



## wwPDB EM Validation Summary Report ⓘ

Nov 4, 2024 – 08:51 PM EST

PDB ID : 8SEO  
EMDB ID : EMD-40423  
Title : Cryo-EM Structure of RyR1 + ATP-gamma-S  
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 : 3.92 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

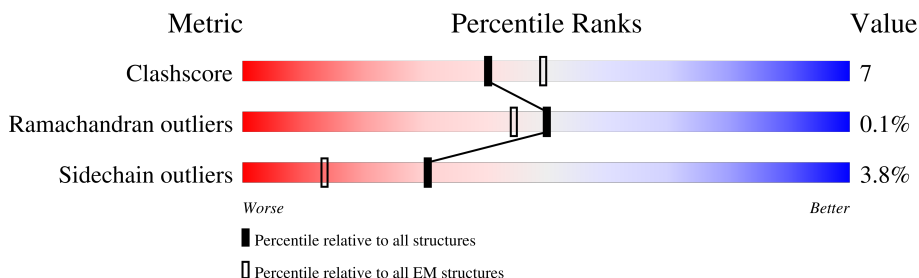
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.92 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>13%</div> <div>69%</div> <div>18%</div> <div>•</div> <div>13%</div> </div>
1	B	5037	<div> <div>13%</div> <div>69%</div> <div>18%</div> <div>•</div> <div>13%</div> </div>
1	C	5037	<div> <div>13%</div> <div>68%</div> <div>18%</div> <div>•</div> <div>13%</div> </div>
1	D	5037	<div> <div>13%</div> <div>69%</div> <div>18%</div> <div>•</div> <div>13%</div> </div>
2	E	350	<div> <div>28%</div> <div>•</div> <div>69%</div> </div>
2	F	350	<div> <div>27%</div> <div>•</div> <div>69%</div> </div>
2	G	350	<div> <div>27%</div> <div>•</div> <div>69%</div> </div>
2	H	350	<div> <div>27%</div> <div>•</div> <div>69%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 143016 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
			34904	22206	6023	6439	236		
1	B	4376	Total	C	N	O	S	9	0
			34904	22206	6023	6439	236		
1	C	4376	Total	C	N	O	S	9	0
			34904	22206	6023	6439	236		
1	D	4376	Total	C	N	O	S	9	0
			34904	22206	6023	6439	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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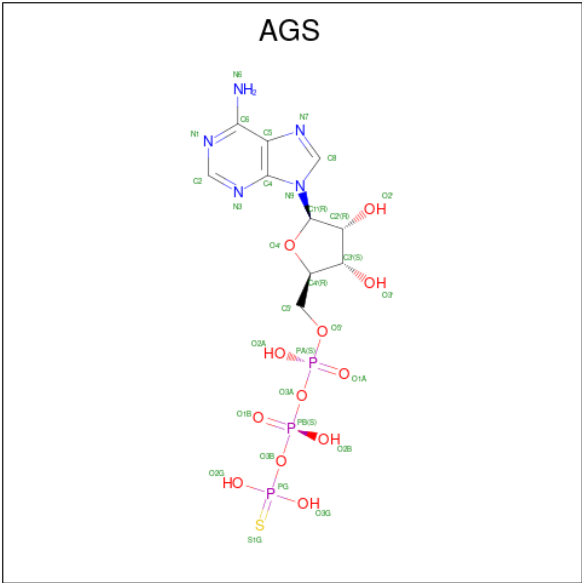
Chain	Residue	Modelled	Actual	Comment	Reference
G	-242	MET	-	expression tag	UNP P08515
G	-241	LYS	-	expression tag	UNP P08515
G	-240	SER	-	expression tag	UNP P08515
G	-239	SER	-	expression tag	UNP P08515
G	-238	HIS	-	expression tag	UNP P08515
G	-237	HIS	-	expression tag	UNP P08515
G	-236	HIS	-	expression 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 PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
3	B	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
3	C	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
3	D	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

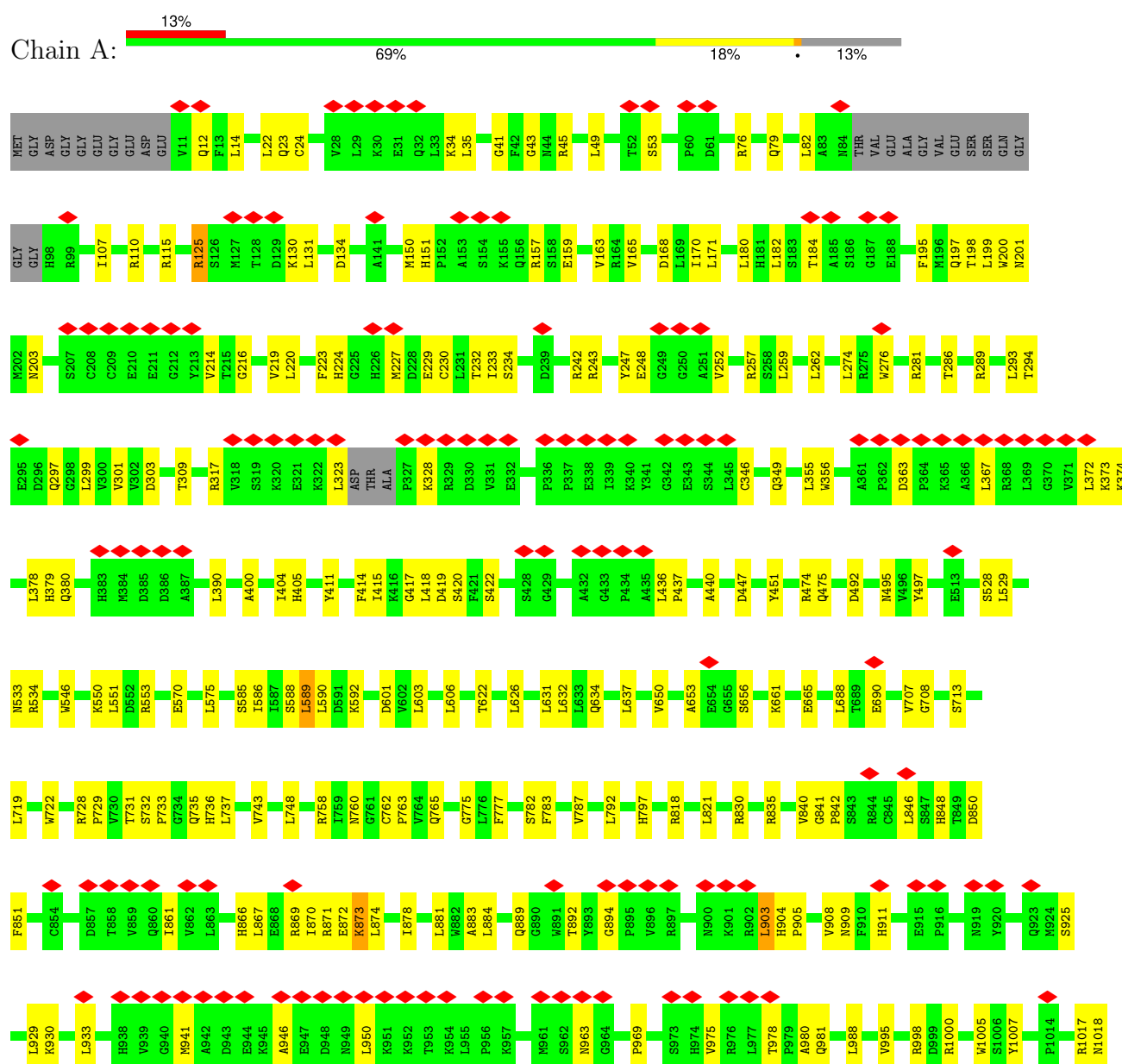
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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.

