



## wwPDB EM Validation Summary Report ⓘ

Oct 15, 2024 – 12:05 AM EDT

PDB ID : 8SER  
EMDB ID : EMD-40426  
Title : Cryo-EM Structure of RyR1 + Adenosine  
Authors : Cholak, S.; Saville, J.W.; Zhu, X.; Berezuk, A.M.; Tuttle, K.S.; Haji-Ghassemi, O.; Van Petegem, F.; Subramaniam, S.  
Deposited on : 2023-04-10  
Resolution : 3.42 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

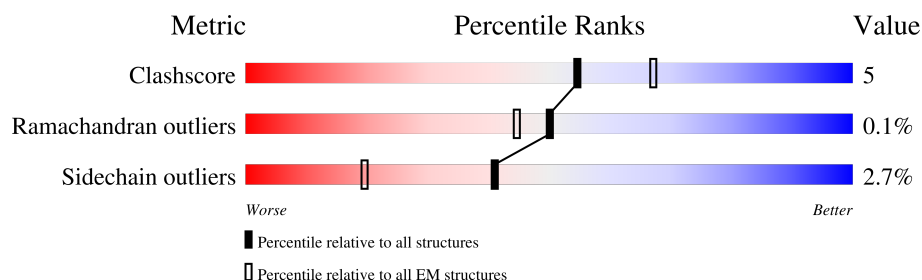
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.42 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	5037	<div> <div>12%</div> <div>74%</div> <div>13%</div> <div>13%</div> </div>
1	B	5037	<div> <div>12%</div> <div>74%</div> <div>13%</div> <div>13%</div> </div>
1	C	5037	<div> <div>13%</div> <div>73%</div> <div>13%</div> <div>13%</div> </div>
1	D	5037	<div> <div>12%</div> <div>74%</div> <div>13%</div> <div>13%</div> </div>
2	E	350	<div> <div>26%</div> <div>5%</div> <div>69%</div> </div>
2	F	350	<div> <div>26%</div> <div>5%</div> <div>69%</div> </div>
2	G	350	<div> <div>26%</div> <div>5%</div> <div>69%</div> </div>
2	H	350	<div> <div>26%</div> <div>5%</div> <div>69%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 142952 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4376	Total	C	N	O	S	9	0
			34900	22201	6022	6441	236		
1	B	4376	Total	C	N	O	S	9	0
			34900	22201	6022	6441	236		
1	C	4376	Total	C	N	O	S	9	0
			34900	22201	6022	6441	236		
1	D	4376	Total	C	N	O	S	9	0
			34900	22201	6022	6441	236		

- Molecule 2 is a protein called Glutathione S-transferase class-mu 26 kDa isozyme,Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	G	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-242	MET	-	expression tag	UNP P08515
E	-241	LYS	-	expression tag	UNP P08515
E	-240	SER	-	expression tag	UNP P08515
E	-239	SER	-	expression tag	UNP P08515
E	-238	HIS	-	expression tag	UNP P08515
E	-237	HIS	-	expression tag	UNP P08515
E	-236	HIS	-	expression tag	UNP P08515
E	-235	HIS	-	expression tag	UNP P08515

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-234	HIS	-	expression tag	UNP P08515
E	-233	HIS	-	expression tag	UNP P08515
E	-232	GLY	-	expression tag	UNP P08515
E	-231	SER	-	expression tag	UNP P08515
E	-230	SER	-	expression tag	UNP P08515
E	-11	GLY	-	linker	UNP P08515
E	-10	ILE	-	linker	UNP P08515
E	-9	GLU	-	linker	UNP P08515
E	-8	GLU	-	linker	UNP P08515
E	-7	ASN	-	linker	UNP P08515
E	-6	LEU	-	linker	UNP P08515
E	-5	TYR	-	linker	UNP P08515
E	-4	PHE	-	linker	UNP P08515
E	-3	GLN	-	linker	UNP P08515
E	-2	SER	-	linker	UNP P08515
E	-1	ASN	-	linker	UNP P08515
E	0	ALA	-	linker	UNP P08515
F	-242	MET	-	expression tag	UNP P08515
F	-241	LYS	-	expression tag	UNP P08515
F	-240	SER	-	expression tag	UNP P08515
F	-239	SER	-	expression tag	UNP P08515
F	-238	HIS	-	expression tag	UNP P08515
F	-237	HIS	-	expression tag	UNP P08515
F	-236	HIS	-	expression tag	UNP P08515
F	-235	HIS	-	expression tag	UNP P08515
F	-234	HIS	-	expression tag	UNP P08515
F	-233	HIS	-	expression tag	UNP P08515
F	-232	GLY	-	expression tag	UNP P08515
F	-231	SER	-	expression tag	UNP P08515
F	-230	SER	-	expression tag	UNP P08515
F	-11	GLY	-	linker	UNP P08515
F	-10	ILE	-	linker	UNP P08515
F	-9	GLU	-	linker	UNP P08515
F	-8	GLU	-	linker	UNP P08515
F	-7	ASN	-	linker	UNP P08515
F	-6	LEU	-	linker	UNP P08515
F	-5	TYR	-	linker	UNP P08515
F	-4	PHE	-	linker	UNP P08515
F	-3	GLN	-	linker	UNP P08515
F	-2	SER	-	linker	UNP P08515
F	-1	ASN	-	linker	UNP P08515
F	0	ALA	-	linker	UNP P08515

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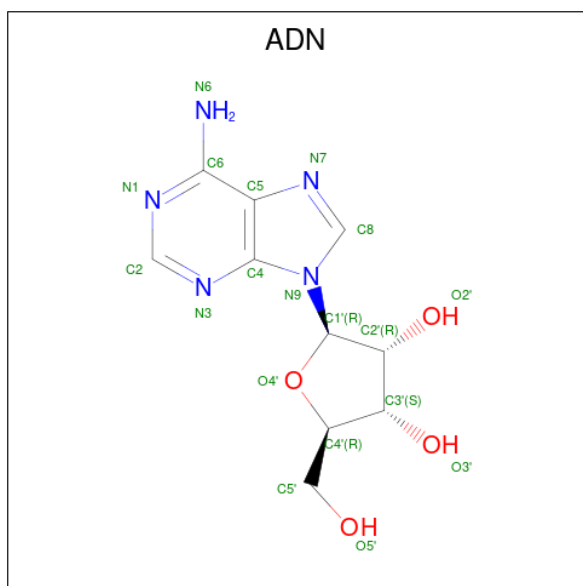
Chain	Residue	Modelled	Actual	Comment	Reference
G	-242	MET	-	expression tag	UNP P08515
G	-241	LYS	-	expression tag	UNP P08515
G	-240	SER	-	expression tag	UNP P08515
G	-239	SER	-	expression tag	UNP P08515
G	-238	HIS	-	expression tag	UNP P08515
G	-237	HIS	-	expression tag	UNP P08515
G	-236	HIS	-	expression tag	UNP P08515
G	-235	HIS	-	expression tag	UNP P08515
G	-234	HIS	-	expression tag	UNP P08515
G	-233	HIS	-	expression tag	UNP P08515
G	-232	GLY	-	expression tag	UNP P08515
G	-231	SER	-	expression tag	UNP P08515
G	-230	SER	-	expression tag	UNP P08515
G	-11	GLY	-	linker	UNP P08515
G	-10	ILE	-	linker	UNP P08515
G	-9	GLU	-	linker	UNP P08515
G	-8	GLU	-	linker	UNP P08515
G	-7	ASN	-	linker	UNP P08515
G	-6	LEU	-	linker	UNP P08515
G	-5	TYR	-	linker	UNP P08515
G	-4	PHE	-	linker	UNP P08515
G	-3	GLN	-	linker	UNP P08515
G	-2	SER	-	linker	UNP P08515
G	-1	ASN	-	linker	UNP P08515
G	0	ALA	-	linker	UNP P08515
H	-242	MET	-	expression tag	UNP P08515
H	-241	LYS	-	expression tag	UNP P08515
H	-240	SER	-	expression tag	UNP P08515
H	-239	SER	-	expression tag	UNP P08515
H	-238	HIS	-	expression tag	UNP P08515
H	-237	HIS	-	expression tag	UNP P08515
H	-236	HIS	-	expression tag	UNP P08515
H	-235	HIS	-	expression tag	UNP P08515
H	-234	HIS	-	expression tag	UNP P08515
H	-233	HIS	-	expression tag	UNP P08515
H	-232	GLY	-	expression tag	UNP P08515
H	-231	SER	-	expression tag	UNP P08515
H	-230	SER	-	expression tag	UNP P08515
H	-11	GLY	-	linker	UNP P08515
H	-10	ILE	-	linker	UNP P08515
H	-9	GLU	-	linker	UNP P08515
H	-8	GLU	-	linker	UNP P08515

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-7	ASN	-	linker	UNP P08515
H	-6	LEU	-	linker	UNP P08515
H	-5	TYR	-	linker	UNP P08515
H	-4	PHE	-	linker	UNP P08515
H	-3	GLN	-	linker	UNP P08515
H	-2	SER	-	linker	UNP P08515
H	-1	ASN	-	linker	UNP P08515
H	0	ALA	-	linker	UNP P08515

- Molecule 3 is ADENOSINE (three-letter code: ADN) (formula:  $C_{10}H_{13}N_5O_4$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			19	10	5	4	
3	B	1	Total	C	N	O	0
			19	10	5	4	
3	C	1	Total	C	N	O	0
			19	10	5	4	
3	D	1	Total	C	N	O	0
			19	10	5	4	

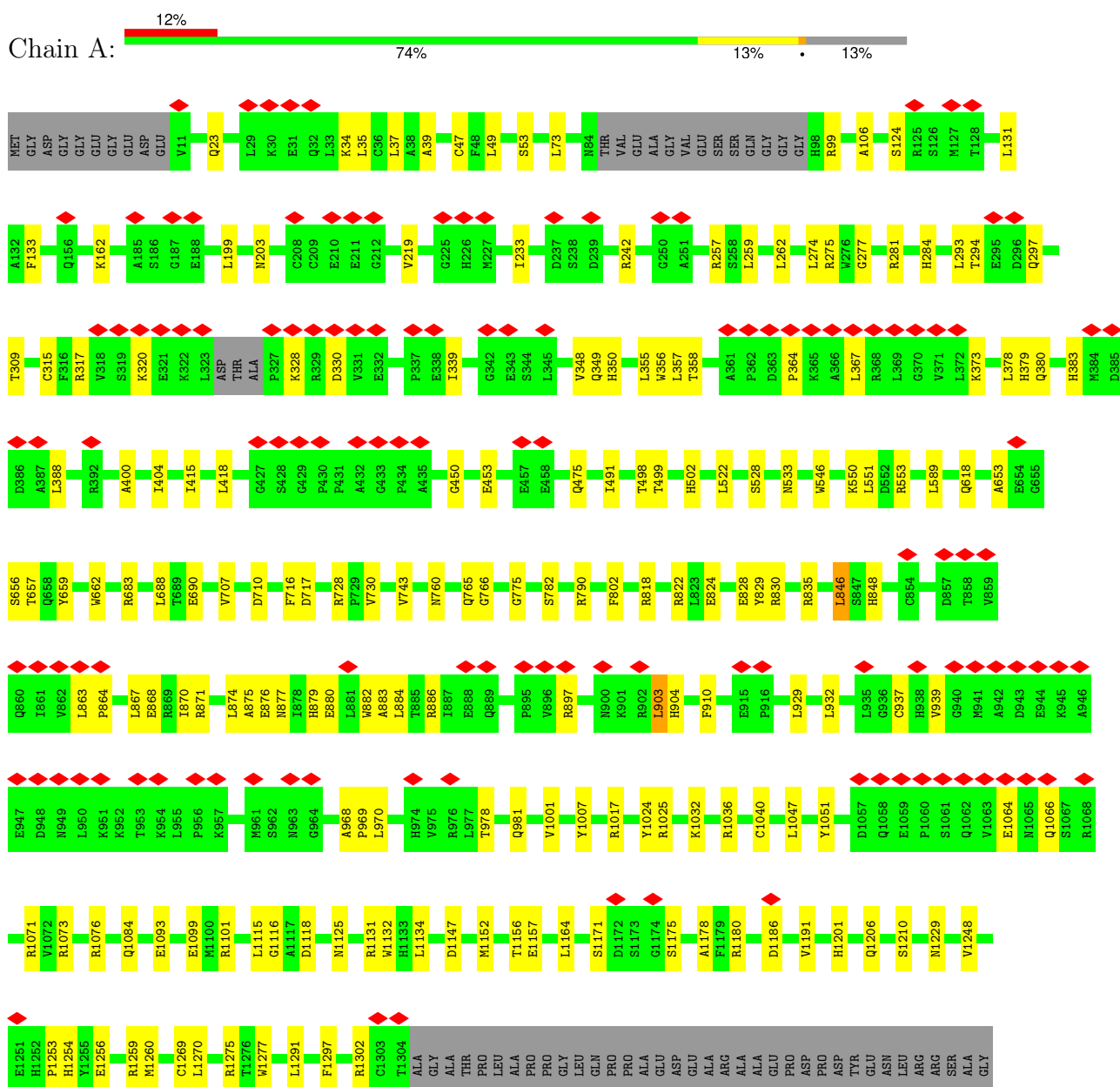
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total 1	Zn 1	0
4	B	1	Total 1	Zn 1	0
4	C	1	Total 1	Zn 1	0
4	D	1	Total 1	Zn 1	0

