



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 01:40 PM UTC

PDB ID : 8RRS / pdb_00008rrs
EMDB ID : EMD-19463
Title : Structure of mouse RyR2 solubilised in detergent in open state in complex with Ca²⁺, ATP, caffeine and Nb9657.
Authors : Li, C.; Efremov, R.G.
Deposited on : 2024-01-23
Resolution : 3.40 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:

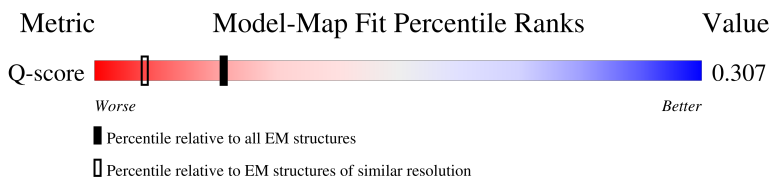
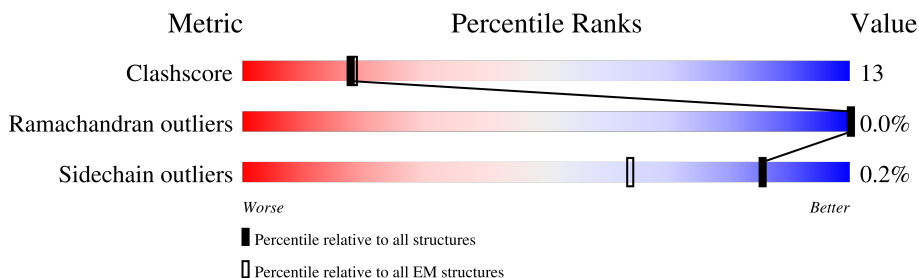
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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

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

The reported resolution of this entry is 3.40 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	-
Q-score	-	25397	14717 (2.90 - 3.90)

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	A	4966	
1	C	4966	
1	E	4966	
1	F	4966	

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Mol	Chain	Length	Quality of chain
2	B	137	37% 64% 28% 8%
2	D	137	36% 65% 27% 8%
2	G	137	36% 64% 28% 8%
2	I	137	36% 64% 28% 8%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 136400 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.

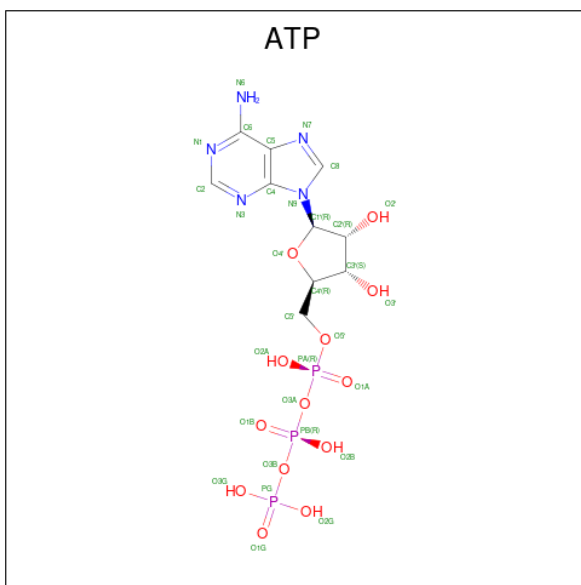
- Molecule 1 is a protein called Ryanodine receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4142	Total	C	N	O	S	0	0
			33088	21113	5650	6106	219		
1	C	4142	Total	C	N	O	S	0	0
			33088	21113	5650	6106	219		
1	E	4142	Total	C	N	O	S	0	0
			33088	21113	5650	6106	219		
1	F	4142	Total	C	N	O	S	0	0
			33088	21113	5650	6106	219		

- Molecule 2 is a protein called Nanobody 9657.