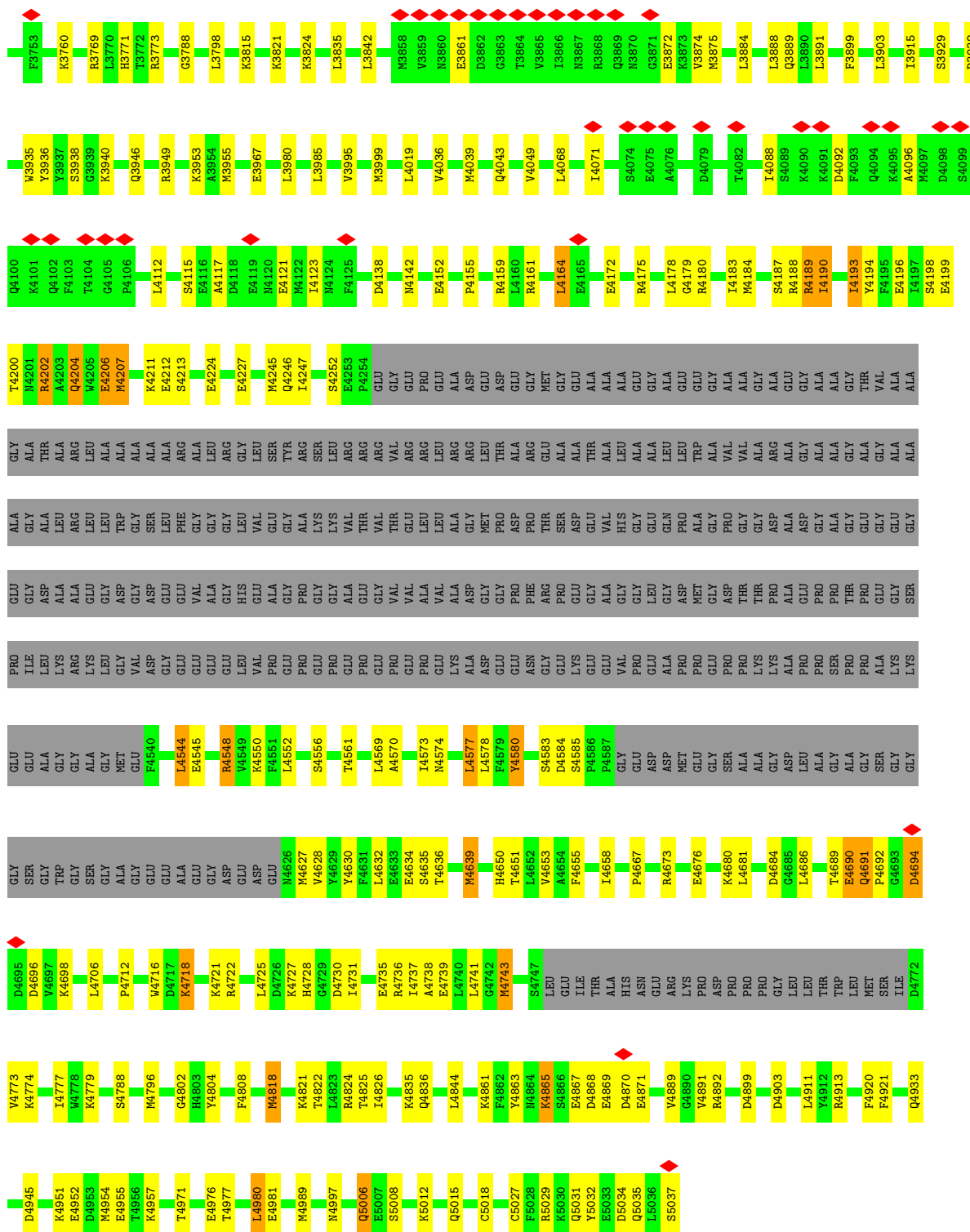
#### • Molecule 1: Ryanodine receptor 1



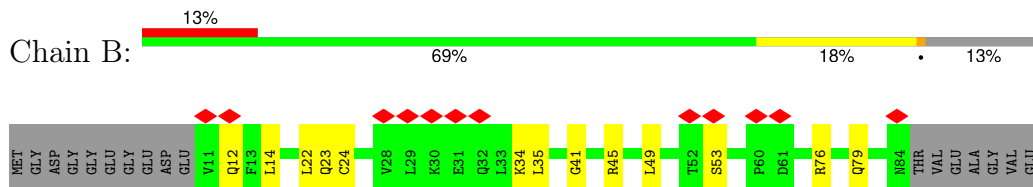


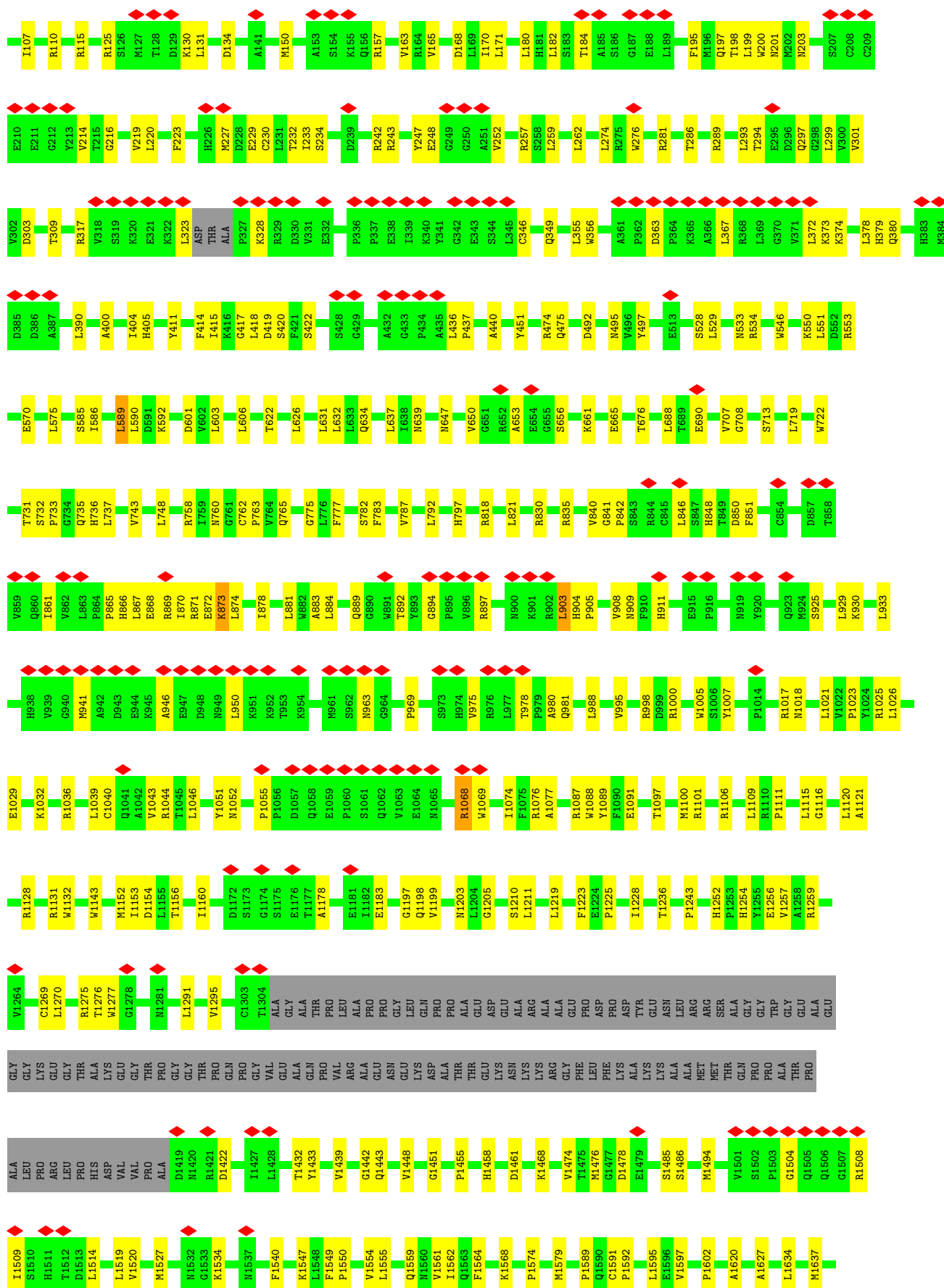
E2413	L2290	PRO	N2007	H1760	P1602	M1494	ALA	E1951	P1111	L1021
N2414	L2296	ALA	R2013	T1769	E1616	V1501	MET	H1282	G1115	L1022
R2415	E2296	GLU	D2014	T1769	E1616	S1502	THR	P1253	L1116	P1023
V2416	E2015	GLU	R1772	P1773	A1620	P1503	GLN	E1254	L1120	Y1024
G2419	V2299	GLU	P1773	P1773	A1627	G1504	PRO	Y1255	L1121	R1025
L2430	L2307	GLU	H1776	H1776	A1628	Q1505	PRO	V1257	L1026	L1027
D2431	Q2308	GLU	A1788	A1788	Q1629	G1506	ALA	R1258	L1027	D1028
R2435	L2313	LYS	G1789	G1789	V1637	Q1507	THR	R1259	E1029	E1029
C2436	L2314	ASP	A1789	A1789	M1637	G1507	ALA	R1264	R1131	K1032
A2437	L2314	ALA	G1790	G1790	P1642	R1508	LEU	W1132	W1143	R1036
L2443	A2315	GLU	V1791	V1791	I1650	I1509	PRO	W1132	W1143	L1039
R2454	D2320	LYS	A1792	A1792	I1653	H1511	THR	R1275	M1152	C1040
L2457	I2321	GLU	E1793	E1793	L1653	T1512	ALA	T1276	I1153	L1043
R2458	R2336	GLU	L1798	L1798	R1656	D1513	VAL	G1278	L1156	R1044
S2459	L2039	GLU	R1808	R1808	Q1660	L1519	THR	N1281	I1160	T1045
L2460	I2044	ALA	D1828	D1828	H1665	V1520	PRO	L1291	I1172	Y1051
D2464	Q2045	GLY	P1829	P1829	L1676	M1527	GLY	L1291	D1172	N1052
L2465	L2046	GLU	V1830	V1830	L1681	K1534	THR	V1295	G1174	P1055
L2466	GLU	GLU	Q1837	Q1837	V1681	N1537	GLY	L1291	S1175	D1057
V2467	GLU	ASP	L1842	L1842	L1685	F1540	PRO	C1303	T1177	Q1058
G2468	PRO	E1944	S1846	S1846	L1694	F1540	GLN	T1304	A1178	P1059
L2469	GLU	E1956	M1851	M1851	L1715	K1547	ALA	ALA	E1181	P1060
I2470	GLU	K1968	G1852	G1852	E1721	F1549	GLM	THR	I1182	S1061
R2471	THR	Y1973	F1854	F1854	R1725	P1550	PRO	PRO	E1183	Q1062
L2472	LEU	Q1973	D1858	D1858	S1726	V1554	ALA	ALA	G1197	V1063
P2473	SER	L1980	V1870	V1870	R1727	L1555	ASN	GLY	V1199	E1064
P2477	SER	A1983	E1874	E1874	L1731	Q1559	GLU	LEU	N1203	N1065
T2478	ARG	F1984	GLU	GLU	L1738	M1560	GLN	GLN	L1204	R1068
L2479	ARG	T1985	GLU	GLU	E1741	V1561	ASP	PRO	G1205	W1069
G2481	LEU	M1986	GLU	GLU	E1742	I1562	ALA	PRO	S1210	I1074
D2482	LEU	S1987	GLU	GLU	R1743	Q1563	THR	ALA	L1211	F1075
G2483	THR	A1988	GLU	GLU	I1744	F1564	GLU	ASP	L1219	R1076
A2484	VAL	A1989	GLU	GLU	L1745	K1568	ALA	GLU	L1219	A1077
L2485	ARG	E1990	GLU	GLU	F1748	Q1569	ARG	ALA	F1223	R1087
K2499	VAL	R1993	GLU	GLU	F1748	K1570	LYS	ARG	E1224	W1088
A2500	LYS	R1994	GLU	GLU	R1752	P1574	LYS	ALA	P1225	Y1089
S2501	LYS	T1995	GLU	GLU	K1753	M1579	ARG	ALA	T1228	F1090
N2502	GLU	R1996	GLU	GLU	G1754	P1589	LYS	ALA	T1236	E1091
R2508	LYS	R1999	GLU	GLU	G1755	Q1591	LYS	ALA	P1243	T1097
V2509	PRO	S2000	GLU	GLU	N1756	P1592	ALA	TYR	P1249	R1101
G2511	GLU	Q2003	ASP	ASP	A1757	L1595	LYS	ASN	P1250	R1106
L2512	GLU	Q2004	GLU	GLU	R1758	E1596	LEU	LEU		L1109
E2513	LEU	I2006	GLU	GLU	R1759	V1597	ALA	ARG		R1110
D2516										
F2517										
L2518										
L2519										





- Molecule 1: Ryanodine receptor 1



















Chain D:





E4203	Q4204	W4205	E4206	M4207	K4211	E4212	S4213	E4224	E4227	M4245	Q4246	S4213	E4224	S4252	E4253	P4254	GLU	GLY	GLU	PRO	GLU	ALA	ASP	GLU	ASP	GLU	GLY	MET	GLY	GLU	ALA	ALA	ALA	GLY	GLY	GLY	GLY	GLY	THR	VAL	ALA	ALA	ALA	ALA	ALA	THR														
S3938	G3939	K3940	E3945	Q3946	R3949	K3953	A3954	M3955	L3965	T3966	E3967	L3980	L3985	V3995	M3999	K4002	L4019	V4036	M4039	Q4043	V4049	L4068	I4071	S4074	E4075	A4076	D4079	T4082	I4088	S4089	K4090	K4091	L4092	F4093	Q4094	K4095	N4096	M4097	D4098																					
L3798	S3803	K3815	L3820	K3821	K3824	L3835	L3842	D3843	L3844	K3858	V3859	N3860	E3861	D3862	T3864	I3865	I3866	N3867	R3868	Q3869	N3870	G3871	K3872	V3874	M3875	D3878	L3884	L3888	Q3889	L3890	L3891	F3899	L3903	T3915	T3919	S3929	D3932	V3935	Y3936	Y3937																				
D3676	L3677	E3682	Q3683	E3684	E3685	E3686	E3687	E3688	E3689	V3690	E3691	E3692	L3698	H3699	Q3700	F3705	T3708	A3730	K3731	S3732	E3736	GLU	GLY	GLY	ASN	GLY	ALA	GLU	GLU	GLU	GLU	V3749	E3750	V3751	S3752	F3753	E3754	E3755	K3760	R3769	L3770	H3771	T3772	R3773	L3780	G3788														
R3582	E3583	E3584	D3585	A3586	D3587	P3589	I3592	R3595	V3596	A3601	Y3604	E3607	E3610	H3611	Y3613	K3614	S3615	K3616	K3617	A3618	V3619	W3620	H3621	K3622	L3623	S3625	K3626	Q3627	R3628	R3629	R3630	A3631	V3632	V3633	A3634	C3635	F3636	R3637	P3640	A3659	A3660	V3661	I3662	L3663	E3670	D3675														
GLU	ARG	THR	LYS	LYS	R3498	R3499	G3500	D3501	R3502	S3503	V3505	Q3506	S3508	L3509	V3511	K3515	N3523	D3531	L3532	I3533	M3534	K3537	T3538	A3541	L3542	K3543	D3544	N3555	N3556	L3557	R3558	L3559	Q3560	K3561	K3562	V3563	E3564	F3565	S3566	L3569	R3570	L3575	Y3576	R3577	P3580	G3581														
E3388	E3389	G3390	E3391	L3392	R3403	Y3409	R3414	Y3415	V3416	K3423	L3424	P3427	T3443	Y3444	V3445	F3451	E3454	N3457	F3458	V3459	V3460	Q3461	N3465	N3466	K3467	S3468	L3470	T3471	A3472	S3474	K3475	S3476	K3477	N3478	LYS	ALA	GLY	ASP	ALA	GLN	SER	GLY	SER	ASP	GLN															
T3264	E3265	T3273	W3284	G3288	P3289	P3292	P3293	P3294	A3295	L3296	P3297	A3298	Q3299	A3300	P3301	P3302	P3303	C3304	T3305	A3306	V3324	I3329	D3330	E3331	A3332	V3340	F3341	A3342	I3345	V3346	S3347	L3354	F3358	T3361	R3364	E3377	R3380	L3381	E3382	A3383	K3384	A3385	E3386	A3387																
G3058	T3059	P3062	V3065	L3075	D3076	A3077	R3078	V3080	M3081	K3082	V3088	D3102	I3103	E3104	V3107	L3110	R3111	L3112	G3113	K3114	V3115	S3116	GLN	ALA	ARG	THR	GLN	VAL	K3123	G3124	T3130	Y3131	T3132	T3133	L3136	H3146	S3032	N3033	Q3151	P3152	G3153	D3154	P3155	V3156	I3157	L3158	V3163													
I2974	L2977	E2978	A2979	V2980	V2981	S2982	S2983	G2984	R2985	V2986	E2987	K2988	S2989	P2990	H2991	E2992	K2996	F2997	F2998	I3001	L3002	L3003	P3004	A2917	L3005	I3006	N3007	L3015	S3019	A3022	K3023	V3024	L3025	G3026	S3027	G3028	A3031	S3032	N3033	K3034	E3035	K3036	E3037	A3048	R3051	H3052	R3053	L3056	F3057											
E2893	L2894	E2895	E2896	E2897	E2898	E2899	E2900	T2901	H2902	F2903	H2904	L2905	V2906	F2907	V2908	D2909	T2910	L2911	T2912	F2917	E2913	K2914	E2915	K2916	A2917	R2918	R2919	R2920	E2921	K2922	E2923	Q2924	E2925	L2926	L2927	K2928	S3027	F2929	L2930	Q2931	E2932	N2933	G2934	V2935	A2936	V2937	T2938	R2939	GLY	LEU	LYS	ASP	MET	GLU	L2946	D2947	T2948	S2949	E2950	D2971





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55892	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	1.268	Depositor
Minimum map value	-0.637	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.064	Depositor
Recommended contour level	0.287	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: ZN, AGS

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	1/35721 (0.0%)	0.65	11/48375 (0.0%)
1	B	0.32	1/35721 (0.0%)	0.65	10/48375 (0.0%)
1	C	0.32	1/35721 (0.0%)	0.65	10/48375 (0.0%)
1	D	0.32	1/35721 (0.0%)	0.65	10/48375 (0.0%)
2	E	0.32	0/834	0.64	0/1123
2	F	0.32	0/834	0.64	0/1123
2	G	0.32	0/834	0.64	0/1123
2	H	0.32	0/834	0.64	0/1123
All	All	0.32	4/146220 (0.0%)	0.65	41/197992 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	904	HIS	C-N	5.54	1.44	1.34
1	B	904	HIS	C-N	5.54	1.44	1.34
1	C	904	HIS	C-N	5.54	1.44	1.34
1	D	904	HIS	C-N	5.54	1.44	1.34

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	903	LEU	CA-CB-CG	6.24	129.64	115.30
1	C	903	LEU	CA-CB-CG	6.24	129.64	115.30
1	D	903	LEU	CA-CB-CG	6.24	129.64	115.30
1	A	903	LEU	CA-CB-CG	6.20	129.56	115.30
1	B	4945	ASP	CB-CG-OD1	6.03	123.73	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	841	GLY	Mainchain
1	B	841	GLY	Mainchain
1	C	841	GLY	Mainchain
1	D	841	GLY	Mainchain

## 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	34904	0	34524	484	0
1	B	34904	0	34524	480	0
1	C	34904	0	34524	489	0
1	D	34904	0	34524	483	0
2	E	818	0	824	5	0
2	F	818	0	824	7	0
2	G	818	0	824	10	0
2	H	818	0	824	7	0
3	A	31	0	12	0	0
3	B	31	0	12	0	0
3	C	31	0	12	0	0
3	D	31	0	12	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	143016	0	141440	1931	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 7.

The worst 5 of 1931 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:C:2283:ASN:HD22	1:C:2286:LEU:HG	1.56	0.71
1:B:2283:ASN:HD22	1:B:2286:LEU:HG	1.56	0.70
1:D:2283:ASN:HD22	1:D:2286:LEU:HG	1.56	0.70
1:B:1561:VAL:HG12	1:B:1562:ILE:HG13	1.74	0.69
1:C:317:ARG:NH2	1:C:349:GLN:OE1	2.25	0.69

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%)	4217 (97%)	131 (3%)	5 (0%)	48	81
1	B	4353/5037 (86%)	4216 (97%)	132 (3%)	5 (0%)	48	81
1	C	4353/5037 (86%)	4216 (97%)	132 (3%)	5 (0%)	48	81
1	D	4353/5037 (86%)	4217 (97%)	131 (3%)	5 (0%)	48	81
2	E	105/350 (30%)	100 (95%)	5 (5%)	0	100	100
2	F	105/350 (30%)	100 (95%)	5 (5%)	0	100	100
2	G	105/350 (30%)	100 (95%)	5 (5%)	0	100	100
2	H	105/350 (30%)	100 (95%)	5 (5%)	0	100	100
All	All	17832/21548 (83%)	17266 (97%)	546 (3%)	20 (0%)	50	81

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3616	LYS
1	B	3616	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	3616	LYS
1	D	3616	LYS
1	A	4694	ASP

### 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	3805/4276 (89%)	3655 (96%)	150 (4%)	27	51
1	B	3805/4276 (89%)	3655 (96%)	150 (4%)	27	51
1	C	3805/4276 (89%)	3655 (96%)	150 (4%)	27	51
1	D	3805/4276 (89%)	3655 (96%)	150 (4%)	27	51
2	E	88/304 (29%)	88 (100%)	0	100	100
2	F	88/304 (29%)	88 (100%)	0	100	100
2	G	88/304 (29%)	88 (100%)	0	100	100
2	H	88/304 (29%)	88 (100%)	0	100	100
All	All	15572/18320 (85%)	14972 (96%)	600 (4%)	30	51

5 of 600 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	2369[A]	ARG
1	D	4871	GLU
1	D	3515	LYS
1	D	2203	MET
1	D	4635	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 82 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	4691	GLN
1	D	2283	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	5031	GLN
1	D	533	ASN
1	D	3214	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	AGS	B	5101	-	28,33,33	0.75	1 (3%)	31,52,52	1.38	5 (16%)
3	AGS	C	5101	-	28,33,33	0.75	1 (3%)	31,52,52	1.38	5 (16%)
3	AGS	A	5101	-	28,33,33	0.75	1 (3%)	31,52,52	1.38	5 (16%)
3	AGS	D	5101	-	28,33,33	0.75	1 (3%)	31,52,52	1.38	5 (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
3	AGS	B	5101	-	-	6/17/38/38	0/3/3/3
3	AGS	C	5101	-	-	6/17/38/38	0/3/3/3
3	AGS	A	5101	-	-	6/17/38/38	0/3/3/3
3	AGS	D	5101	-	-	6/17/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	5101	AGS	PG-S1G	2.09	1.95	1.90
3	B	5101	AGS	PG-S1G	2.09	1.95	1.90
3	C	5101	AGS	PG-S1G	2.09	1.95	1.90
3	D	5101	AGS	PG-S1G	2.09	1.95	1.90

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	5101	AGS	PB-O3B-PG	-3.64	119.86	133.17
3	A	5101	AGS	PB-O3B-PG	-3.64	119.86	133.17
3	B	5101	AGS	PB-O3B-PG	-3.64	119.86	133.17
3	C	5101	AGS	PB-O3B-PG	-3.64	119.86	133.17
3	C	5101	AGS	O5'-C5'-C4'	3.12	119.63	108.99

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

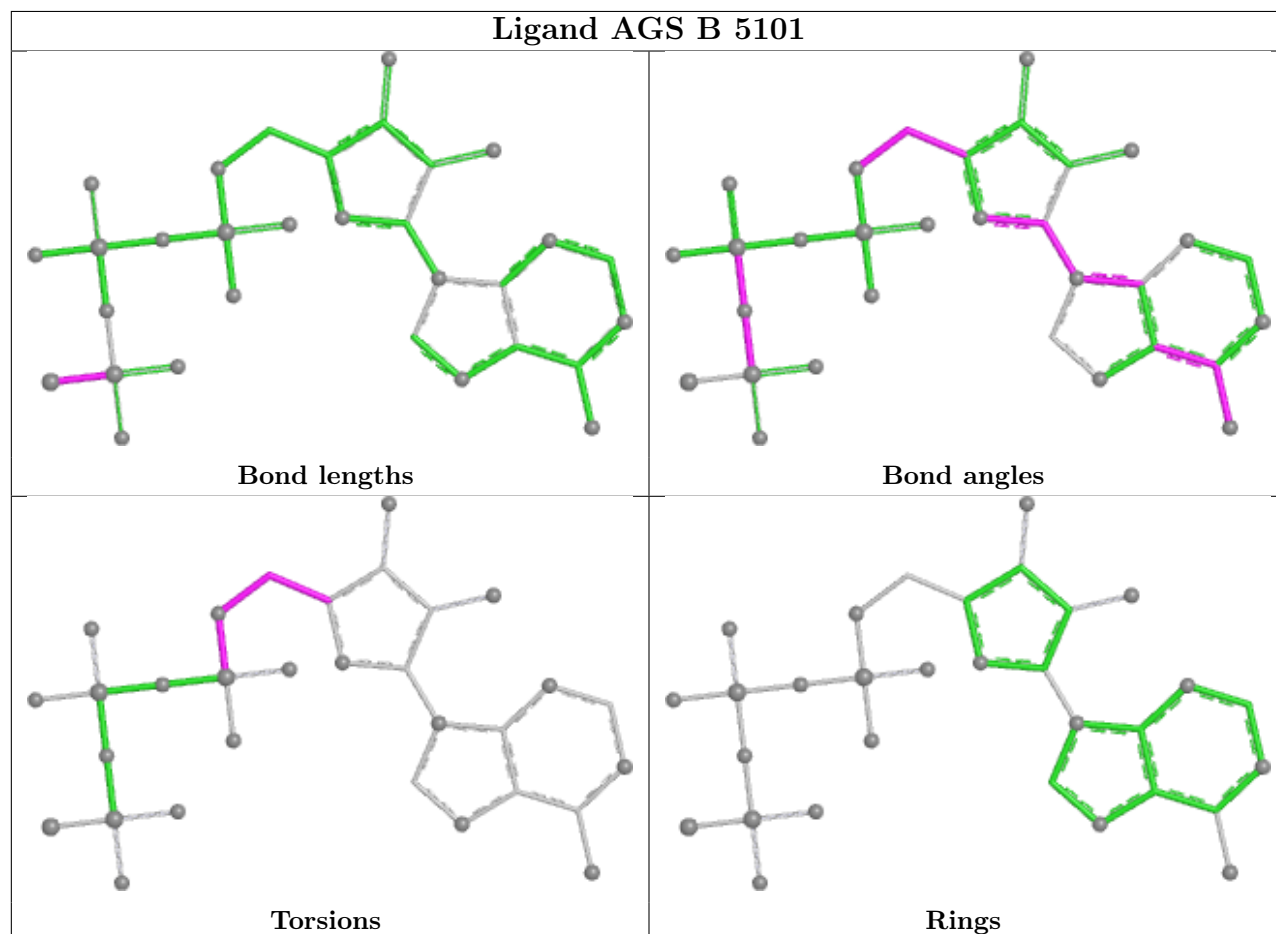
Mol	Chain	Res	Type	Atoms
3	A	5101	AGS	C5'-O5'-PA-O3A
3	A	5101	AGS	C4'-C5'-O5'-PA
3	A	5101	AGS	O4'-C4'-C5'-O5'
3	B	5101	AGS	C5'-O5'-PA-O3A
3	B	5101	AGS	C4'-C5'-O5'-PA