### 3 Residue-property plots

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

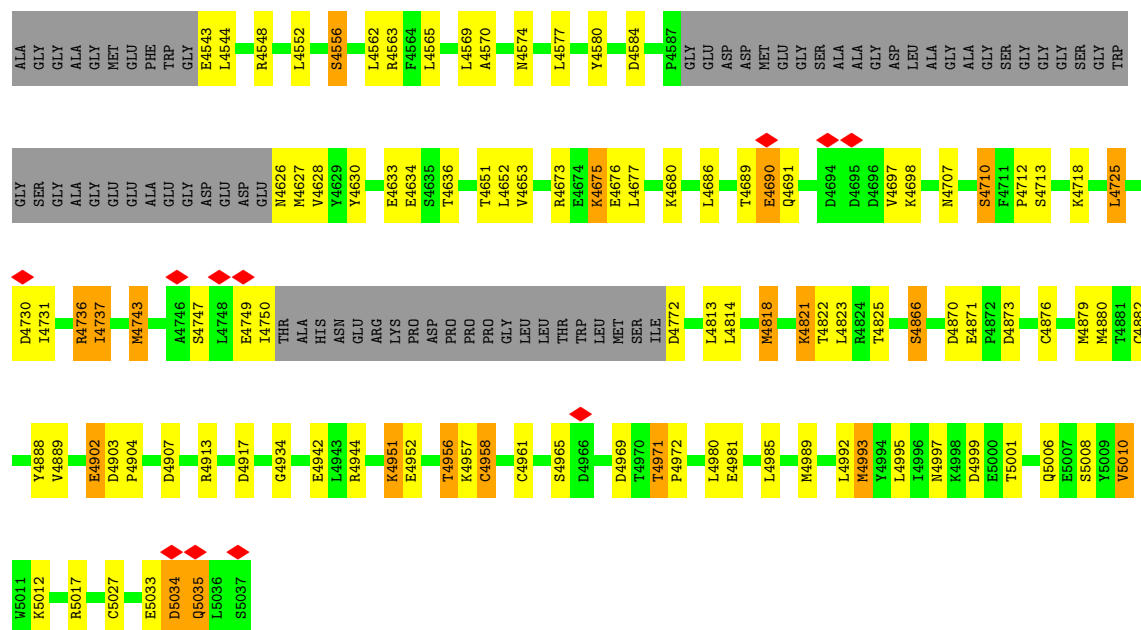
#### • Molecule 1: Ryanodine receptor 1



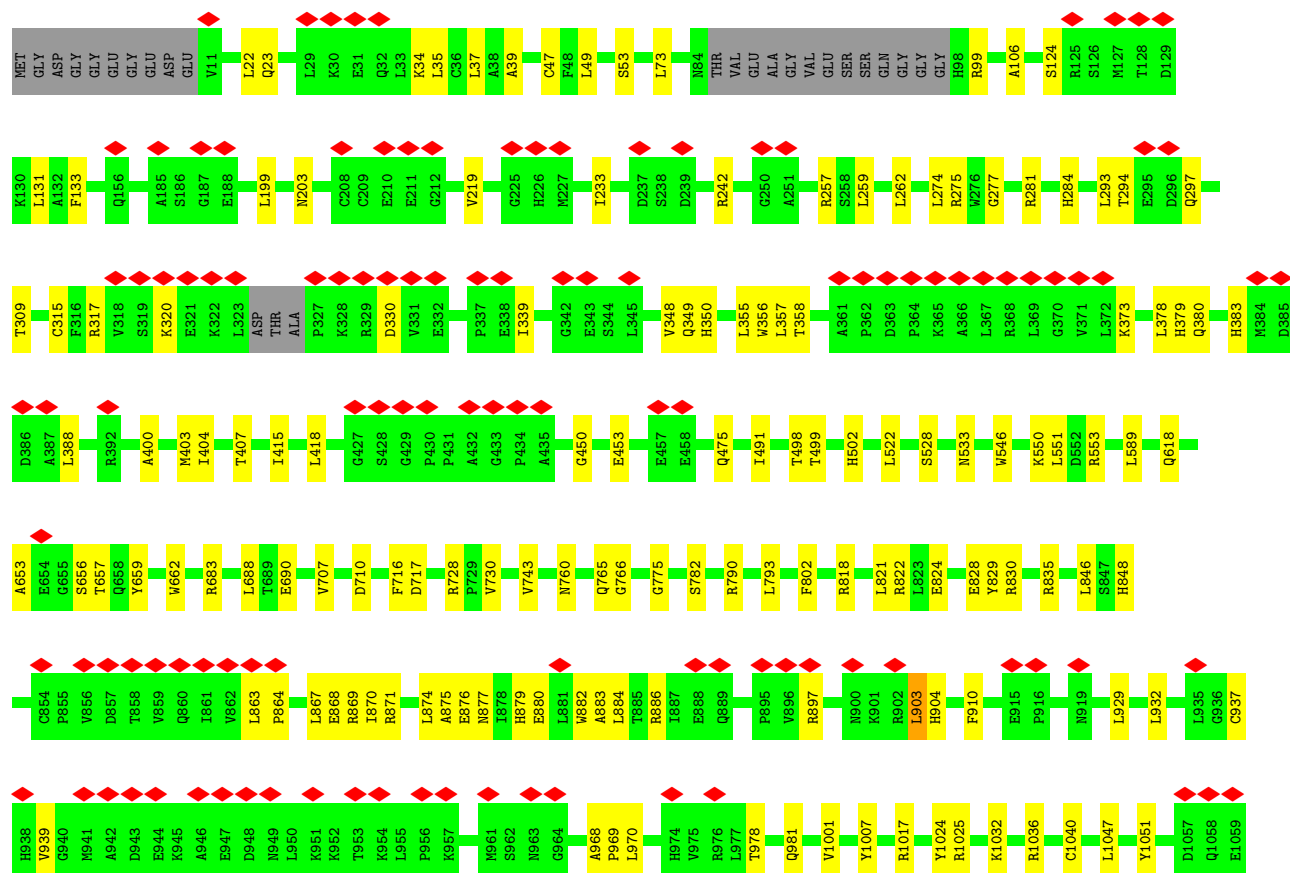








• Molecule 1: Ryanodine receptor 1



K2795	F2735	S2590	ARG	I2167	K2045	GLU	G1754	G1507	LYS	LEU	S1210	P1060
T2796	D2736	R2593	ASP	N2176	L2046	GLU	G1755	R1509	ALA	ARG	N1229	S1061
F2797	P2737	S2594	ARG	N2196	GLU	GLY	M1756	I1509	ALA	SER	R1232	Q1062
S2798	R2738	L2595	ARG	R2199	GLU	GLU	A1768	H1510	ALA	GLY	V1248	V1063
E2799	P2739	R2600	HIS	E2205	GLU	GLU	A1789	H1511	THR	GLY	E1064	E1065
D2801	V2740	M2618	PHE	R2208	GLU	GLU	G1790	T1512	GLN	TRP	P1253	Q1066
K2802	E2741	V2627	GLY	E2206	PRO	GLU	A1792	V1520	ALA	GLY	H1254	S1067
E2803	L2742	G2217	GLU	M2208	GLU	GLU	E1793	D1521	THR	GLU	E1256	R1068
L2804	M2743	G2218	THR	G2217	GLU	THR	R1808	A1523	ALA	GLY	R1259	R1071
R2805	P2744	G2219	LEU	G2218	GLU	LEU	R1827	K1534	LEU	LYS	V1072	R1073
R2806	E2745	E2219	SER	E2218	SER	SER	D1828	P1550	ARG	GLU	M1260	R1076
M2807	L2746	T2220	ARG	T2220	ARG	ARG	I1853	V1554	LEU	THR	C1269	R1076
P2808	M2414	K2221	LEU	K2221	LEU	LEU	Q1861	Q1559	HIS	ALA	E1093	E1093
L2809	L2474	L2236	ARG	L2236	ARG	ARG	M1865	V1561	ASP	LYS	R1275	E1099
K2810	T2478	M2250	SER	M2250	SER	SER	E1874	I1562	VAL	GLY	T1276	E1099
E2811	L2479	L2265	LEU	L2265	LEU	LEU	GLU	Q1563	VAL	GLY	W1277	M1100
S2812	G2480	L2268	THR	L2268	THR	THR	GLU	F1564	ALA	PRO	L1291	R1101
L2813	K2481	A2277	GLU	A2277	GLU	GLU	R1584	A1578	ALA	GLY	F1297	L1115
K2814	D2482	I2281	VAL	I2281	VAL	VAL	R1585	R1585	THR	THR	R1302	G1116
A2815	G2483	L2307	ARG	L2307	ARG	ARG	E1874	K1585	PRO	GLN	C1303	A1117
M2816	F2679	C2310	LYS	C2310	LYS	LYS	GLU	GLU	ALA	GLY	T1304	D1118
L2817	L2682	L2313	LYS	L2313	LYS	LYS	GLU	GLU	ALA	GLY	M125	M125
A2818	F2683	D2320	LYS	D2320	LYS	LYS	GLU	GLU	ALA	GLY	R1131	R1131
M2819	S2684	R2330	LYS	R2330	LYS	LYS	GLU	GLU	ALA	GLY	W1132	W1132
E2820	L2686	R2336	LYS	R2336	LYS	LYS	GLU	GLU	ALA	GLY	H1133	H1133
M2821	A2687	L2368	LYS	L2368	LYS	LYS	GLU	GLU	ALA	GLY	L1134	L1134
L2822	H2688	R2369	LYS	R2369	LYS	LYS	GLU	GLU	ALA	GLY	D147	D147
L2823	L2706	G2370	LYS	G2370	LYS	LYS	GLU	GLU	ALA	GLY	M152	M152
E2824	A2707	E2371	LYS	E2371	LYS	LYS	GLU	GLU	ALA	GLY	T1156	T1156
K2825	P2712	G2372	LYS	G2372	LYS	LYS	GLU	GLU	ALA	GLY	E1157	E1157
A2826	L2717	G2373	LYS	G2373	LYS	LYS	GLU	GLU	ALA	GLY	L1164	L1164
R2827	S2718	L2376	LYS	L2376	LYS	LYS	GLU	GLU	ALA	GLY	S1171	S1171
E2828	Y2719	R2385	LYS	R2385	LYS	LYS	GLU	GLU	ALA	GLY	D1172	D1172
G2829	S2720	A2391	LYS	A2391	LYS	LYS	GLU	GLU	ALA	GLY	S1175	S1175
E2830	S2721	R2392	LYS	R2392	LYS	LYS	GLU	GLU	ALA	GLY	A1178	A1178
GLU	K2770	G2396	LYS	G2396	LYS	LYS	GLU	GLU	ALA	GLY	F1179	F1179
ARG	D2771	V2397	LYS	V2397	LYS	LYS	GLU	GLU	ALA	GLY	R1180	R1180
THR	Q2772	ARG	LYS	ARG	LYS	LYS	GLU	GLU	ALA	GLY	D1186	D1186
GLU	N2773		LYS		LYS	LYS	GLU	GLU	ALA	GLY	V1191	V1191
LYS	M2774		LYS		LYS	LYS	GLU	GLU	ALA	GLY	H1201	H1201
LYS	S2775		LYS		LYS	LYS	GLU	GLU	ALA	GLY	Q1206	Q1206
LYS	Q2776		LYS		LYS	LYS	GLU	GLU	ALA	GLY		
THR	Y2777		LYS		LYS	LYS	GLU	GLU	ALA	GLY		
ARG	E2778		LYS		LYS	LYS	GLU	GLU	ALA	GLY		
LYS	P2779		LYS		LYS	LYS	GLU	GLU	ALA	GLY		
THR	M2780		LYS		LYS	LYS	GLU	GLU	ALA	GLY		
THR	V2781		LYS		LYS	LYS	GLU	GLU	ALA	GLY		
GLN	D2782		LYS		LYS	LYS	GLU	GLU	ALA	GLY		
ALA	E2783		LYS		LYS	LYS	GLU	GLU	ALA	GLY		
THR	E2784		LYS		LYS	LYS	GLU	GLU	ALA	GLY		
TYR	L2785		LYS		LYS	LYS	GLU	GLU	ALA	GLY		
ASP	K2786		LYS		LYS	LYS	GLU	GLU	ALA	GLY		
PRO	T2787		LYS		LYS	LYS	GLU	GLU	ALA	GLY		
ARG	H2788		LYS		LYS	LYS	GLU	GLU	ALA	GLY		
GLY	P2789		LYS		LYS	LYS	GLU	GLU	ALA	GLY		
	M2790		LYS		LYS	LYS	GLU	GLU	ALA	GLY		
	L2791		LYS		LYS	LYS	GLU	GLU	ALA	GLY		
	R2792		LYS		LYS	LYS	GLU	GLU	ALA	GLY		
	P2793		LYS		LYS	LYS	GLU	GLU	ALA	GLY		
	Y2794		LYS		LYS	LYS	GLU	GLU	ALA	GLY		