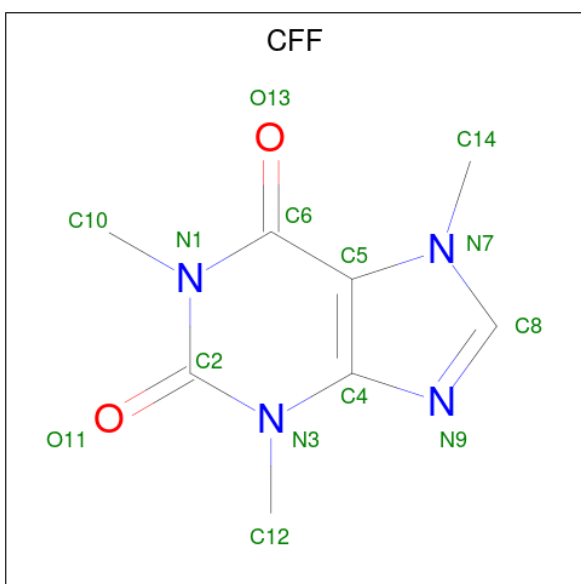
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	126	Total	C	N	O	S	0	0
			965	595	170	195	5		
2	D	126	Total	C	N	O	S	0	0
			965	595	170	195	5		
2	G	126	Total	C	N	O	S	0	0
			965	595	170	195	5		
2	I	126	Total	C	N	O	S	0	0
			965	595	170	195	5		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	F	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 4 is CAFFEINE (CCD ID: CFF) (formula: $C_8H_{10}N_4O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	4	2	
4	C	1	Total	C	N	O	0
			14	8	4	2	
4	E	1	Total	C	N	O	0
			14	8	4	2	
4	F	1	Total	C	N	O	0
			14	8	4	2	

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Zn	0
			1	1	
5	C	1	Total	Zn	0
			1	1	
5	E	1	Total	Zn	0
			1	1	
5	F	1	Total	Zn	0
			1	1	

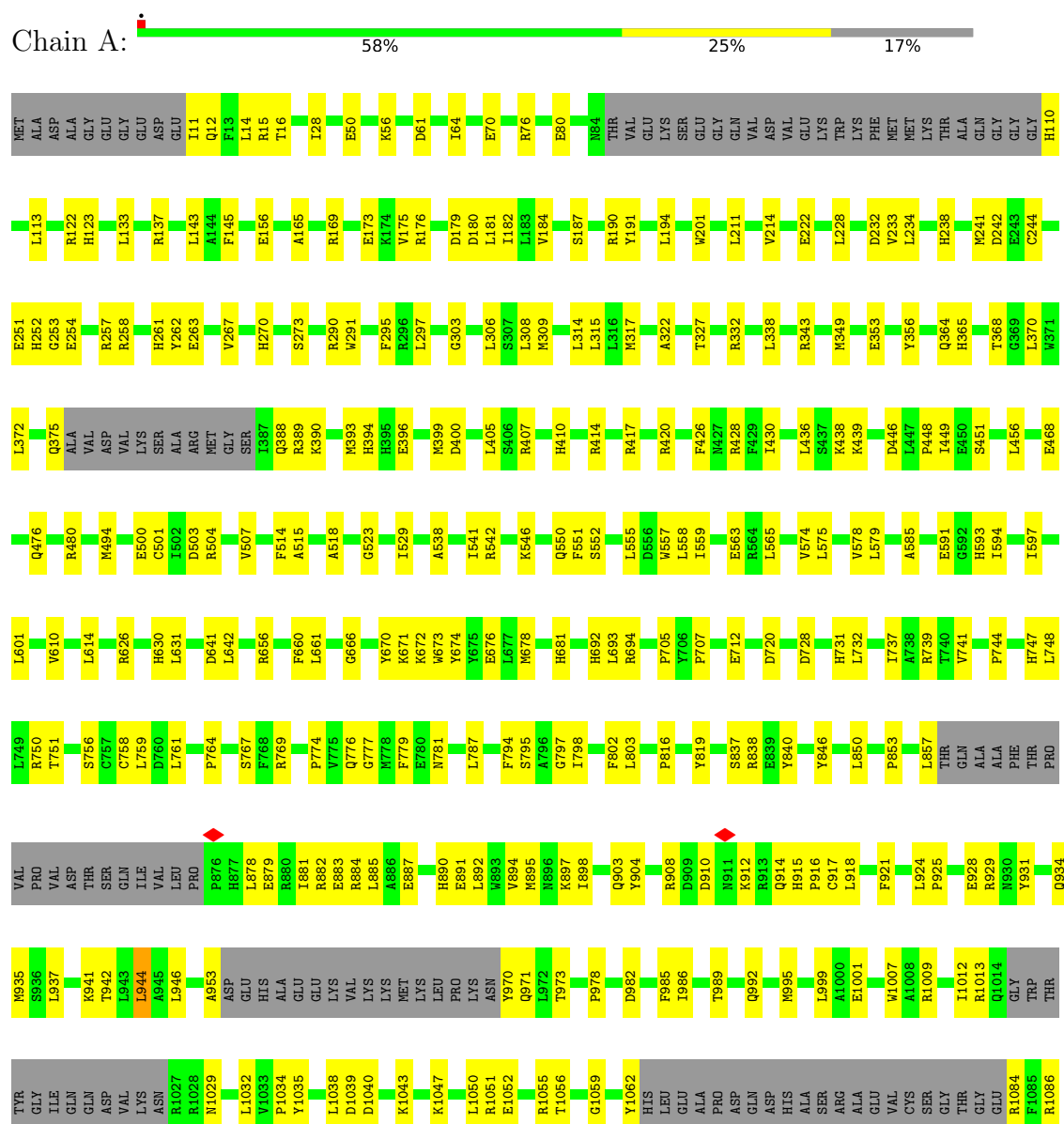
- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Ca	0
			1	1	
6	C	1	Total	Ca	0
			1	1	
6	E	1	Total	Ca	0
			1	1	
6	F	1	Total	Ca	0
			1	1	