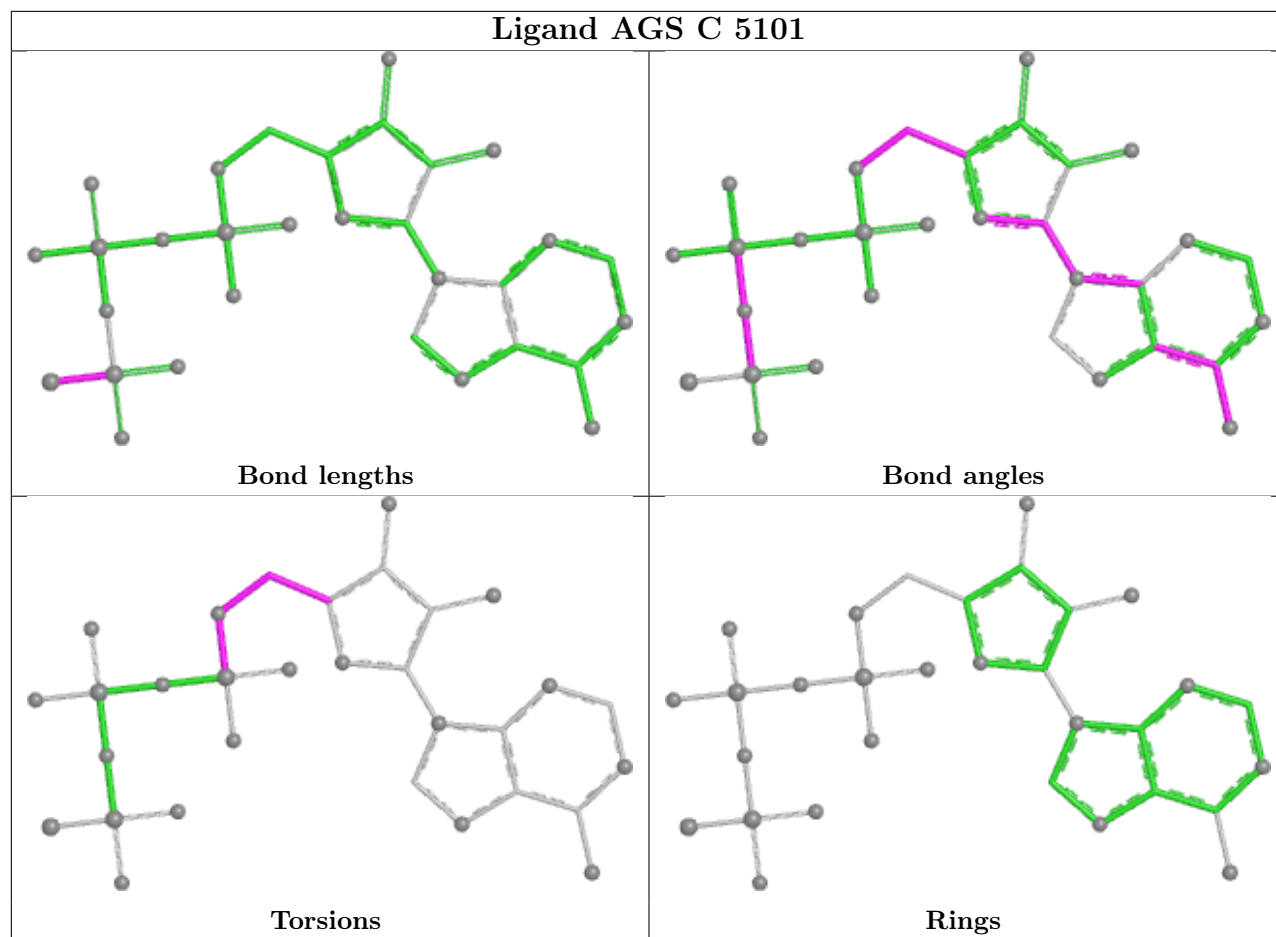
There are no ring outliers.

No monomer is involved in short contacts.

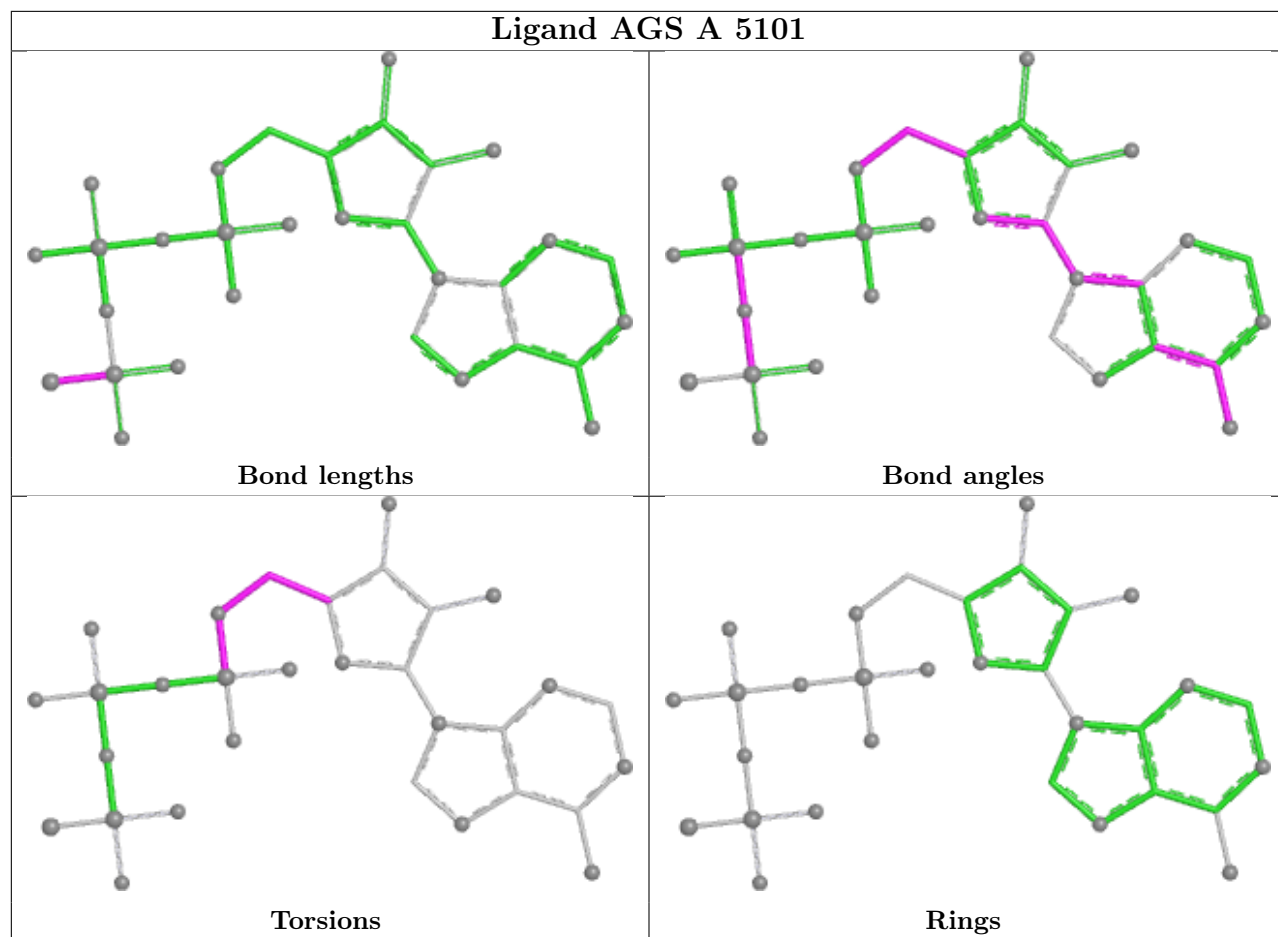
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

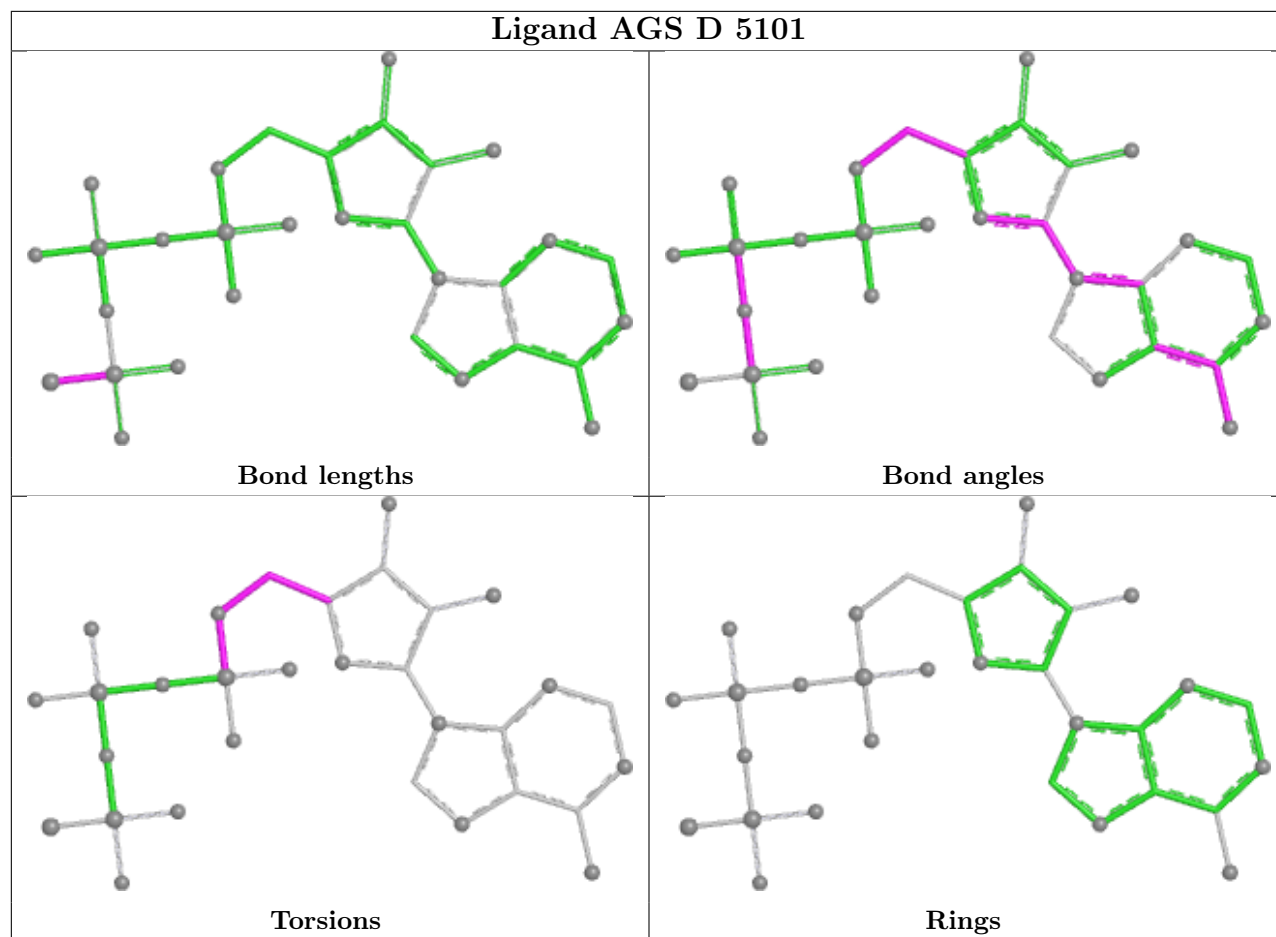
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers 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.