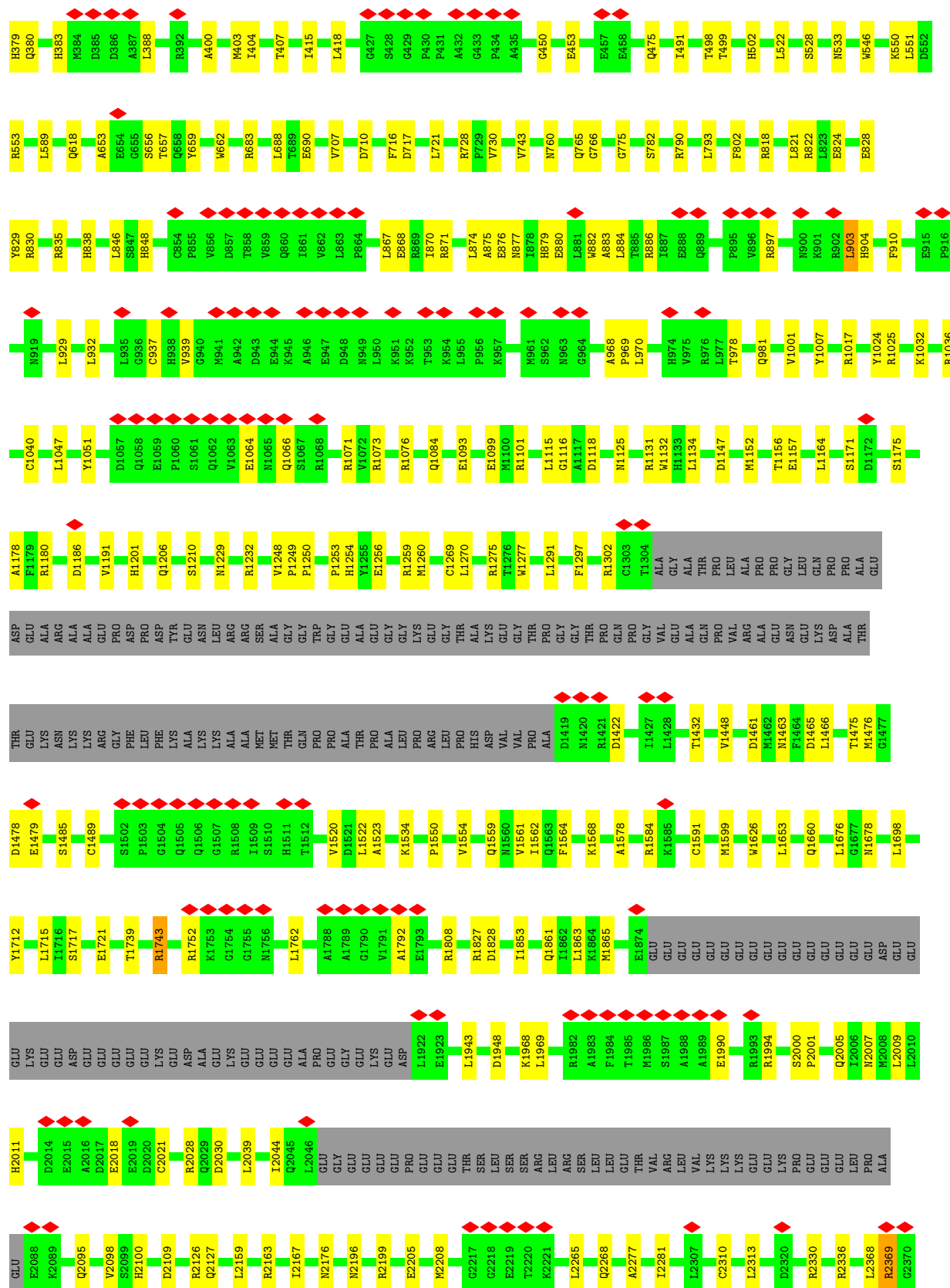




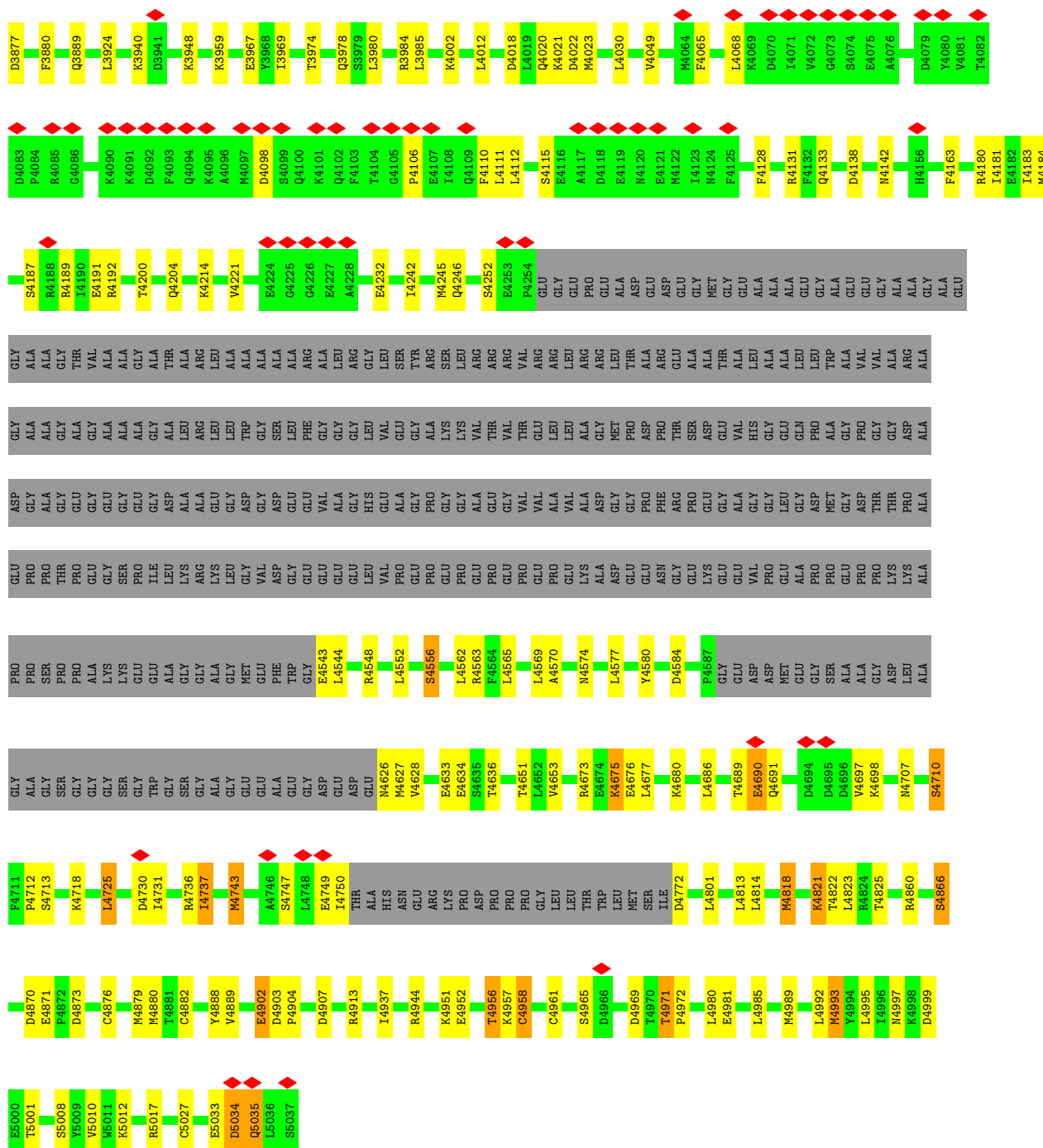
K4002	S3768	A3618	L3514	D3404	G3288	R3167	H3052	S2949	R2888	R2827	A2767	L2686
L4012	R3769	V3619	N3523	Y3409	P3292	T3166	R3053	L2960	K2889	E2828	F2768	A2687
D4018	L3770	W3620	M3524	R3414	P3293	S3171	G3058	L2963	K2890	G2829	D2769	H2688
L4019	H3771	H3621	H3533	H5449	A3295	N3180	T3059	M2967	K2891	E2830	K2770	I2706
Q4020	R3772	L3622	T3538	N3450	L3296	V3183	P3062	S2970	Q2892	GLU	I2771	A2707
K4021	R3773	L3624	T3538	E3454	P3297	E3184	V3065	Q2971	E2893	ARG	Q2772	P2711
M4023	L3835	S3625	T3538	E3454	A3298	K3185	L3068	F2972	L2894	THR	N2773	P2712
L4030	S3840	Q3626	A3541	N3457	G3299	Q3209	L3075	F2973	E2895	LYS	N2774	A2717
V4049	K3852	R3627	L3542	Q3461	A3300	L3210	E3086	E2978	K2896	LYS	W2775	S2718
M4064	G3857	R3628	K3543	N3462	P3301	A3215	E3087	A2979	G2898	THR	Y2777	Y2719
F4065	M3858	R3629	D3544	N3463	P3302	C3216	V3088	V2980	G2899	ARG	G2778	S2720
L4066	R3859	A3631	D3546	I3464	P3303	S3217	L3087	V2981	G2900	ILE	S2776	S2721
L4068	N3860	V3632	E3548	N3465	L3316	Y3218	D3102	S2982	T2901	SER	N2780	K2722
K4069	E3861	V3633	N3555	N3466	T3322	Y3219	T3103	G2984	H2902	GLN	V2781	A2723
D4070	D3862	A3634	N3556	N3467	N3325	T3220	V3107	Q2985	P2903	THR	E2782	E2724
L4072	G3863	F3636	L3557	F3469	N3326	T3221	L3110	V2986	L2905	ALA	D2783	K2725
G4073	T3864	R3637	H3558	S3470	T3329	S3223	L3111	E2987	L2906	THR	E2784	LYS
S4074	V3865	A3659	Q3560	A3472	D3330	P3224	R3112	K2988	V2907	THR	L2785	ALA
F4075	N3866	L3663	G3561	D3473	N3335	R3225	G3113	K2989	P2908	ASP	K2786	THR
A4076	R3867	L3663	K3562	S3474	R3337	E3226	V3114	P2990	D2909	ARG	T2787	VAL
D4079	Q3868	G3681	E3564	K3475	V3346	A3228	G3115	H2991	T2910	GLU	H2788	ALA
V4080	N3870	E3682	G3565	K3477	L3354	I3229	V3116	E2992	L2911	GLY	P2789	GLY
T4082	D3877	A3684	L3579	M3478	L3354	L3230	GLN	N2855	L2912	N2857	M2790	N2734
P4083	F3880	E3685	P3580	A3479	L3354	G3231	ARG	E2915	T2913	Q2858	L2791	F2735
P4084	L3888	E3686	G3581	GLY	F3358	L3232	THR	K2914	K2915	P2859	R2792	D2736
R4085	Q3889	E3687	E3582	ALA	R3368	N3234	GLN	E2916	K2916	Q2860	P2793	R2738
G4086	L3924	E3688	E3583	ASP	K3371	S3235	VAL	Q3009	P2860	D2861	K2794	P2739
K4090	K3940	E3689	D3585	GLN	V3245	V3236	G3123	F3010	L2862	L2863	T2796	V2740
L4091	D3941	E3691	A3586	GLY	R3248	V3236	G3124	T3011	S2863	Q2864	F2797	E2741
D4092	K3948	E3692	D3587	GLY	Q3378	M3239	G3124	N3012	E2918	E2865	S2798	T2742
F4093	K3948	P3695	I3592	ASP	L3379	V3245	Y3131	H3013	D2919	T2866	E2799	L2743
K4095	K3959	D3696	V3596	GLN	R3380	V3245	T3132	F3017	E2920	L2867	K2800	N2744
M4097	E3967	Q3700	S3599	THR	L3381	G3260	H3146	T3020	K2922	S2868	D2801	V2745
D4098	Y3968	E3736	A3601	GLY	E3376	T3264	D3154	P3021	A2923	E2869	E2802	I2746
L4100	I3969	GLY	V3602	LYS	E3377	E3265	D3154	A3022	Q2924	E2870	I2747	I2747
K4101	T3974	GLY	H3605	LYS	Q3378	M3266	T3157	G3024	A2875	L2871	R2806	K2750
D4102	Q3976	GLY	E3610	R3498	L3379	V3269	L3157	L3025	E2876	W2807	W2807	L2751
F4103	S3978	GLY	E3611	R3499	L3381	I3270	D3158	S3027	E2876	P2808	D2752	D2752
T4104	L3980	GLY	H3611	G3500	E3382	E3271	D3159	G3026	Q2877	L2809	S2753	S2753
G4105	R3984	ALA	P3612	D3501	E3388	T3273	V3160	K3036	L2878	K2810	F2754	F2754
P4106	L3985	GLY	F3613	D3502	E3389	P3275	Q3162	E3037	A2879	E2811	I2755	I2755
F4107	L4107	GLY	Y3613	R3503	E3390	M3276	S3163	K3045	E2880	S2812	I2756	I2756
T4108	L4108	GLY	K3614	Y3503	E3391	E3286	V3164	A3048	E2881	K2814	K2757	K2757
D4109	F4109	GLY	S3615	Q3506	L3392	R3287	S3164	A3048	E2884	A2815	F2758	F2758
F4110	E3750	GLY	K3616	Q3506	L3393	E3287	S3164	A3048	E2885	E2816	A2769	A2769
L4111	F3753	GLY	F3617	T3510	R3403	R3287	S3164	A3048	E2886	I2817	E2760	E2760
										A2818	Y2761	Y2761
										W2819	T2762	T2762
										W2820	H2763	H2763
										W2821	E2764	E2764
										T2822	K2765	K2765
										E2824	A2766	A2766
										K2825		
										A2826		