3 Residue-property plots

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

• Molecule 1: Ryanodine receptor 2



A2522	LYS	THR	H2233	R2089	D1929	F1852	L1754	M1602	I1446	TYR	LYS	M1216	E1091
P2525	ASP	SER	H2237	Q2090	V1932	G1853	L1758	V1609	H1451	ALA	SER	F1217	K1092
L2526	GLY	GLY	T2237	I2094	I1935	ALA	R1759	R1611	D1458	GLN	VAL	G1218	T1093
T2527	LYS	SER	P2238	L2094	L1935	ALA	P1760	S1610	D1459	LYS	ALA	L1219	Y1094
R2528	VAL	LYS	L2239	V2098	Q1939	VAL	P1767	G1617	D1460	PRO	GLY	D1220	K1097
C2530	F2452	THR	A2244	R2099	R1942	PRO	SER	G1620	R1461	ARG	PRO	V1221	K1098
C2531	D2454	LEU	D2258	A2100	R1942	GLU	PHE	V1620	R1466	GLY	PRO	Y1236	A1099
F2534	N2455	ASP	P2259	L2101	M1947	GLU	VAL	C1622	V1467	LYS	GLY	N1242	R1100
A2535	S2456	ILE	E2258	K2102	M1947	GLU	SER	C1622	T1468	GLN	ALA	Y1102	W1101
G2536	A2457	GLU	T2104	T2104	S1953	GLY	ILE	L1623	T1468	ARG	PHE	R1245	F1103
T2537	G2458	GLU	Y2105	Y2105	A1954	THR	SER	E1636	G1470	PHE	TYR	D1246	E1104
H2540	F2459	LEU	K2263	S2121	A1955	PRO	ASN	E1637	D1471	LEU	GLY	I1247	M1113
A2541	C2460	ASP	V2264	I2125	L1956	GLU	C1776	R1638	E1472	LEU	LYS	T1248	R1114
S2542	H2463	D2379	R2266	I2125	R1959	LYS	D1786	D1641	H1477	THR	ASN	L1251	W1117
L2543	K2464	H2382	C2276	V2131	K1960	ILE	LYS	D1641	T1480	LYS	LEU	R1254	W1117
I2544	N2467	N2383	Q2277	R2132	T1961	SER	K1789	E1644	K1481	PRO	GLU	P1120	P1120
D2545	G2384	G2385	M2278	M2133	R1962	ILE	A1790	E1644	R1482	ASP	ASP	Q1257	P1124
S2546	A2386	A2387	L2279	E2137	R1965	GLU	K1791	E1649	S1483	TYR	PHE	F1258	P1124
L2548	I2387	I2387	W2289	E2137	S1966	ASP	M1795	E1649	N1484	THR	VAL	P1262	E1127
H2549	A2392	A2392	K2290	L2145	P1967	LYS	LYS	C1666	C1485	GLY	ASP	H1265	L1128
Y2552	W2405	W2405	P2291	M2149	P1968	LEU	K1801	L1677	Y1486	HIS	SER	A1136	A1136
R2553	H2406	H2406	R2296	F2154	Q1971	GLY	E1802	L1677	M1487	ALA	ASP	H1266	H1266
L2554	L2407	L2407	F2300	F2154	I1972	ALA	L1805	V1681	E1507	ARG	PHE	H1267	H1267
S2555	I2408	I2408	F2300	F2154	I1972	GLU	L1805	V1681	E1507	GLU	GLY	F1137	F1137