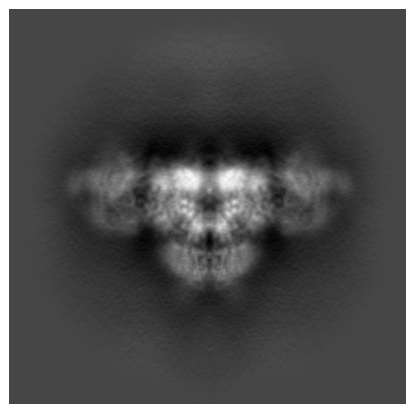
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40423. These allow visual inspection of the internal detail of the map and identification of artifacts.

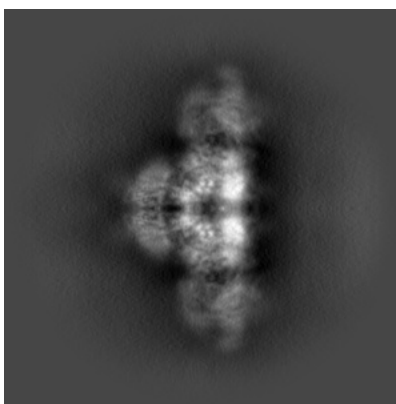
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

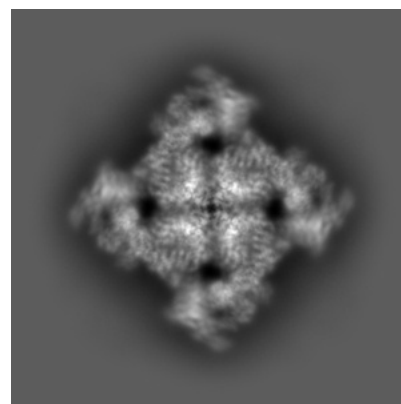
#### 6.1.1 Primary map



X

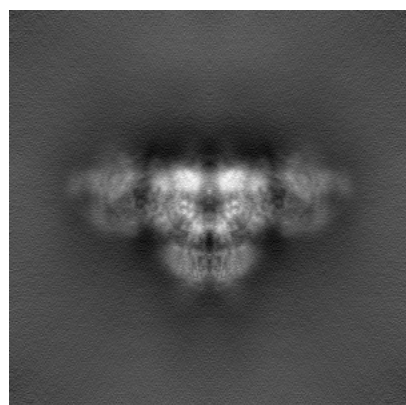


Y

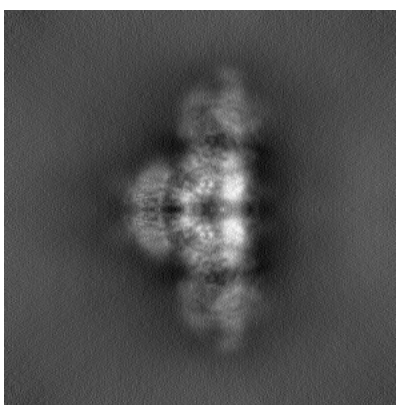


Z

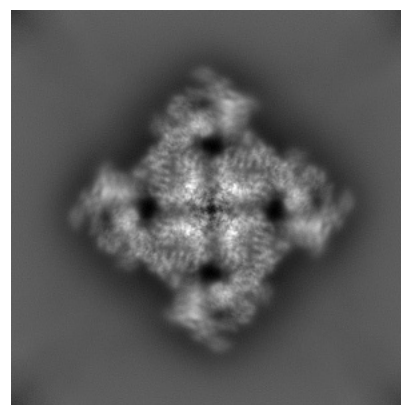
#### 6.1.2 Raw map



X



Y

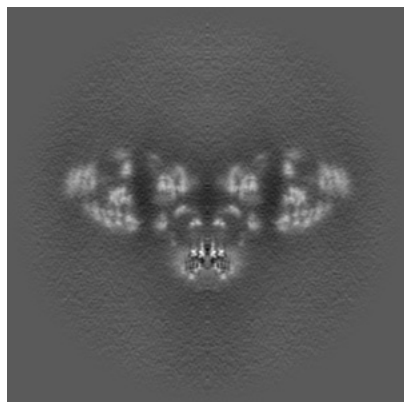


Z

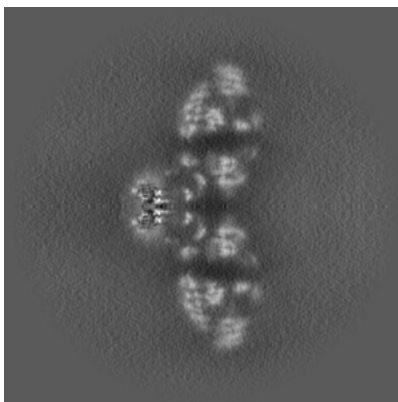
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

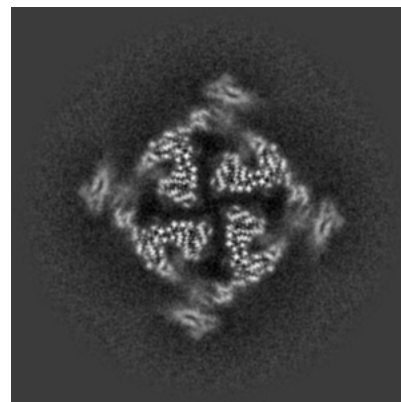
### 6.2.1 Primary map



X Index: 200

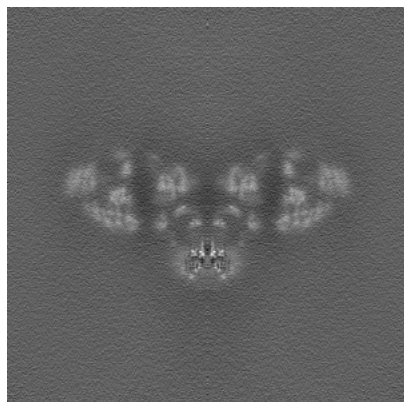


Y Index: 200

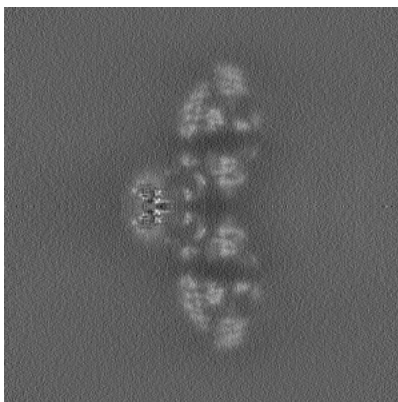


Z Index: 200

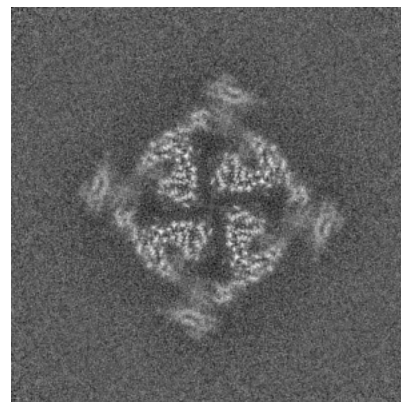
### 6.2.2 Raw map



X Index: 200



Y Index: 200

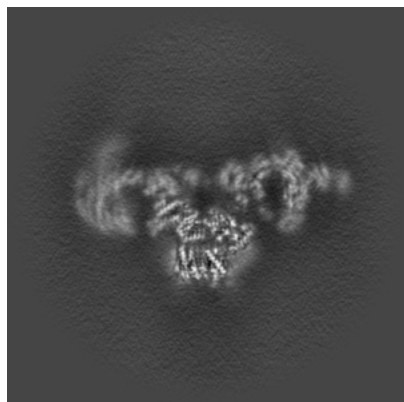


Z Index: 200

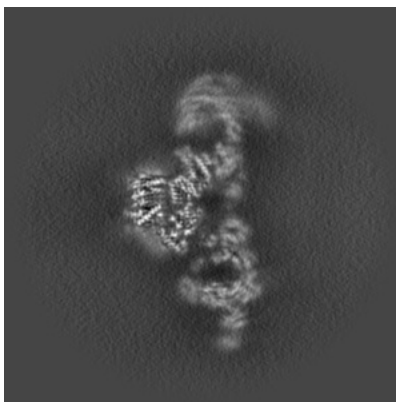
The images above show central slices of the map in three orthogonal directions.