Chain E:

26%

5%

69%

MET	LEU
LYS	GLY
SER	LEU
GLU	PHE
HIS	PRO
HIS	ASN
HIS	LEU
HIS	PRO
HIS	TYR
GLY	TYR
SER	ILE
SER	ASP
MET	GLY
SER	ASP
PRO	VAL
ILE	LYS
LEU	LEU
LEU	THR
GLN	GLN
TRP	SER
LYS	MET
ILE	ALA
LYS	ILE
GLY	ILE
LEU	ARG
VAL	TYR
GLN	ILE
ALA	PRO
THR	ASP
ARG	LYS
LEU	HIS
LEU	LEU
LEU	ASN
GLY	LEU
TYR	GLY
LEU	GLY
GLU	CYS
GLU	PRO
LYS	LYS
GLU	GLU
GLU	ARG
ALA	ALA
HIS	GLU
LEU	ILE
TYR	SER
GLU	MET
ASP	LEU
GLY	GLY
ALA	ALA
ASP	VAL
LYS	LEU
TRP	ASP
ARG	ILE
ASN	ARG
LYS	TYR
LYS	GLY
PHE	VAL
ALA	SER



[illegible]

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	51504	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 ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.346	Depositor
Minimum map value	-0.409	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.073	Depositor
Recommended contour level	0.387	Depositor
Map size (Å)	515.2, 515.2, 515.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.288, 1.288, 1.288	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADN, 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	A	0.32	0/35714	0.62	6/48365 (0.0%)
1	B	0.32	0/35714	0.62	6/48365 (0.0%)
1	C	0.32	0/35714	0.62	6/48365 (0.0%)
1	D	0.32	0/35714	0.62	6/48365 (0.0%)
2	E	0.34	0/834	0.62	0/1123
2	F	0.34	0/834	0.62	0/1123
2	G	0.34	0/834	0.62	0/1123
2	H	0.34	0/834	0.62	0/1123
All	All	0.32	0/146192	0.62	24/197952 (0.0%)

There are no bond length outliers.

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	903	LEU	CA-CB-CG	6.63	130.54	115.30
1	B	903	LEU	CA-CB-CG	6.63	130.54	115.30
1	C	903	LEU	CA-CB-CG	6.63	130.54	115.30
1	D	903	LEU	CA-CB-CG	6.63	130.54	115.30
1	C	2790	MET	CA-CB-CG	5.77	123.11	113.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	34900	0	34530	340	0
1	B	34900	0	34530	336	0
1	C	34900	0	34530	349	0
1	D	34900	0	34530	336	0
2	E	818	0	824	8	0
2	F	818	0	824	8	0
2	G	818	0	824	8	0
2	H	818	0	824	8	0
3	A	19	0	13	0	0
3	B	19	0	13	0	0
3	C	19	0	13	0	0
3	D	19	0	13	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
All	All	142952	0	141468	1384	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 1384 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3335:MET:SD	1:A:3403:ARG:NH1	2.64	0.70
1:B:3335:MET:SD	1:B:3403:ARG:NH1	2.64	0.69
1:D:3335:MET:SD	1:D:3403:ARG:NH1	2.65	0.68
1:C:3335:MET:SD	1:C:3403:ARG:NH1	2.65	0.68
1:B:3889:GLN:HG3	1:B:3967:GLU:HG3	1.78	0.65

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	
1	A	4353/5037 (86%)	4168 (96%)	182 (4%)	3 (0%)	48	78
1	B	4353/5037 (86%)	4168 (96%)	182 (4%)	3 (0%)	48	78
1	C	4353/5037 (86%)	4167 (96%)	183 (4%)	3 (0%)	48	78
1	D	4353/5037 (86%)	4167 (96%)	183 (4%)	3 (0%)	48	78
2	E	105/350 (30%)	98 (93%)	7 (7%)	0	100	100
2	F	105/350 (30%)	98 (93%)	7 (7%)	0	100	100
2	G	105/350 (30%)	98 (93%)	7 (7%)	0	100	100
2	H	105/350 (30%)	98 (93%)	7 (7%)	0	100	100
All	All	17832/21548 (83%)	17062 (96%)	758 (4%)	12 (0%)	50	78

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3616	LYS
1	A	4712	PRO
1	B	3616	LYS
1	B	4712	PRO
1	C	3616	LYS

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	3806/4276 (89%)	3697 (97%)	109 (3%)	37	61
1	B	3806/4276 (89%)	3697 (97%)	109 (3%)	37	61
1	C	3806/4276 (89%)	3697 (97%)	109 (3%)	37	61
1	D	3806/4276 (89%)	3697 (97%)	109 (3%)	37	61
2	E	88/304 (29%)	87 (99%)	1 (1%)	70	81
2	F	88/304 (29%)	87 (99%)	1 (1%)	70	81
2	G	88/304 (29%)	87 (99%)	1 (1%)	70	81
2	H	88/304 (29%)	87 (99%)	1 (1%)	70	81

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	15576/18320 (85%)	15136 (97%)	440 (3%)	41 62

5 of 440 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	2369[A]	ARG
1	C	4743	MET
2	G	25	HIS
1	D	4813	LEU
1	C	3053	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 64 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	3419	ASN
1	D	3895	HIS
1	B	3052	HIS
1	B	2971	GLN
1	D	4201	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\# Z  > 2$
3	ADN	D	5101	-	17,21,21	0.72	0	17,31,31	0.80	1 (5%)
3	ADN	A	5101	-	17,21,21	0.72	0	17,31,31	0.79	1 (5%)
3	ADN	B	5101	-	17,21,21	0.72	0	17,31,31	0.79	1 (5%)
3	ADN	C	5101	-	17,21,21	0.72	0	17,31,31	0.79	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADN	D	5101	-	-	2/2/22/22	0/3/3/3
3	ADN	A	5101	-	-	2/2/22/22	0/3/3/3
3	ADN	B	5101	-	-	2/2/22/22	0/3/3/3
3	ADN	C	5101	-	-	2/2/22/22	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	5101	ADN	C5-C6-N6	2.26	123.75	120.31
3	A	5101	ADN	C5-C6-N6	2.26	123.75	120.31
3	C	5101	ADN	C5-C6-N6	2.26	123.75	120.31
3	B	5101	ADN	C5-C6-N6	2.26	123.75	120.31

There are no chirality outliers.

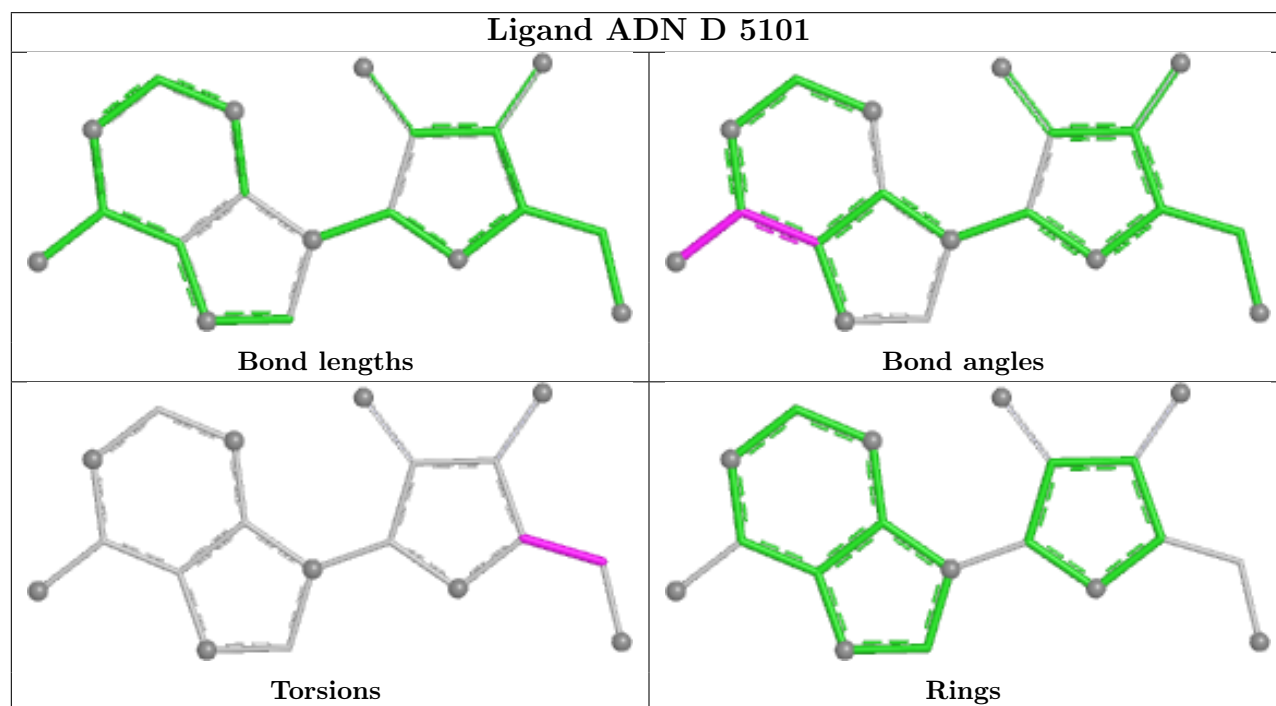
5 of 8 torsion outliers are listed below:

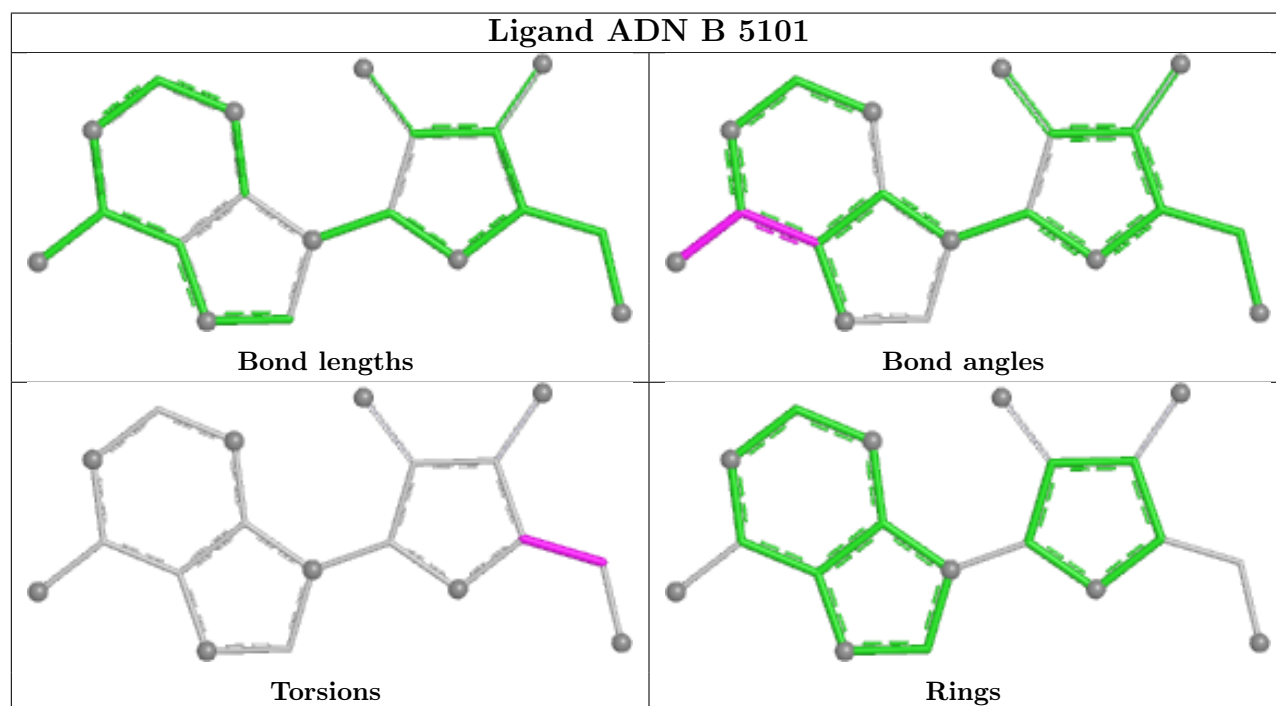
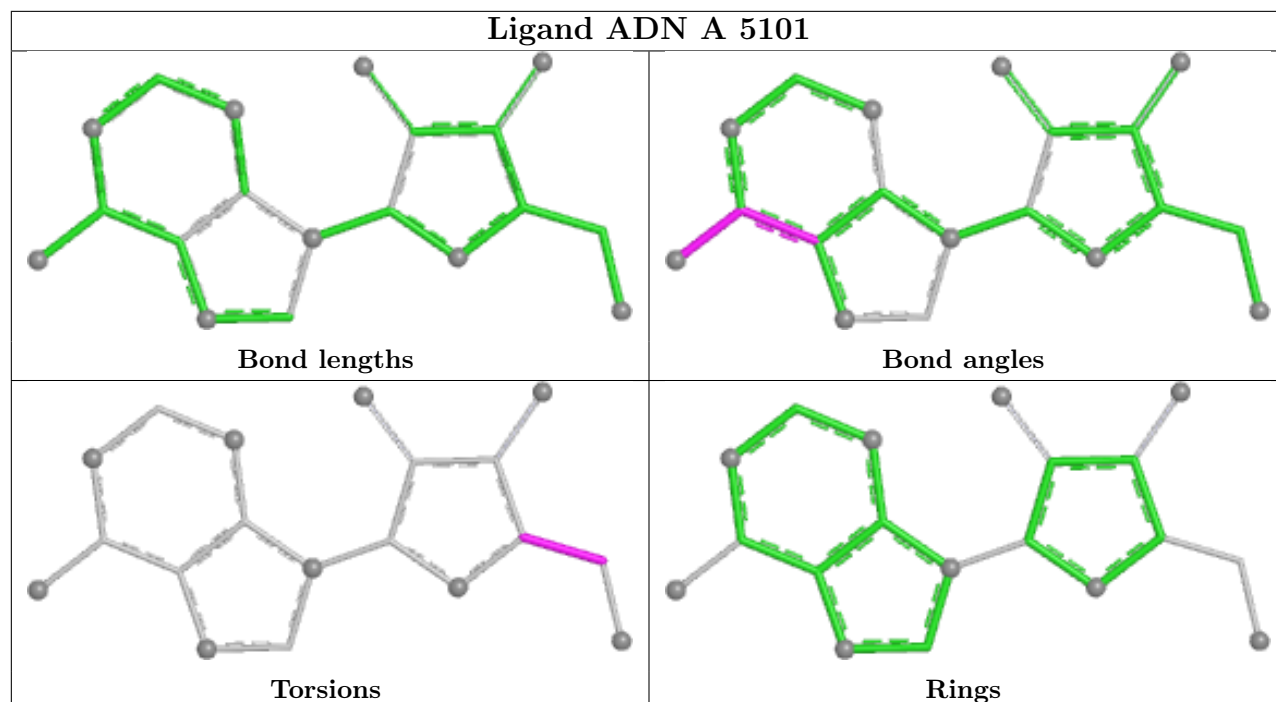
Mol	Chain	Res	Type	Atoms
3	A	5101	ADN	C3'-C4'-C5'-O5'
3	B	5101	ADN	C3'-C4'-C5'-O5'
3	C	5101	ADN	C3'-C4'-C5'-O5'
3	D	5101	ADN	C3'-C4'-C5'-O5'
3	A	5101	ADN	O4'-C4'-C5'-O5'

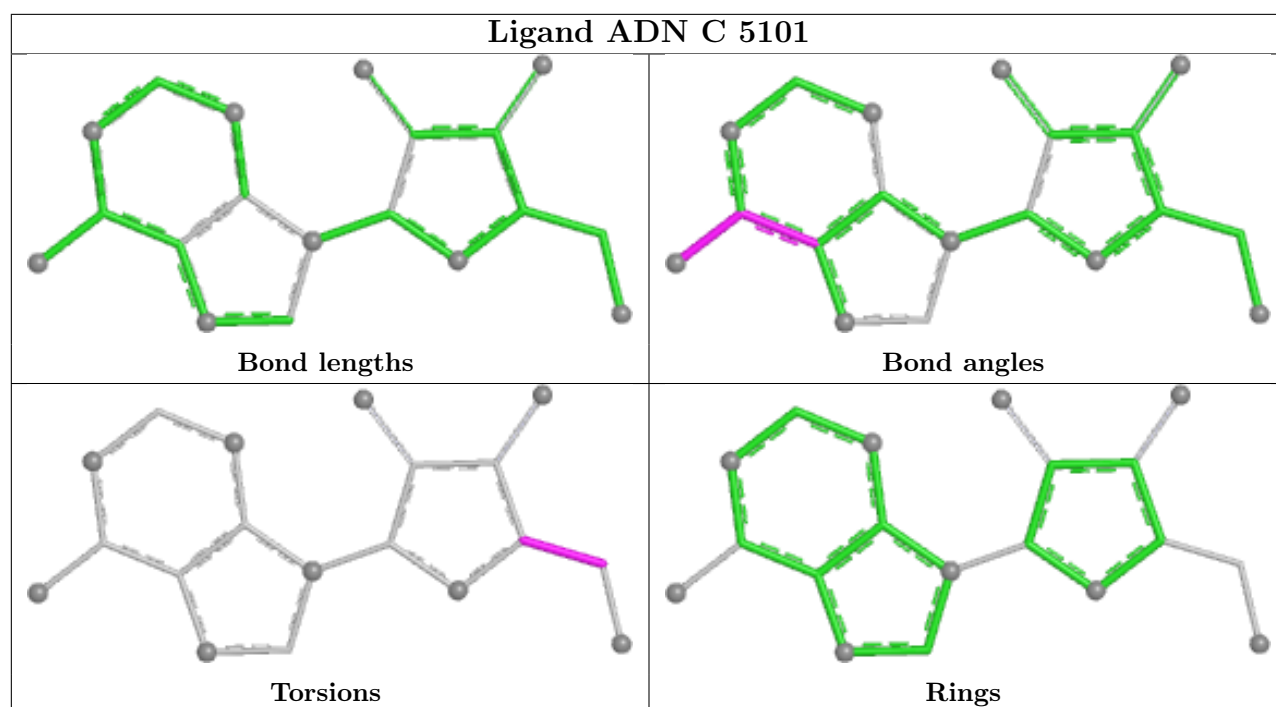
There are no ring outliers.

No monomer is involved in short contacts.

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.

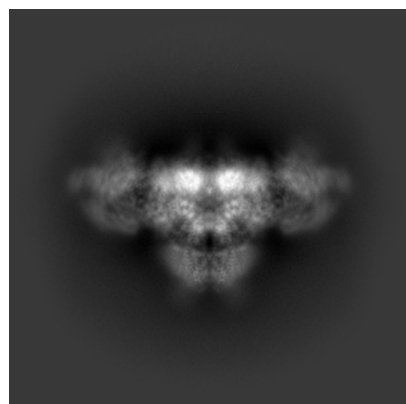
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40426. These allow visual inspection of the internal detail of the map and identification of artifacts.

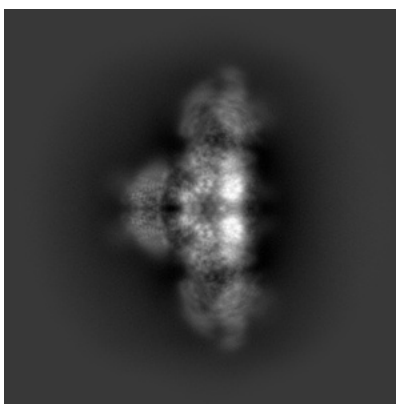
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