K2556	K2412	K2412	N2317	P2158	L1975	GLU	R1808	L1686	C1510	LEU	VAL	D1138	D1138
T2561	G2413	G2413	W2159	N2159	F1978	GLU	D1809	L1686	C1510	THR	LEU	E1269	E1269
Q2564	E2414	E2414	L2160	L2160	K1979	LYS	P1811	Y1694	E1535	ASP	LYS	R1272	R1272
R2565	A2415	A2415	M2161	M2161	K1979	GLY	S1814	Y1704	T1538	VAL	THR	D1274	D1274
D2566	I2418	I2418	G2165	G2165	C1985	ARG	T1815	D1705	V1553	ALA	HIS	GLY	C1164
S2567	R2419	R2419	N2186	N2186	P1988	PRO	E1816	L1706	F1554	ASP	GLY	THR	M165
I2568	R2423	R2423	F22175	F22175	E1989	LYS	F1817	L1707	F1554	ASP	HIS	ILE	V1166
E2569	S2424	S2424	P2175	P2175	E1990	GLU	L1818	D1709	E1557	ARG	LEU	ASP	D1167
V2570	L2425	L2425	P2189	P2189	I1991	GLU	L1818	I1710	E1557	VAL	VAL	SER	M1168
L2573	I2426	I2426	K2191	K2191	R1992	GLU	P1821	I1710	E1557	PRO	PRO	SER	SER
Q2578	D2430	D2430	N2191	N2191	L1995	LYS	Y1827	S1713	R1560	ARG	ASP	PRO	M1173
L2579	L2431	L2431	V2192	V2192	L1995	GLU	Y1827	S1713	I1561	ARG	ARG	CYS	M1174
R2580	G2432	G2432	A2193	A2193	F1998	ILE	I1831	A1718	K1582	ILE	ASP	LEU	L1177
P2581	C2433	C2433	R2197	R2197	H1999	PRO	I1831	A1718	N1583	ASP	LYS	K1284	L1177
S2582	V2434	V2434	F2198	F2198	E2000	LYS	I1834	M1721	H1576	LYS	ASP	V1285	L1182
M2583	I2435	I2435	K2351	K2351	D2001	GLU	N1837	M1722	K1577	GLY	LYS	Q1287	L1182
H2584	S2436	S2436	L2352	L2352	C2006	M1905	E1838	I1727	C1583	THR	GLU	Q1293	L1190
Q2585	I2437	I2437	A2353	A2353	G2007	C1906	D1839	V1728	P1584	PRO	PRO	F1192	A1191
H2586	G2438	G2438	E2354	E2354	I2008	L1907	L1840	P1729	P1585	LYS	LYS	N1294	F1192
L2587	F2439	F2439	D2355	D2355	GLU	L1907	K1841	E1733	H1588	PRO	PRO	N1295	F1201
L2588	Q2440	Q2440	L2079	L2079	ASP	L1909	H1842	E1733	V1589	GLY	GLY	R1303	F1201
L2591	N2441	N2441	Q2210	Q2210	LEU	L1909	H1842	L1739	Q1590	PHE	PHE	L1304	L1202
V2592	P2442	P2442	M2213	M2213	GLU	C1913	L1844	L1739	Q1590	ASN	ASN	S1305	L1207
L2608	THR	THR	F2261	F2261	GLU	C1913	L1844	L1739	Q1590	ASN	ASN	G1268	G1268
	ILE	ILE	SER	SER	ASP	R1920	Q1845	L1749	V1595	HIS	HIS	V1209	V1209
	ALA	ALA	PRO	PRO	GLY	R1920	L1846	P1760	W1597	LYS	LYS	Q1211	Q1211
					SER		I1847			ASP	ASP		