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

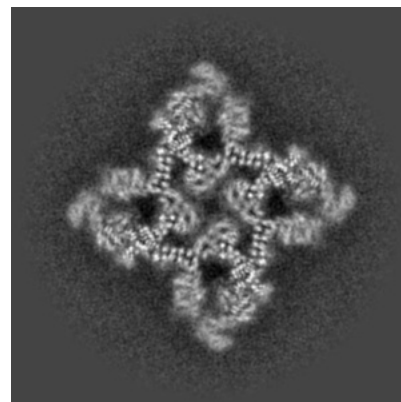
### 6.3.1 Primary map



X Index: 186

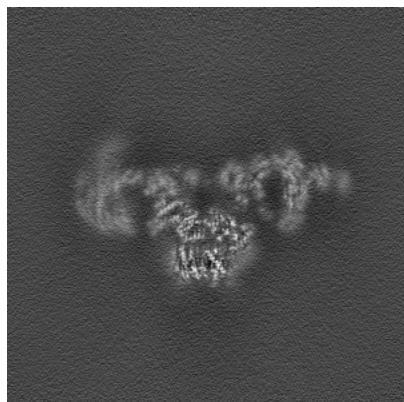


Y Index: 186

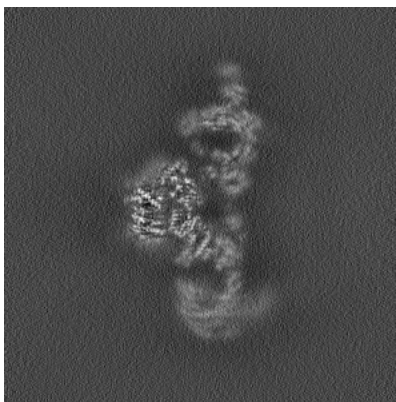


Z Index: 225

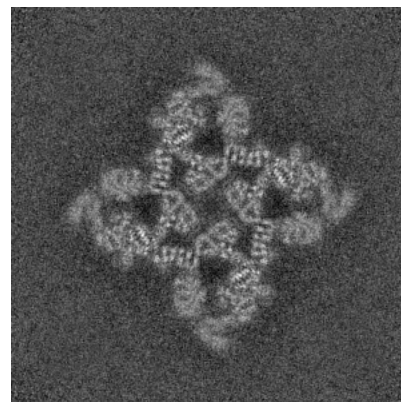
### 6.3.2 Raw map



X Index: 186



Y Index: 214



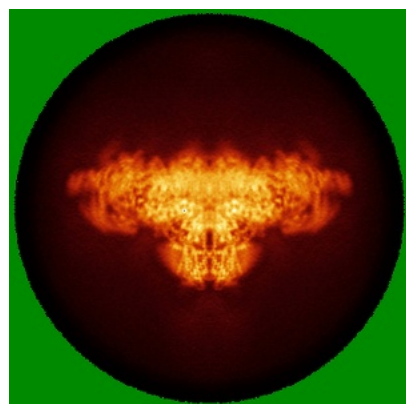
Z Index: 223

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

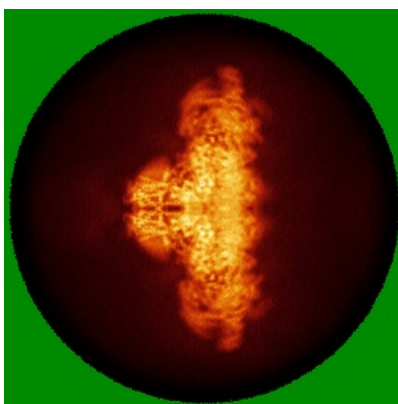


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

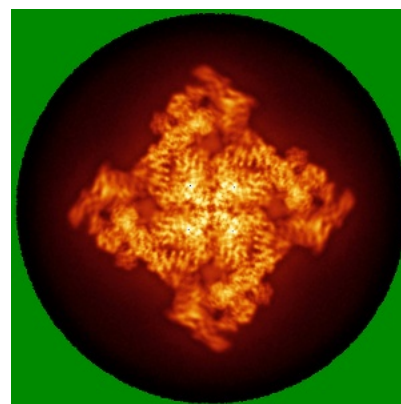
### 6.4.1 Primary map



X

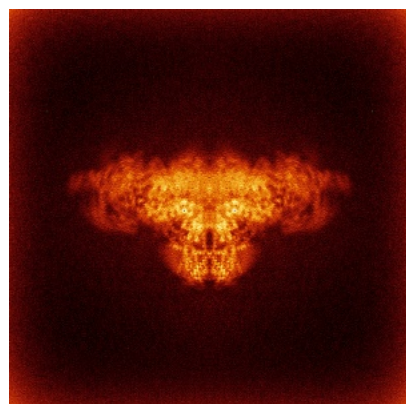


Y

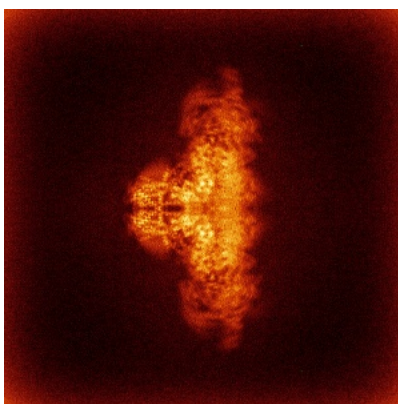


Z

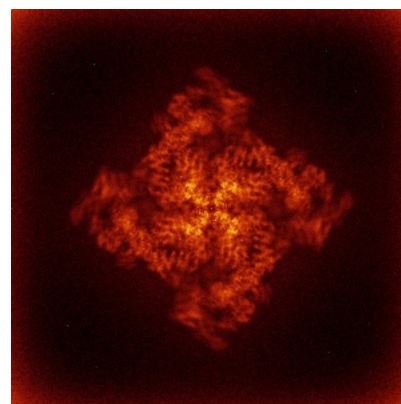
### 6.4.2 Raw map



X



Y

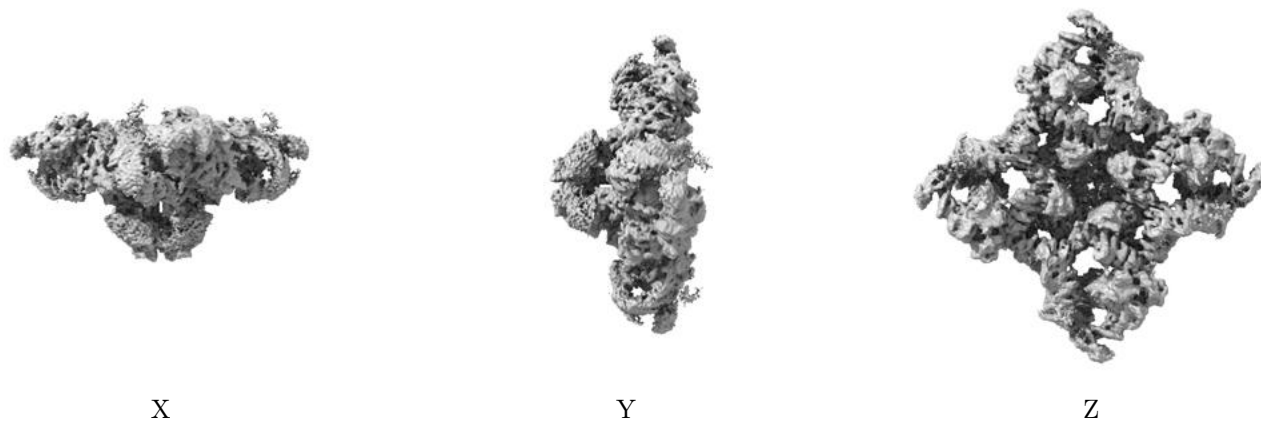


Z

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.

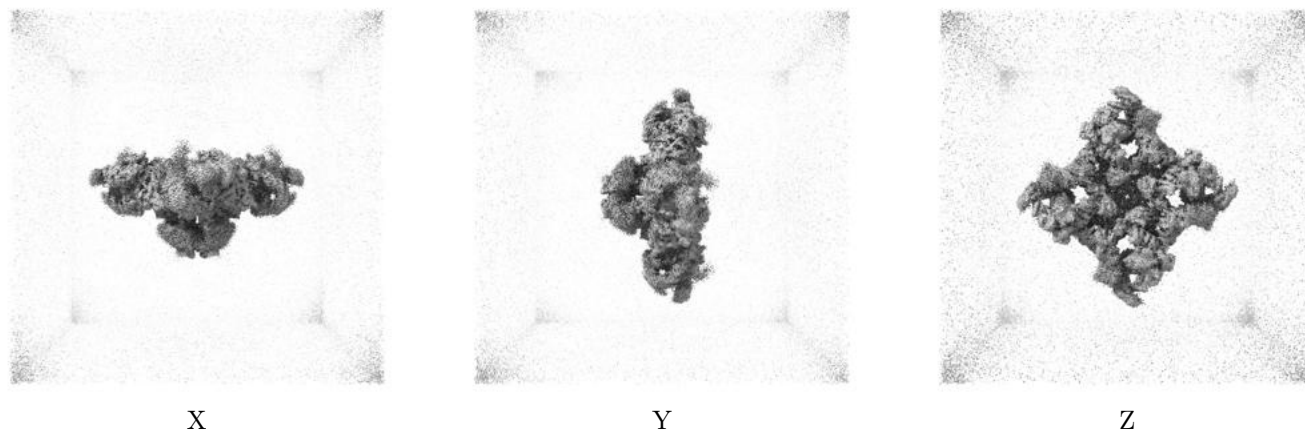
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.287. 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.

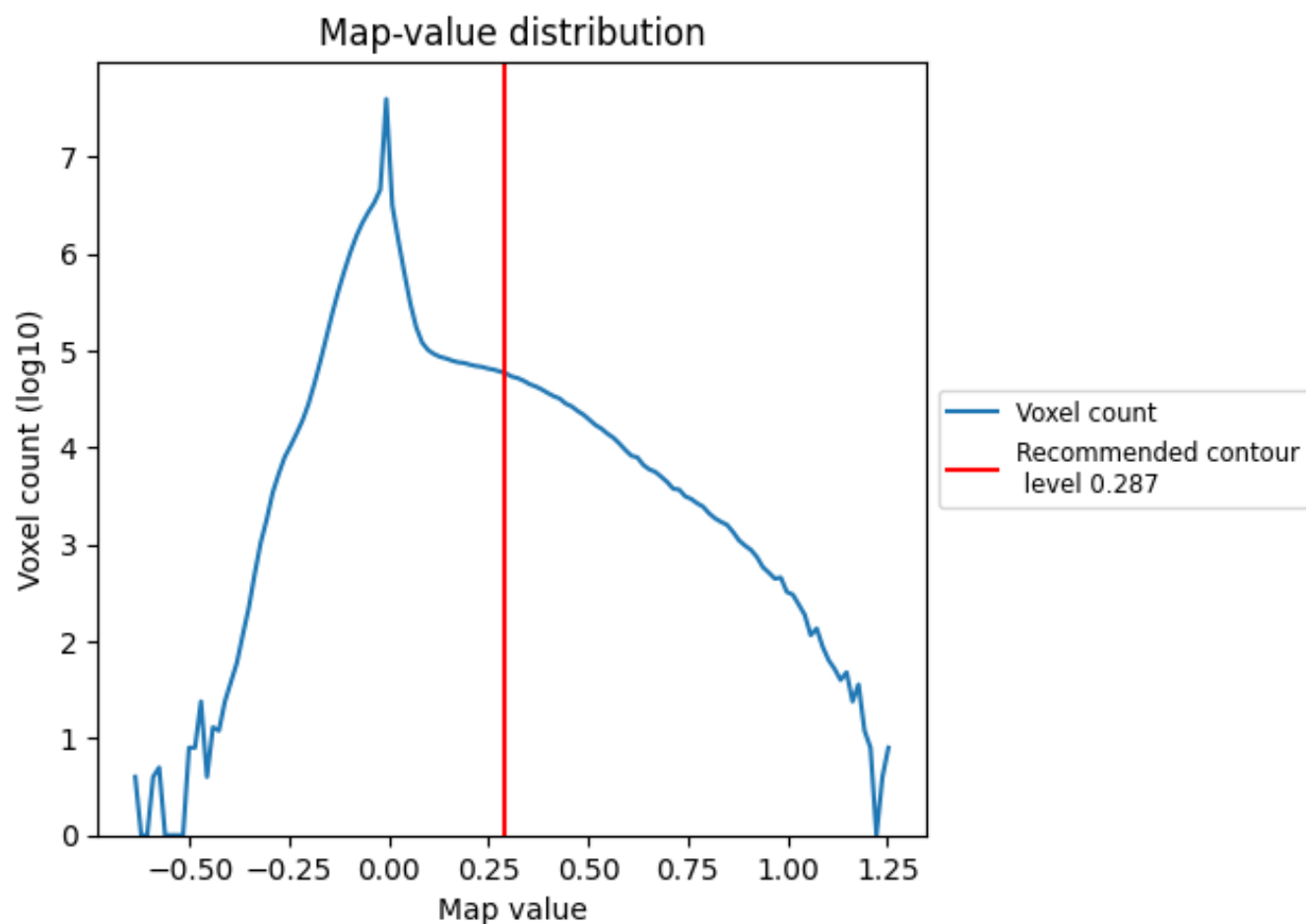
## 6.6 Mask visualisation [i](#)

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.