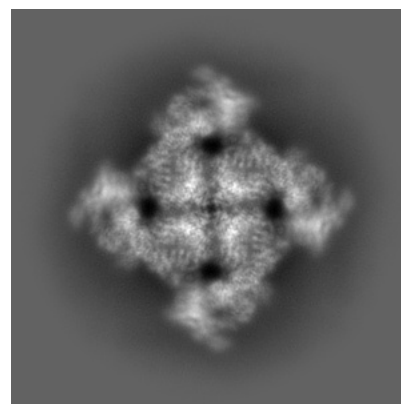
#### 6.1.1 Primary map



X

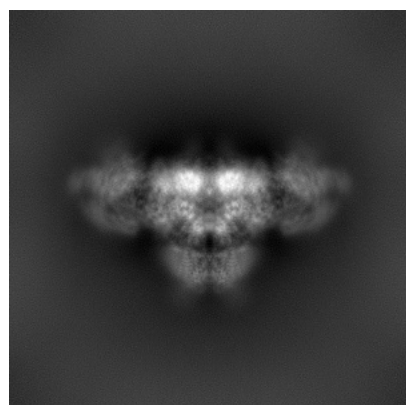


Y

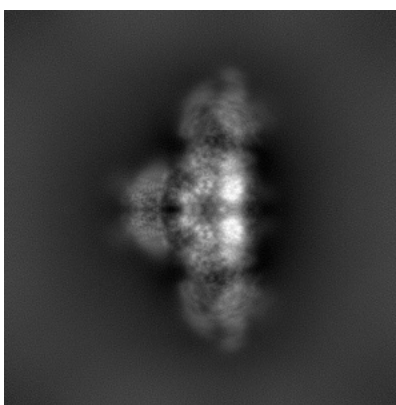


Z

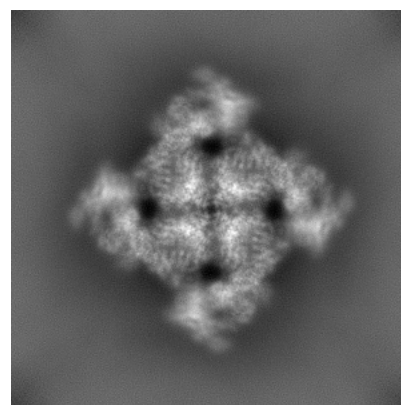
#### 6.1.2 Raw map



X



Y



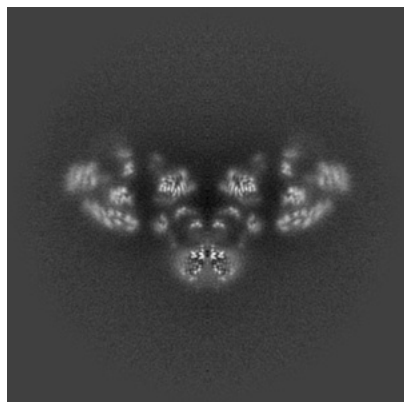
Z

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

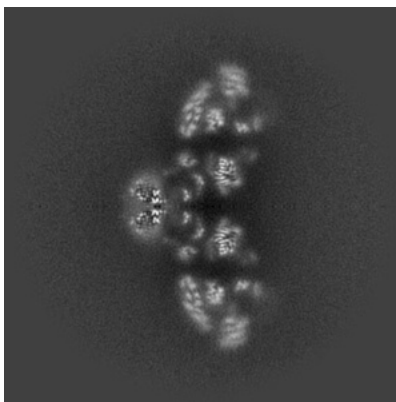


## 6.2 Central slices [i](#)

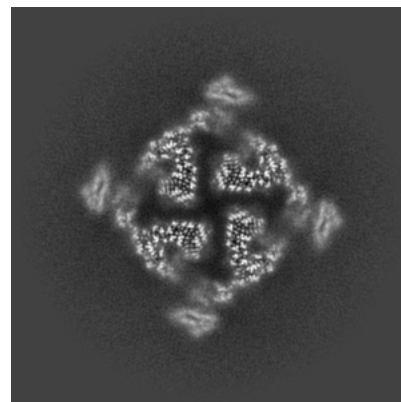
### 6.2.1 Primary map



X Index: 200

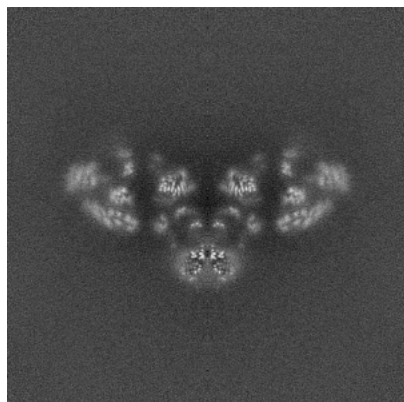


Y Index: 200

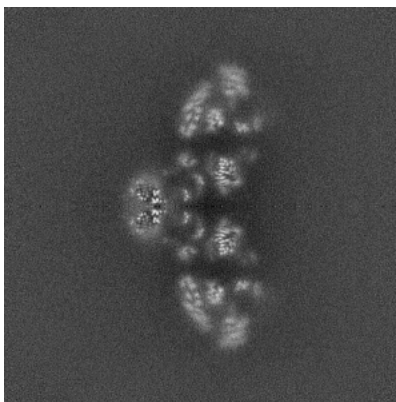


Z Index: 200

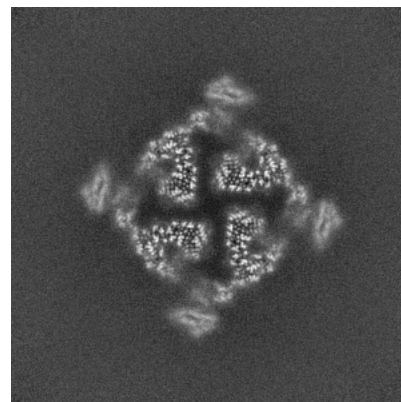
### 6.2.2 Raw map



X Index: 200



Y Index: 200

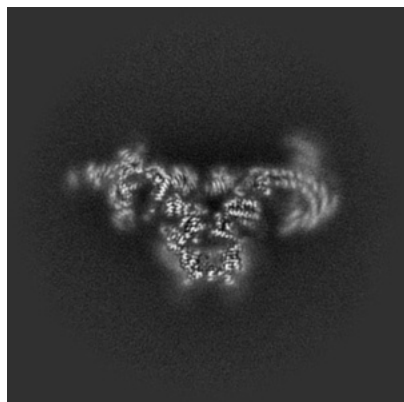


Z Index: 200

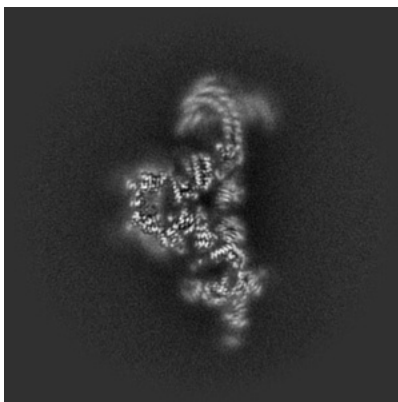
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

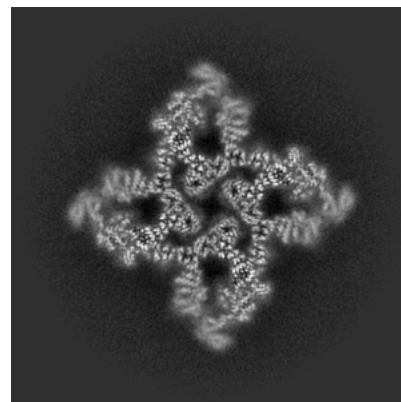
### 6.3.1 Primary map



X Index: 218

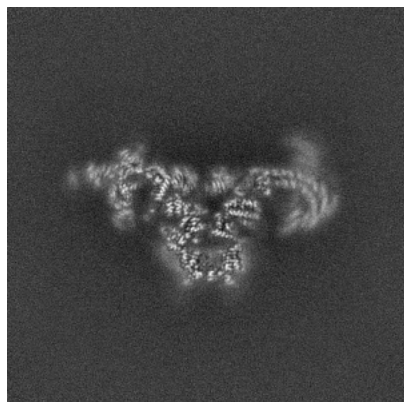


Y Index: 182

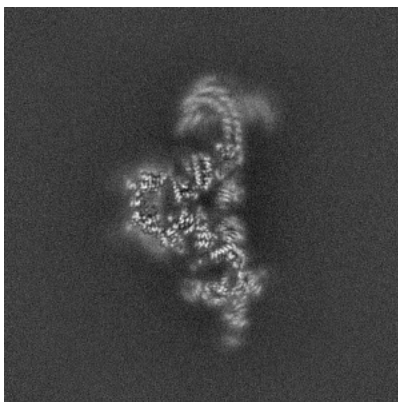


Z Index: 225

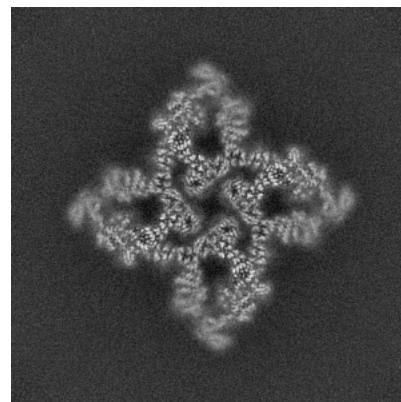
### 6.3.2 Raw map



X Index: 218



Y Index: 182

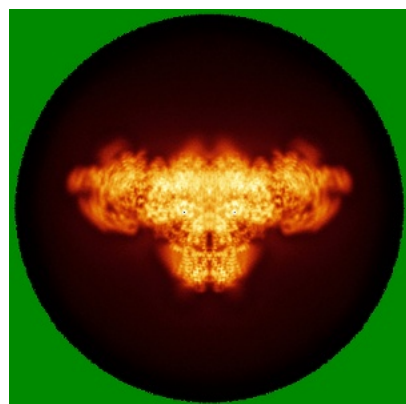


Z Index: 225

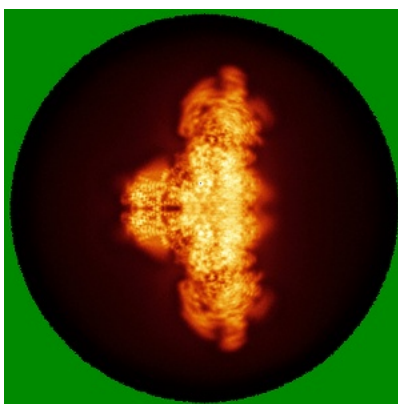
The images above show the largest variance slices of the map in three orthogonal directions.

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

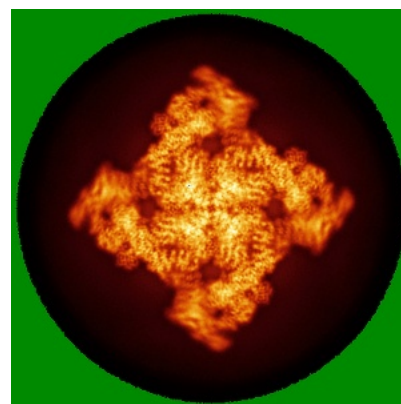
### 6.4.1 Primary map



X

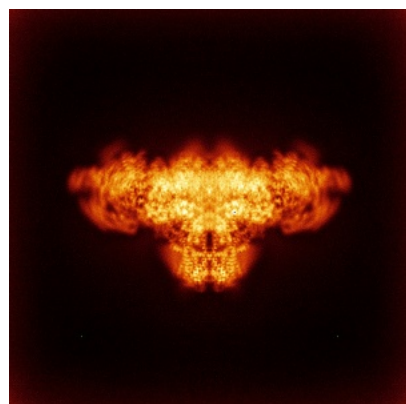


Y

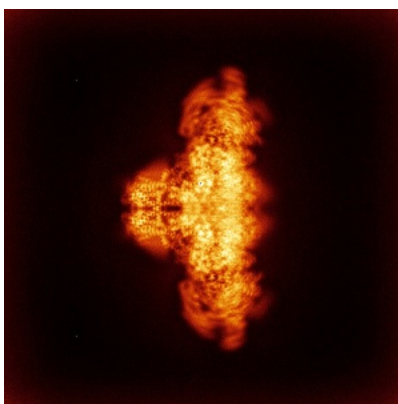


Z

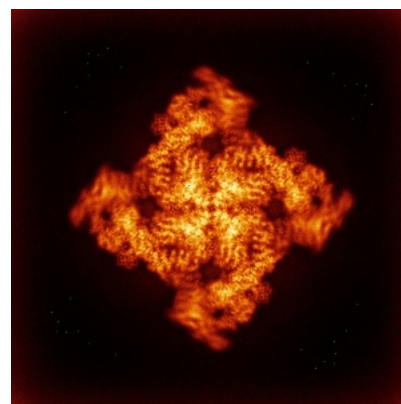
### 6.4.2 Raw map



X



Y

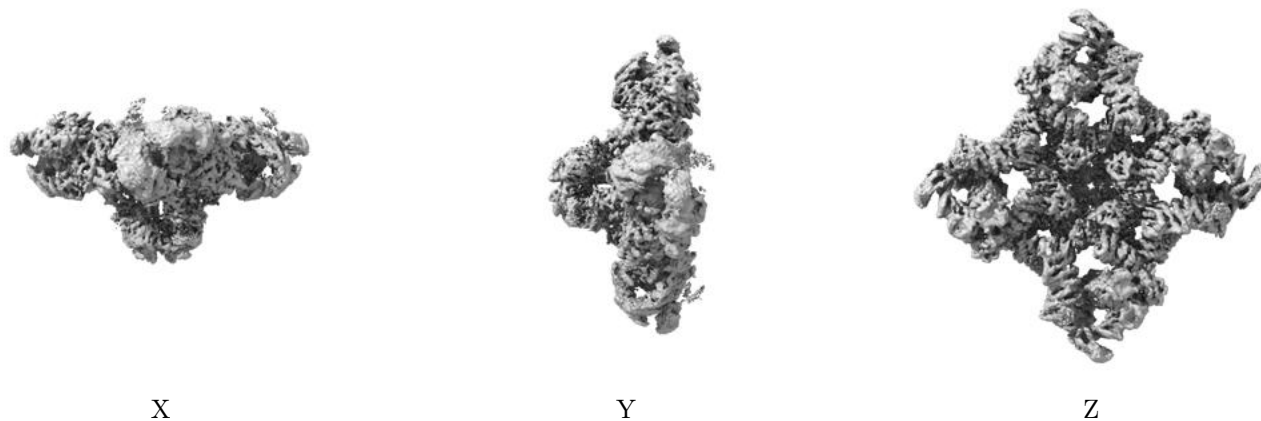


Z

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.