L2609	L2613	L2614	L2615	L2618	L2619	L2620	L2621	L2622	L2625	F2629	S2633	L2637	L2638	R2641	L2642	L2643	F2644	W2645	L2646	L2647	E2657	L2658	L2660	F2661	K2662	S2669	A2670	V2671	G2673	A2674	L2675	L2676	P2677	K2680	GLU	SER	ASN	TYR	VAL	SER	VAL	SER	VAL	GLU	GLN	SER					
SER	MET	ASP	SER	GLY	ASN	PHE	ASN	PRO	GLN	PRO	VAL	ASP	THR	TRP	ASN	ILE	THR	ILE	P2713	E2714	K2715	L2716	Y2723	S2727	W2731	S2732	K2735	N2738	G2739	W2740	I2741	E2744	I2745	I2746	S2747	D2748	S2749	S2750	K2751	I2752	Q2753	P2754	L2755	M2756	LYS	PRO	GLU	GLN	SER		
K2765	E2766	E2767	E2768	R2771	L2774	L2778	W2781	V2784	GLY	TRP	ARG	ILE	GLU	ARG	THR	ASP	SER	MET	ALA	LEU	TYR	ASN	ARG	THR	ARG	ILE	SER	GLN	THR	SER	GLN	VAL	SER	ILE	ASP	ALA	ASP	HIS	GLY	TYR	SER	PRO	ARG	ALA	ILE	ASP	MET	SER	ASN	VAL	
THR	LEU	SER	ARG	D2835	W2839	W2851	A2852	K2855	K2856	L2857	E2858	L2859	E2860	S2861	K2862	G2863	G2864	G2865	H2867	P2868	L2869	T2877	A2878	K2881	Q2889	D2890	I2891	F2892	K2893	G2905	PHE	LYS	ASP	LEU	LEU	ASP	ASP	THR	THR	SER	I2916	E2917	K2918	R2919	Y2922	S2923	F2924	L2925	Q2926	Q2927	
L2928	L2929	R2930	V2931	V2932	E2933	A2935	L2936	Q2937	Y2938	K2949	G2950	Y2955	F2962	V2965	L2966	L2967	T2970	D2971	Q2972	Y2973	F2974	H2977	R2978	L2979	Y2980	F2981	L2982	S2983	ALA	ALA	SER	ARG	PRO	LEU	CYS	THR	GLY	GLY	HIS	S2996	N2997	K2998	E2999	K3000	E3001	M3002	V3003	L3006	F3007		
L3010	L3013	V3014	L3018	A3025	L3028	V3029	K3030	C3031	L3032	H3033	I3034	T3038	L3039	D3040	R3041	T3043	K3046	T3047	G3048	L3049	D3050	S3051	V3052	K3053	R3057	E3065	K3069	T3070	M3071	L3074	Q3078	S3083	S3084	Q3085	V3089	I3093	N3094	Y3095	T3096	T3097	S3105	F3108									
E3109	H3110	F3116	G3117	L3120	I3121	L3122	E3123	D3124	V3125	Q3126	C3129	L3133	T3134	S3135	A3138	Y3146	V3147	R3151	G3155	E3156	A3159	A3160	F3161	P3166	I3167	T3172	N3178	V3179	Y3180	Y3183	N3184	T3185	R3186	R3189	P3197	E3201	D3202	V3203	P3208	L3210	E3211										
K3212	L3213	M3214	I3217	L3220	T3225	R3226	M3230	M3233	M3234	E3235	V3236	V3237	L3238	P3239	M3240	L3241	Y3244	M3245	S3246	W3247	W3248	W3249	E3250	E3254	N3255	H3256	M3262	H3271	M3272	N3273	T3274	L3275	L3276	I3279	L3280	I3283	N3286	L3287	G3288	D3289	D3290	E3291	G3292	A3293	W3294	M3295					
L3298	F3301	S3302	Q3303	L3306	R3307	V3308	V3309	K3310	L3313	L3314	K3315	H3317	F3318	L3319	P3320	L3321	M3322	E3323	K3324	L3325	K3326	K3327	K3328	M3331	V3332	E3335	L3339	K3340	A3341	E3342	A3343	R3344	G3345	D3346	M3347	S3348	E3351	L3352	L3353	I3354	L3356	A3362	R3363	D3364	L3365	F3368	Y3369	L3372			
V3376	D3377	V3378	N3379	R3380	L3381	K3382	W3383	L3384	K3385	E3386	P3387	N3388	P3389	E3390	A3391	E3392	E3393	L3394	F3395	R3396	M3397	V3398	A3399	E3400	V3401	F3402	I3403	N3425	N3426	K3427	S3428	F3429	L3430	K3435	S3436	S3439	K3440	I3443	E3447	K3450	K3454	R3457	S3463	L3464	I3465	V3466	K3470	R3471			
L3472	L3473	P3474	I3475	I3479	C3480	A3481	P3482	G3483	D3484	Q3485	E3486	L3487	A3488	L3489	A3491	K3492	R3505	I3508	I3512	G3516	K3517	L3518	A3522	W3525	Q3526	M3527	Y3530	L3533	P3534	N3535	R3536	T3537	E3538	D3539	P3540	V3547	E3548	R3549	V3550	L3551	G3552	I3553	A3554	N3555	V3556	L3557	F3558	H3559			
L3560	E3561	S3564	LYS	TYR	THR	GLY	ARG	GLY	TYR	PHE	SER	LEU	VAL	GLU	HIS	PRO	GLN	ARG	SER	LYS	LYS	ALA	VAL	TRP	HIS	LEU	LEU	SER	LYS	ALA	VAL	VAL	CYS	PHE	ARG	MET	ALA	PRO	TYR	ASN	LEU	P3611	R3612	H3613	R3614	A3615	V3616	N3617	L3618	F3619	L3620
Y3623	W3627	E3636	D3637	K3638	P3646	G3647	A3648	E3649	LEU	PRO	GLU	GLU	ASP	GLU	ALA	MET	K3658	R3659	V3660	H3664	E3677	D3684	M3688	I3693	K3696	S3697	C3698	H3699	ASP	GLU	GLU	ASP	ASP	ASP	GLY	GLU	GLU	VAL	LYS	S3712	E3717	Q3721	Q3727	A3728	F3729						