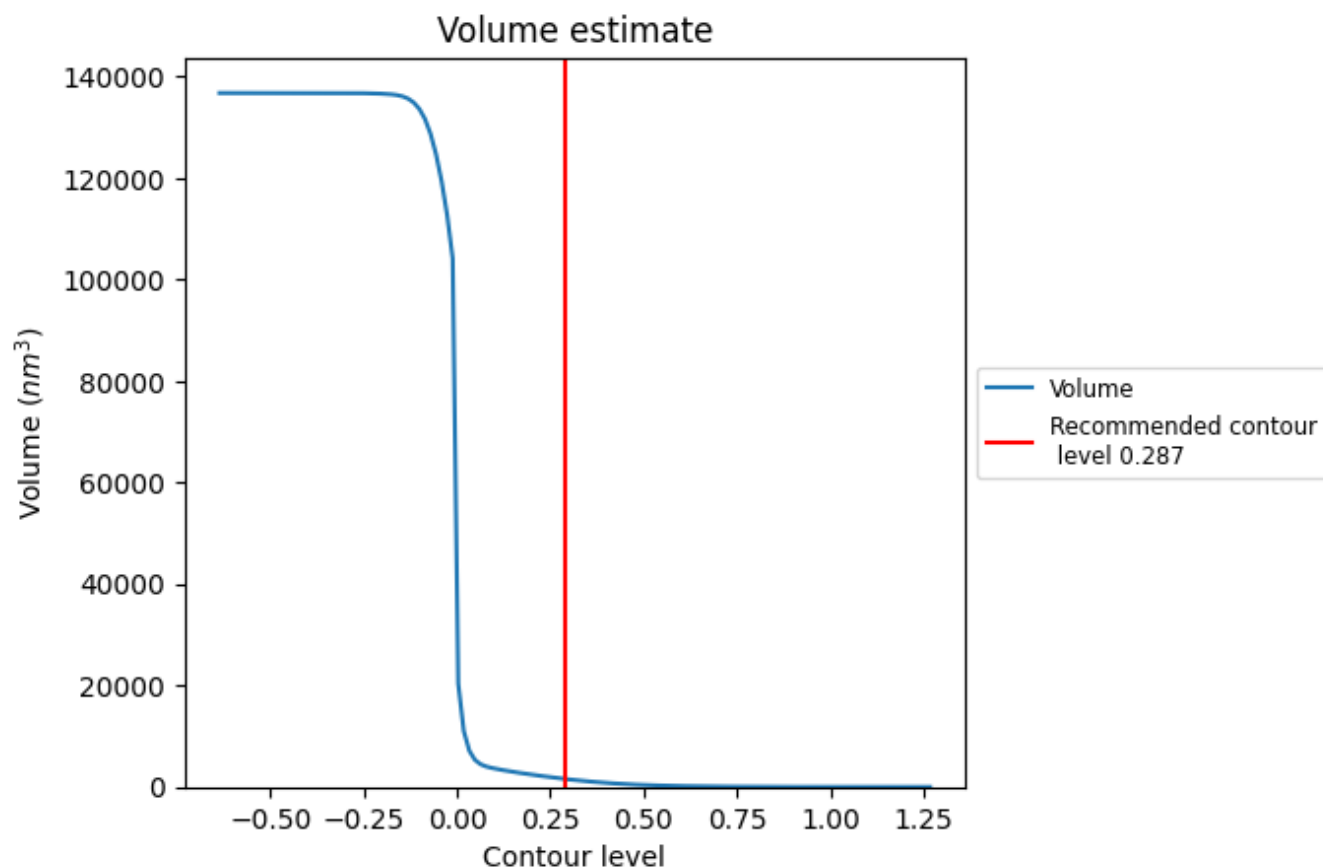
### 7.1 Map-value distribution [i](#)



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.



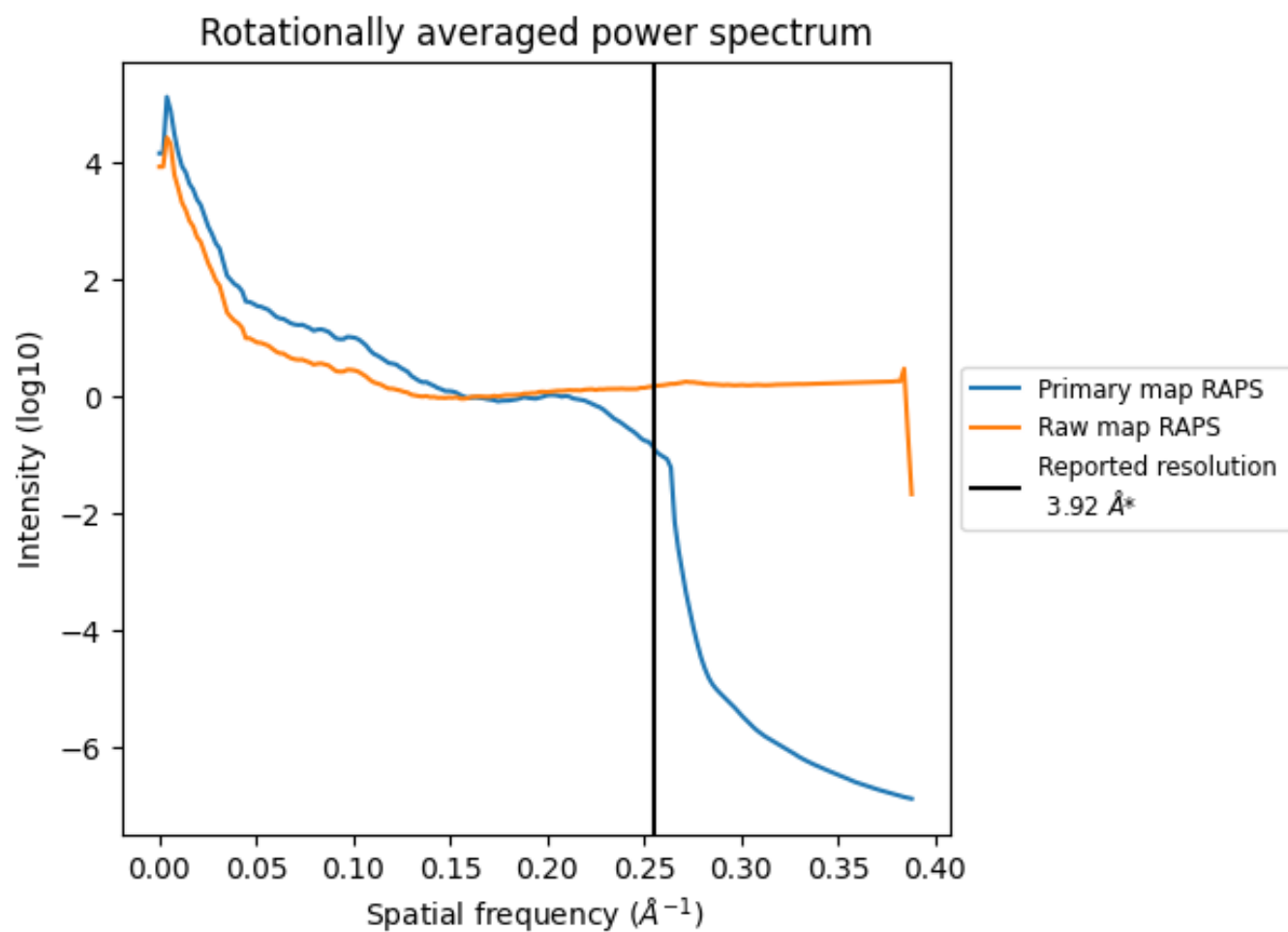
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1594  $\text{nm}^3$ ; this corresponds to an approximate mass of 1440 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 ⓘ