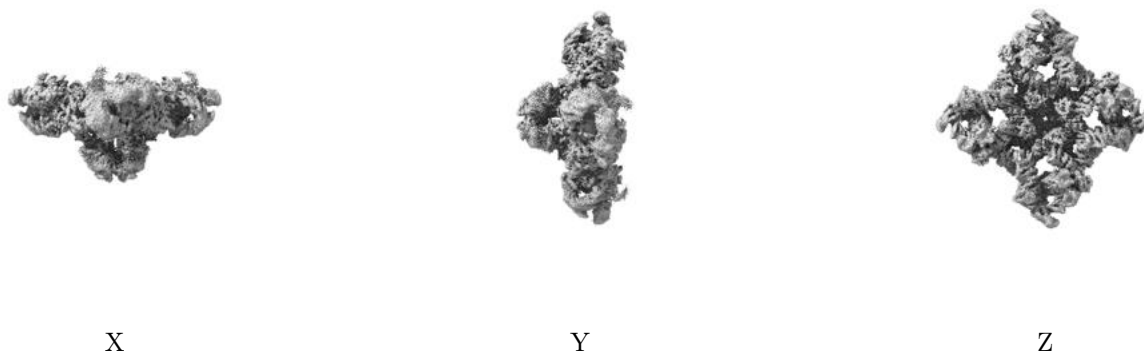
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.387. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

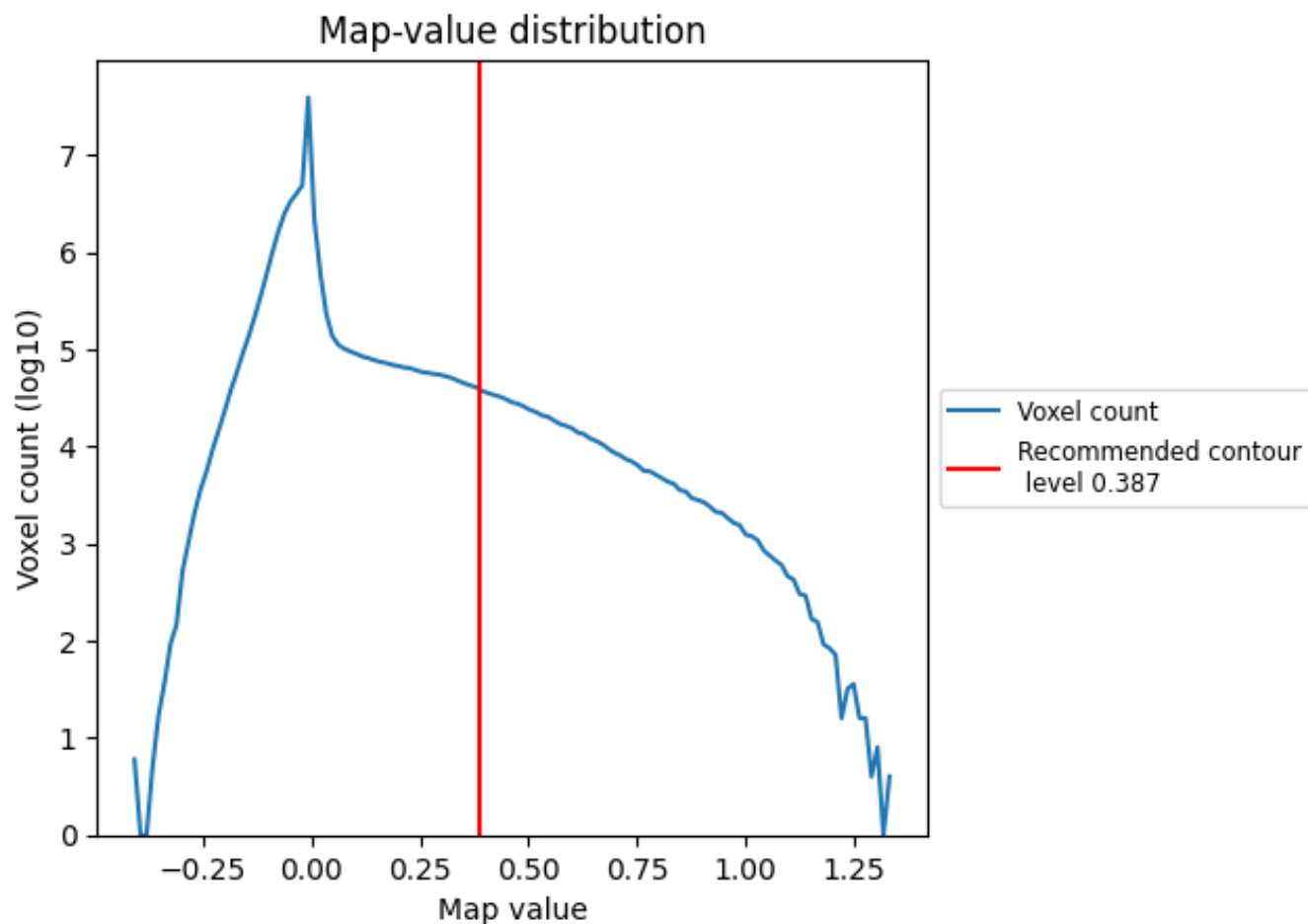
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

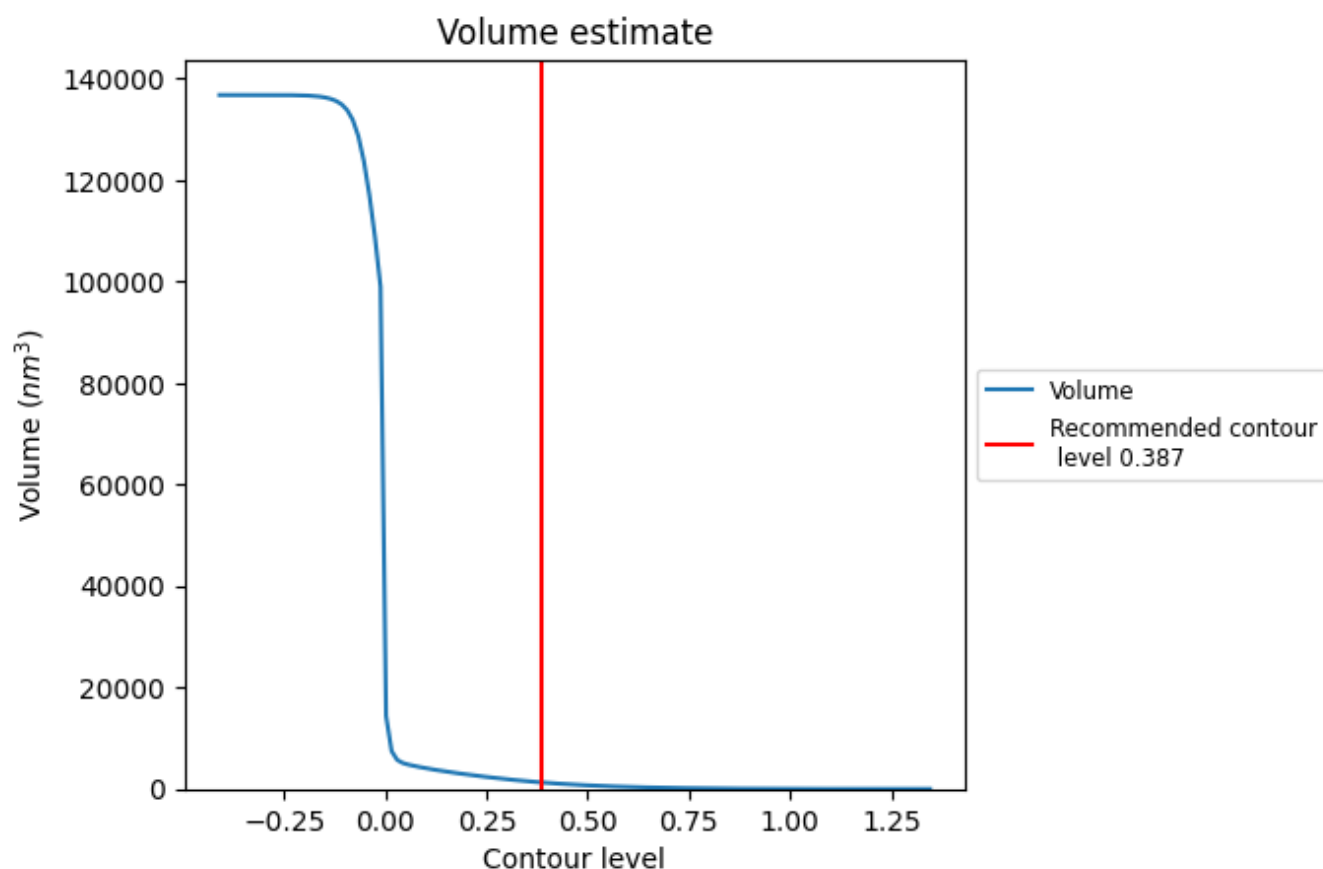
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

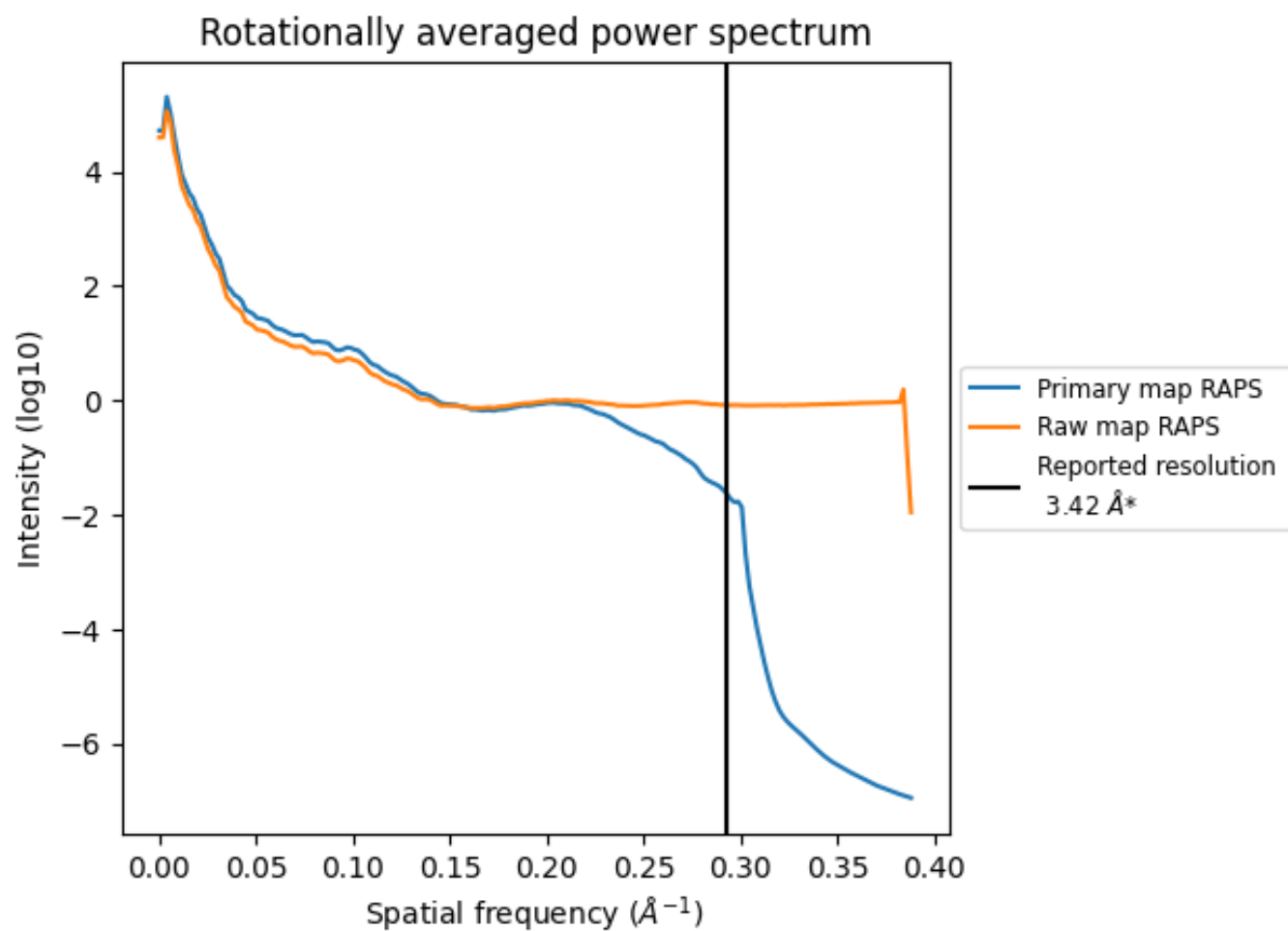
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1280  $\text{nm}^3$ ; this corresponds to an approximate mass of 1156 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 ⓘ