- Molecule 1: Ryanodine receptor 2

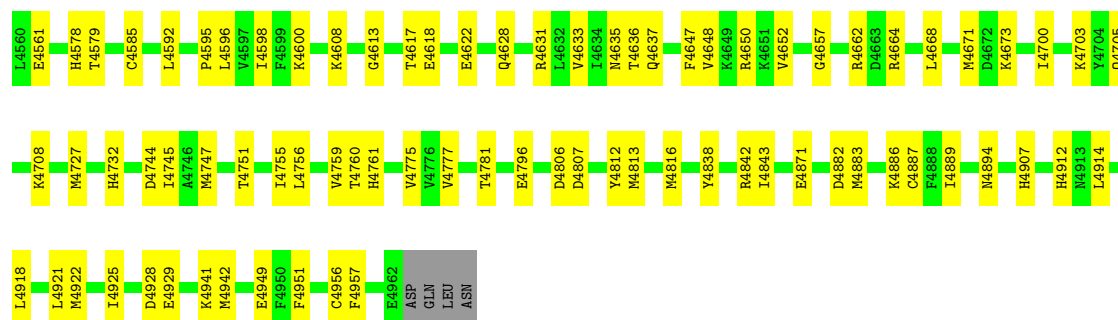
Frequency	Percentage
Daily	59%
Weekly	25%
Monthly	17%



