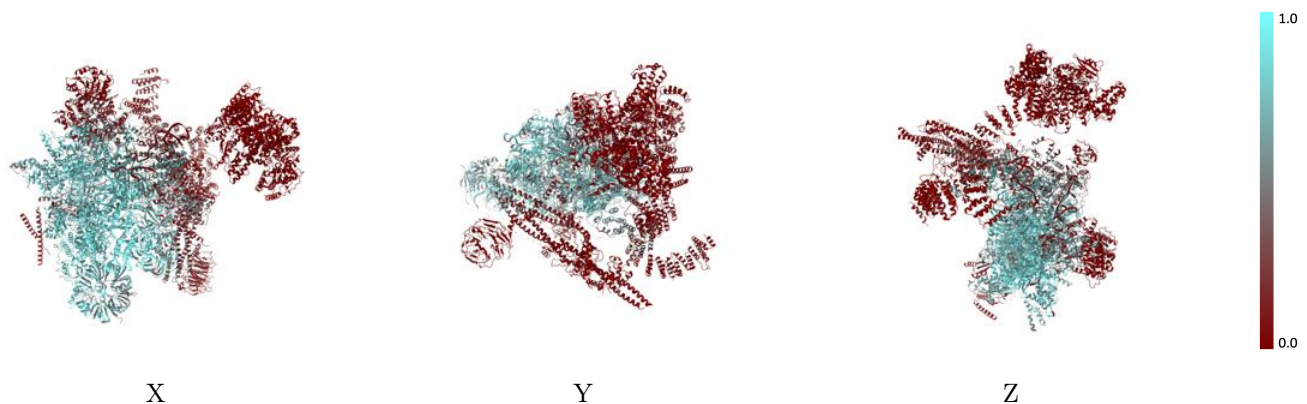
The images above show the 3D surface view of the map at the recommended contour level 3.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



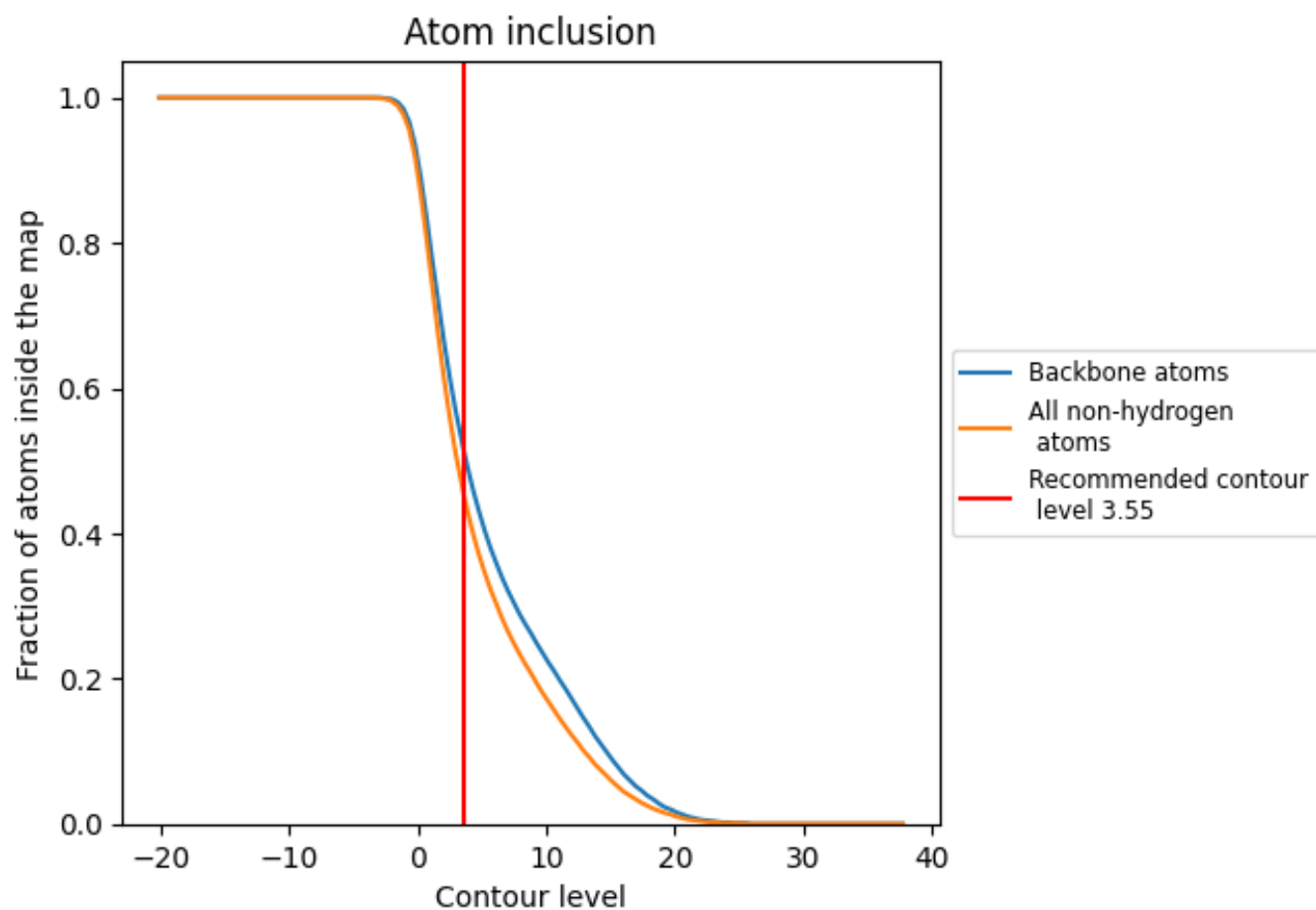
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.55).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 52% of all backbone atoms, 46% 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 (3.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4560	 0.3240
1	 0.4260	 0.3460
2	 0.4240	 0.3160
5	 0.8960	 0.5180
6	 0.5250	 0.3510
A	 0.8180	 0.5270
B	 0.8010	 0.5140
C	 0.6820	 0.4410
D	 0.8140	 0.5290
E	 0.7040	 0.4790
F	 0.6540	 0.4320
G	 0.6130	 0.3800
H	 0.7050	 0.4650
I	 0.7230	 0.4510
J	 0.7460	 0.5120
K	 0.8210	 0.5120
L	 0.6500	 0.4400
M	 0.3530	 0.3180
N	 0.0010	 0.0390
O	 0.7960	 0.5120
P	 0.4460	 0.3400
Q	 0.7420	 0.5080
R	 0.3340	 0.2400
S	 0.0210	 0.0950
T	 0.0830	 0.1130
U	 0.0550	 0.1060
V	 0.0350	 0.0900
W	 0.3780	 0.2880
X	 0.0550	 0.0880
Y	 0.2010	 0.2840
Z	 0.1880	 0.1880
a	 0.5000	 0.3400
b	 0.2540	 0.2530
c	 0.7340	 0.4730
d	 0.4530	 0.3460



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
f	 0.2270	 0.2320
m	 0.1690	 0.3020
r	 0.1580	 0.1660
y	 0.3800	 0.2950
z	 0.1960	 0.1910