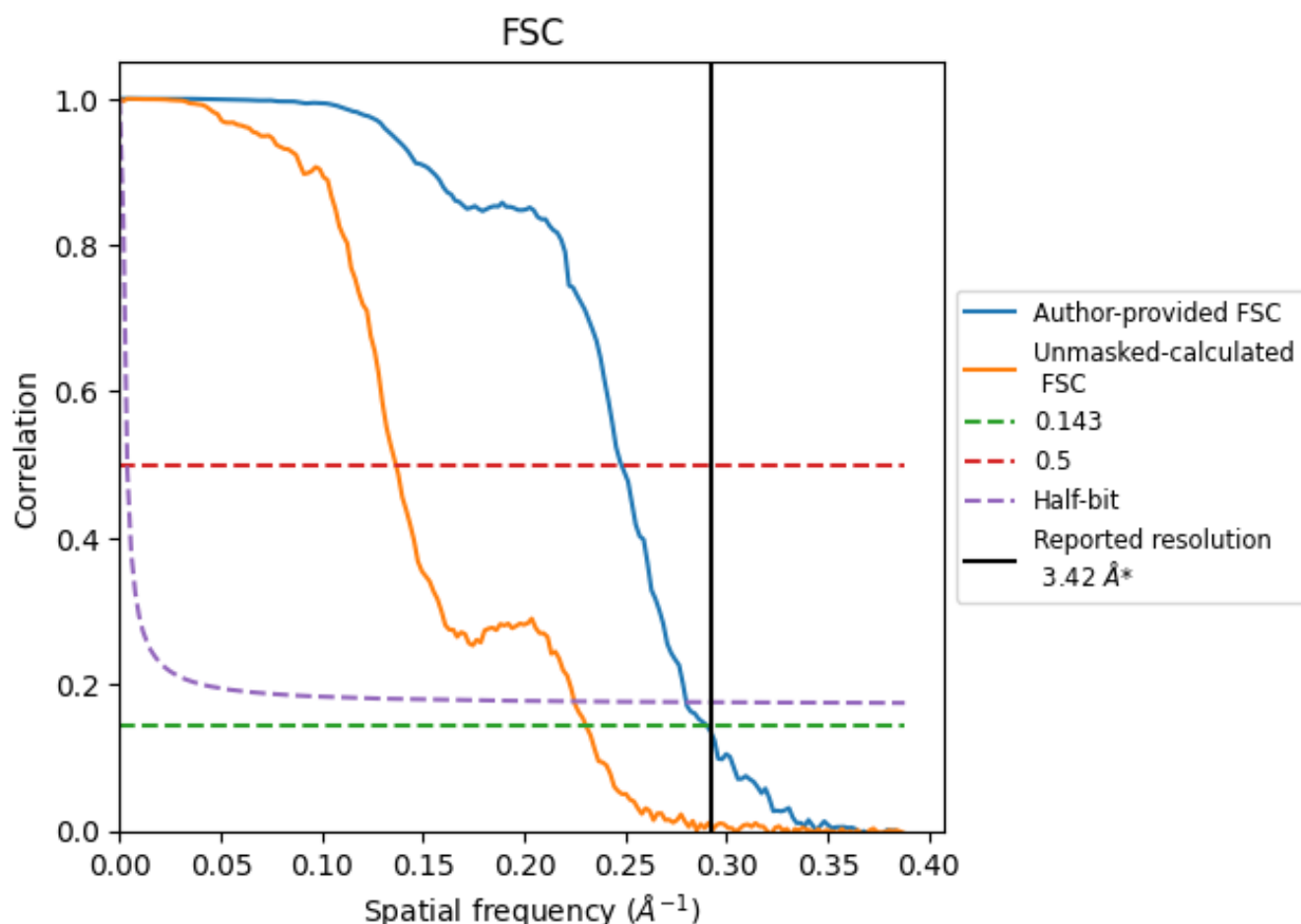
\*Reported resolution corresponds to spatial frequency of 0.292  $\text{\AA}^{-1}$



## 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 0.292  $\text{\AA}^{-1}$



## 8.2 Resolution estimates [i](#)

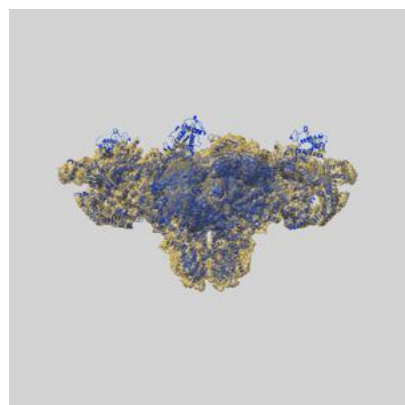
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.42	-	-
Author-provided FSC curve	3.44	4.03	3.57
Unmasked-calculated*	4.33	7.32	4.45

\*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 4.33 differs from the reported value 3.42 by more than 10 %

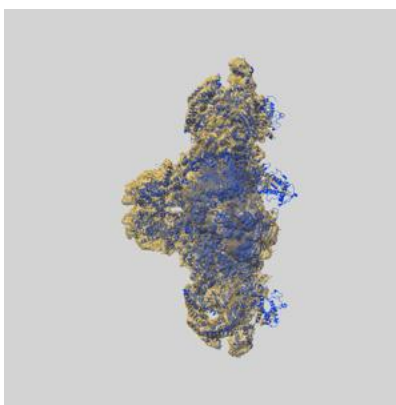
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-40426 and PDB model 8SER. Per-residue inclusion information can be found in section [3](#) on page [8](#).

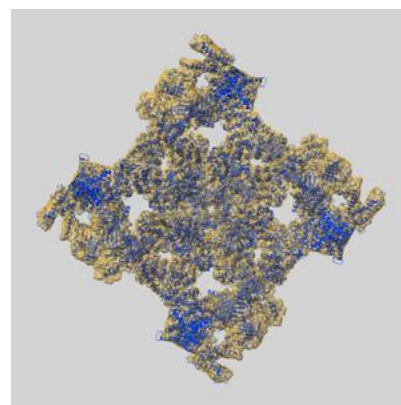
### 9.1 Map-model overlay [i](#)



X



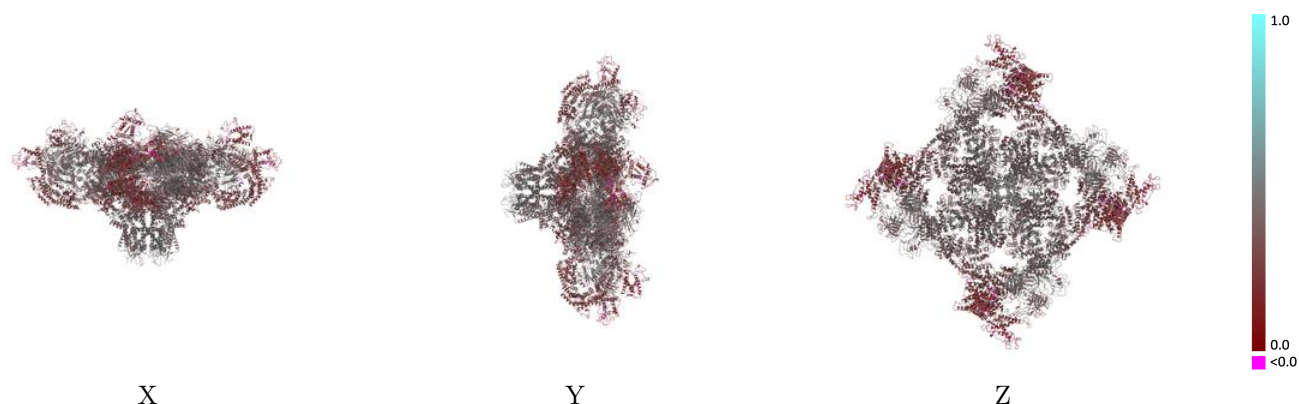
Y



Z

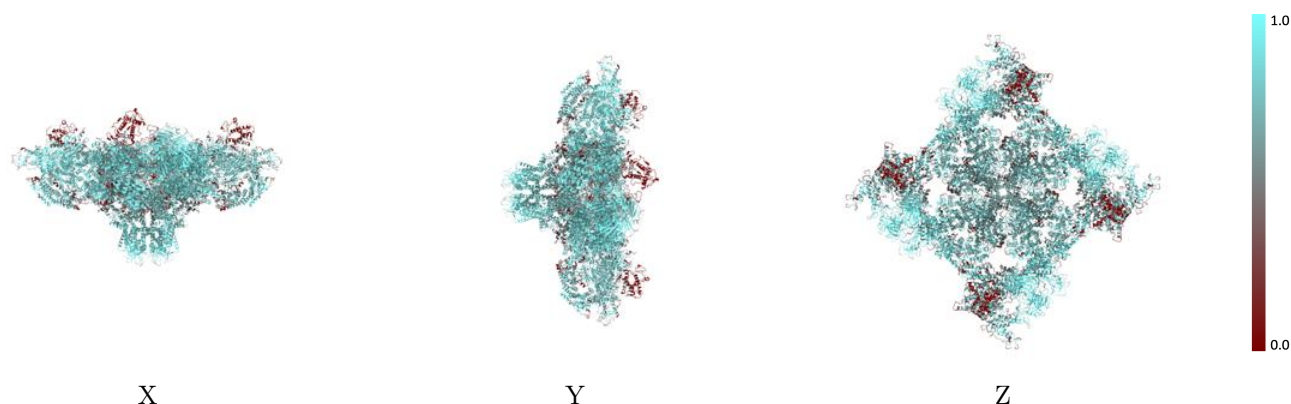
The images above show the 3D surface view of the map at the recommended contour level 0.387 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



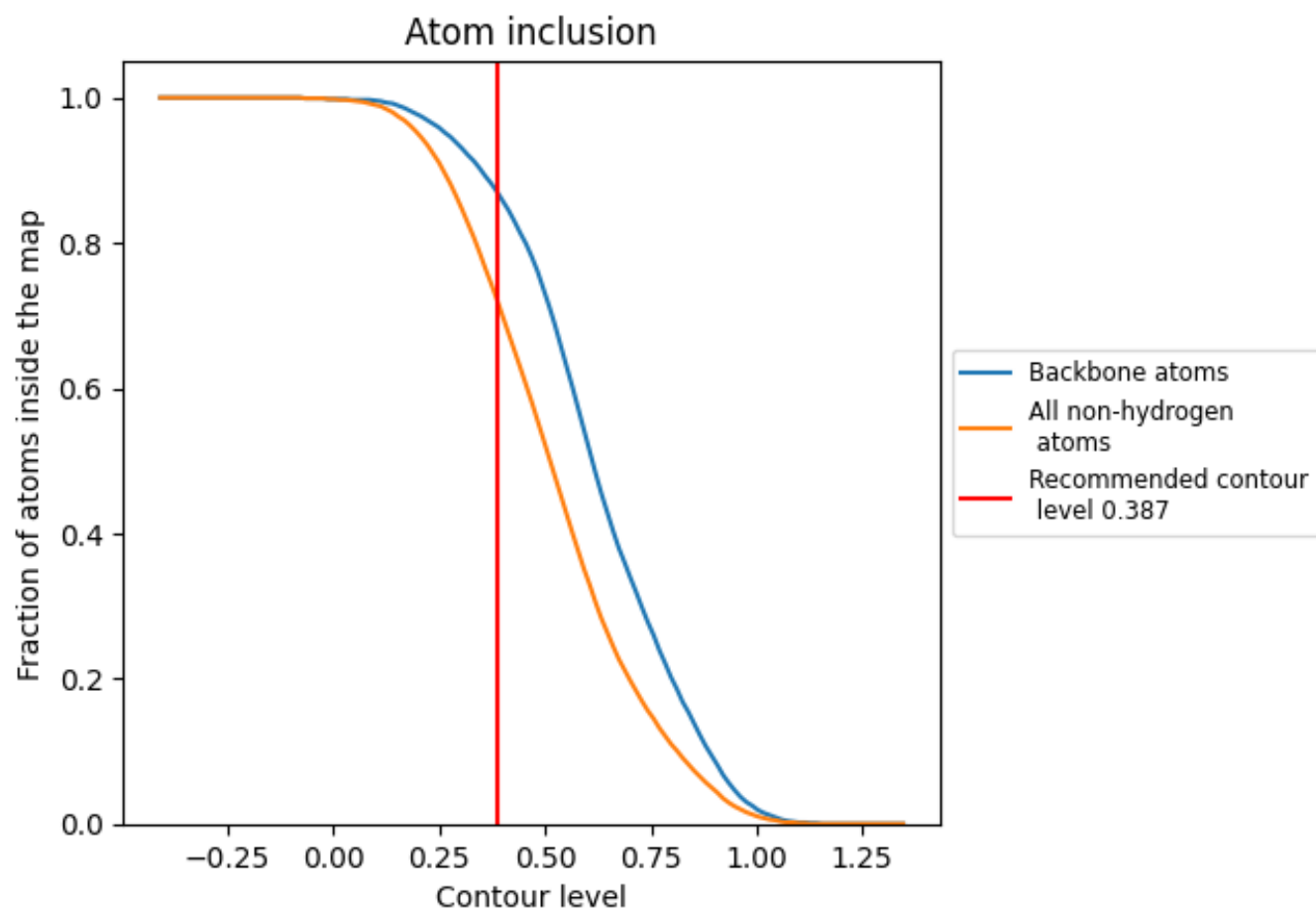
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.387).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.387) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7210	<div></div> 0.3530
A	<div></div> 0.7170	<div></div> 0.3510
B	<div></div> 0.7170	<div></div> 0.3510
C	<div></div> 0.7170	<div></div> 0.3510
D	<div></div> 0.7170	<div></div> 0.3520
E	<div></div> 0.8730	<div></div> 0.4230
F	<div></div> 0.8730	<div></div> 0.4230
G	<div></div> 0.8730	<div></div> 0.4240
H	<div></div> 0.8730	<div></div> 0.4250

1.0

0.0

<0.0