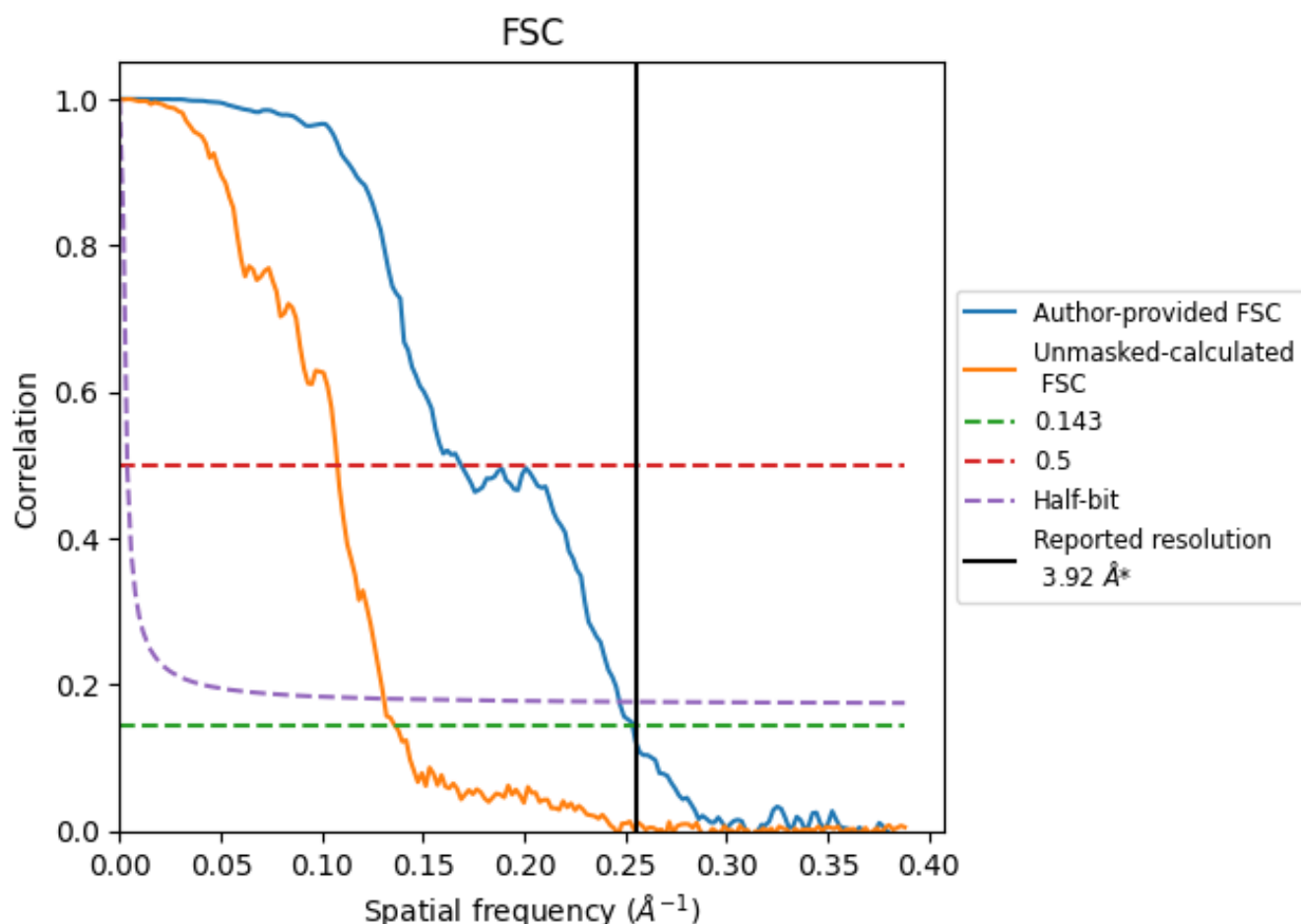


\*Reported resolution corresponds to spatial frequency of 0.255 Å<sup>-1</sup>

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

## 8.2 Resolution estimates [i](#)

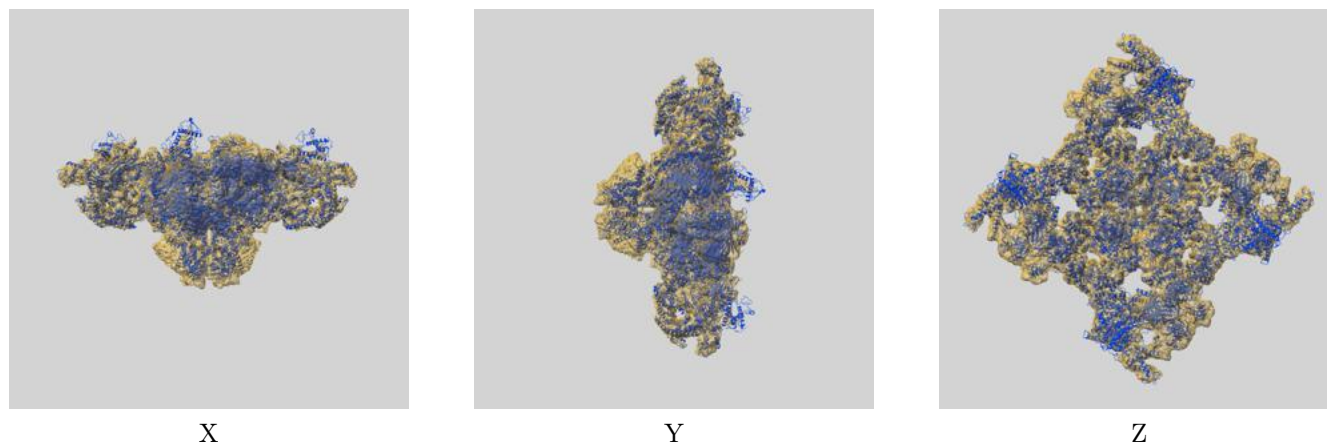
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.92	-	-
Author-provided FSC curve	3.94	5.92	4.05
Unmasked-calculated*	7.34	9.29	7.65

\*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 7.34 differs from the reported value 3.92 by more than 10 %

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

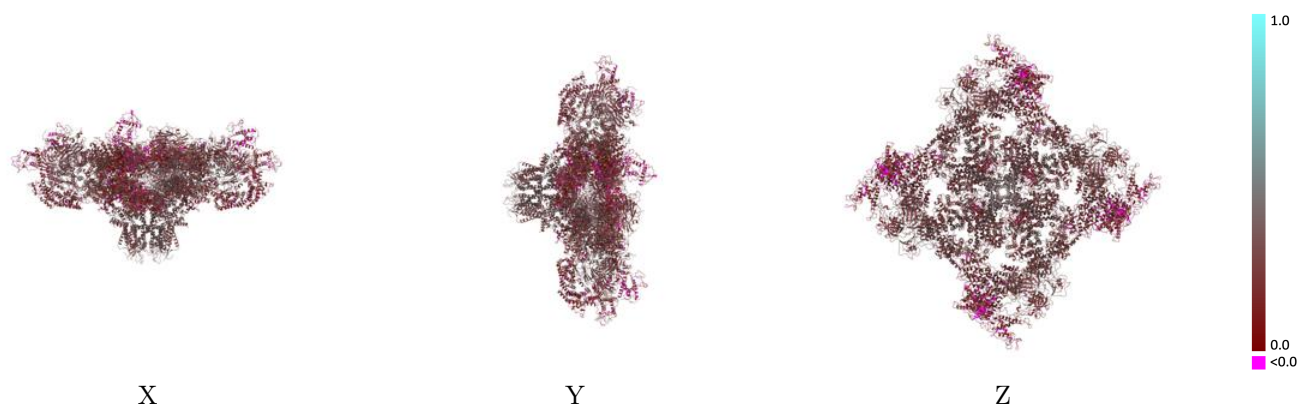
This section contains information regarding the fit between EMDB map EMD-40423 and PDB model 8SEO. Per-residue inclusion information can be found in section [3](#) on page [8](#).

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



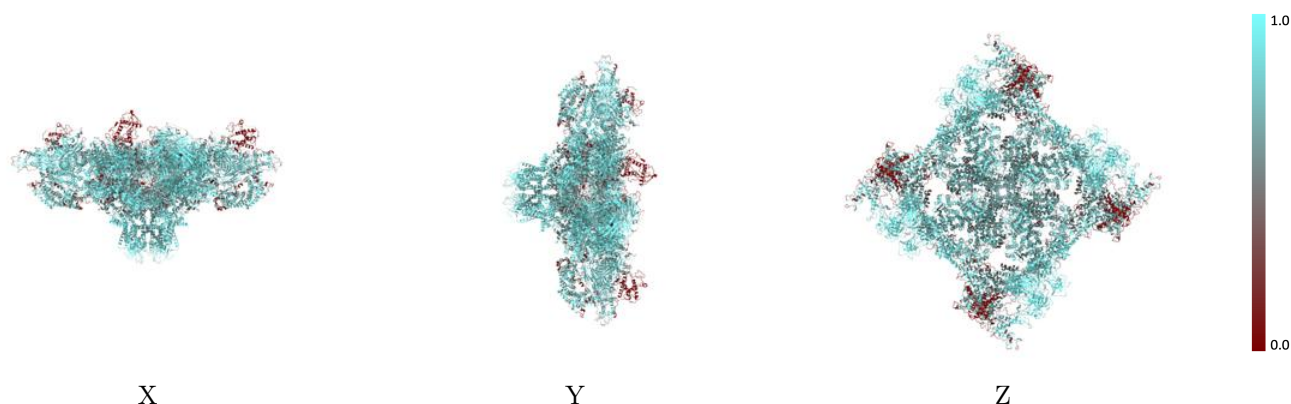
The images above show the 3D surface view of the map at the recommended contour level 0.287 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



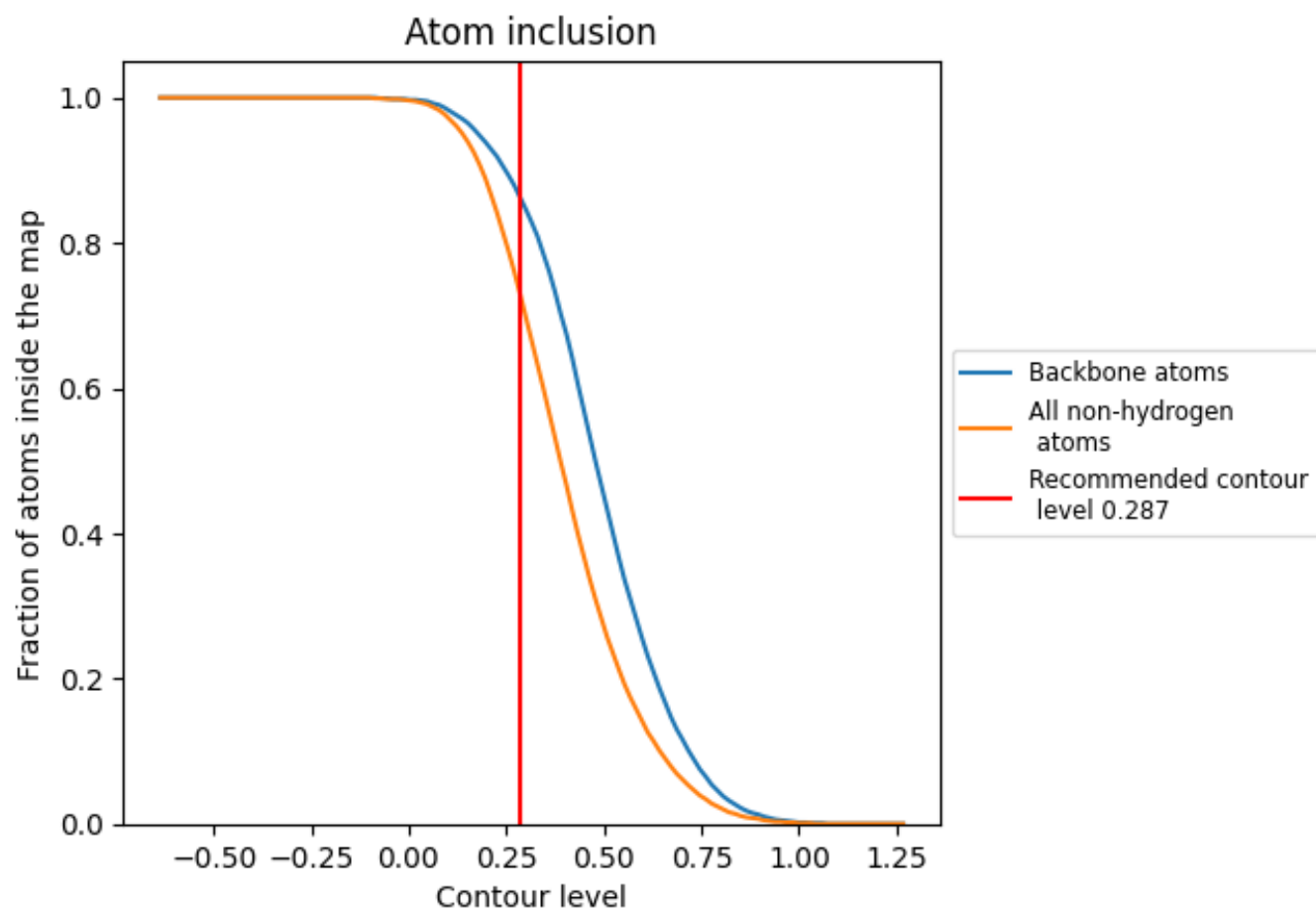
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.287).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 73% 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 (0.287) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.7270</div>	<div><div></div>0.2530</div>
A	<div><div></div>0.7230</div>	<div><div></div>0.2520</div>
B	<div><div></div>0.7230</div>	<div><div></div>0.2530</div>
C	<div><div></div>0.7230</div>	<div><div></div>0.2520</div>
D	<div><div></div>0.7230</div>	<div><div></div>0.2520</div>
E	<div><div></div>0.8870</div>	<div><div></div>0.3060</div>
F	<div><div></div>0.8870</div>	<div><div></div>0.3060</div>
G	<div><div></div>0.8870</div>	<div><div></div>0.3060</div>
H	<div><div></div>0.8870</div>	<div><div></div>0.3080</div>

1.0

0.0

<0.0