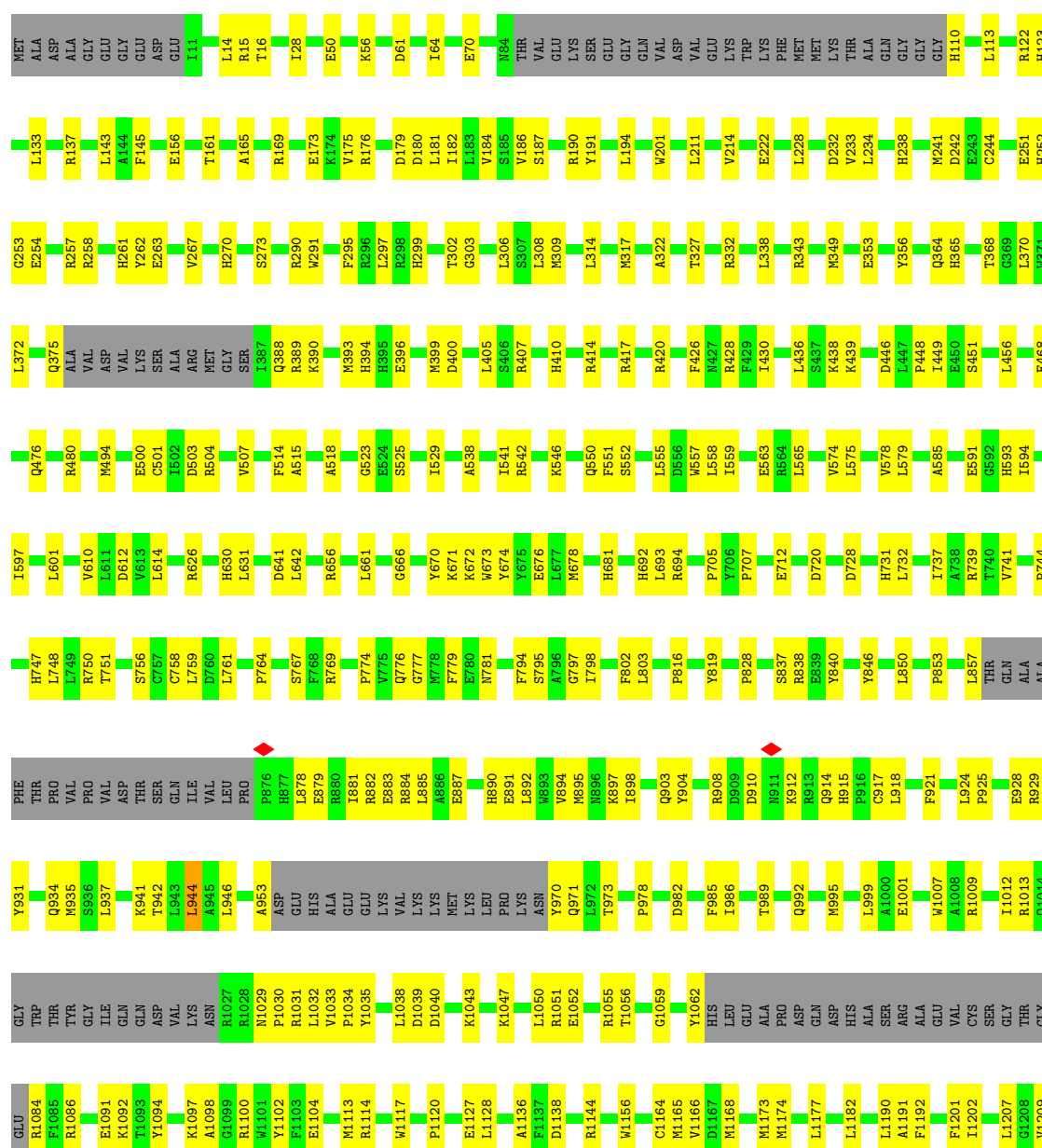
GLU	GLY	PHE	G1617	L1459	D1220	T1093	GLN	L937	VAL	T751	L601	Q476	Q375
THR	THR	VAL	V1620	D1460	V1221	Y1094	ASP	K941	THR	S756	L610	R480	ALA
PRO	ILE	ILE	C1621	GLY	Y1236	K1097	THR	T941	ASP	C757	V610	SER	VAL
GLU	GLU	GLN	L1622	GLY	Y1466	A1098	LYS	L943	GLN	C758	M494	ASP	ASP
LYS	LYS	ARG	T1467	PHE	M1242	G1099	ASN	L944	ILE	L759	L614	VAL	VAL
GLU	GLU	ARG	T1468	TYR	R1245	R1100	R1027	L945	VAL	D760	R626	E500	LYS
ILE	ILE	LEU	T1469	GLY	D1246	W1101	R1028	L946	LEU	L761	R626	C501	SER
ILE	ILE	LEU	G1470	GLY	D1247	Y1102	M1029	A953	PRO	P764	H630	I502	ALA
ILE	ILE	ARG	D1471	GLY	T1248	F1103	L1032	R877	ARG	P767	L631	D503	ALA
ASP	ASP	ARG	D1472	ASN	L1251	E1104	P1033	R878	MET	R768	L631	R504	ARG
ASP	ASP	THR	H1477	LEU	L1254	M1113	P1034	R879	GLY	S767	D641	V507	GLY
ALA	ALA	LYS	T1480	GLU	R1254	R1114	Y1035	R880	SER	R769	L642	V507	SER
LYS	LYS	PRO	K1481	ASP	R1257	W1117	L1038	I881	THR	F768	D641	V507	GLY
LEU	LEU	TYR	S1482	PHE	Q1257	Y1117	D1039	R882	GLN	S767	L642	V507	GLY
GLU	GLU	SER	C1666	ASP	F1258	P1120	D1040	R883	GLY	P774	R656	H513	GLN
GLU	GLU	THR	M1484	VAL	F1258	P1120	D1040	R884	LYS	Q776	L661	D516	GLN
GLY	GLY	THR	C1485	VAL	F1258	P1120	D1040	R885	LYS	G777	G666	V517	GLN
GLY	GLY	GLY	C1486	ASP	F1262	E1127	K1043	R886	LYS	R778	G666	A518	GLN
GLY	GLY	GLY	Y1486	ASP	P1262	E1128	K1047	R887	LYS	F779	G666	A518	GLN
ALA	ALA	ALA	M1487	ASP	H1265	A1136	L1047	R890	LYS	S767	D641	V507	GLY
GLY	GLY	ALA	E1507	PHE	H1266	A1136	L1050	R891	LYS	F768	D641	V507	GLY
GLY	GLY	ARG	C1510	GLY	H1267	F1137	L1051	R892	LYS	R769	L642	V507	GLY
GLY	GLY	LEU	C1510	GLY	H1268	D1138	R1051	R893	LYS	P774	R656	H513	GLN
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R894	LYS	Q776	L661	D516	GLN
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R895	LYS	G777	L661	D516	GLN
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R896	LYS	R778	G666	A518	GLN
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R897	LYS	F779	G666	A518	GLN
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R898	LYS	S767	D641	V507	GLY
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R899	LYS	R769	L642	V507	GLY
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R900	LYS	P774	R656	H513	GLN
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R901	LYS	Q776	L661	D516	GLN
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R902	LYS	G777	L661	D516	GLN
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R903	LYS	R778	G666	A518	GLN
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R904	LYS	F779	G666	A518	GLN
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R905	LYS	S767	D641	V507	GLY
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R906	LYS	R769	L642	V507	GLY
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R907	LYS	P774	R656	H513	GLN
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R908	LYS	Q776	L661	D516	GLN
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R909	LYS	G777	L661	D516	GLN
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R910	LYS	R778	G666	A518	GLN
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R911	LYS	F779	G666	A518	GLN
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R912	LYS	S767	D641	V507	GLY
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R913	LYS	R769	L642	V507	GLY
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R914	LYS	P774	R656	H513	GLN
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R915	LYS	Q776	L661	D516	GLN
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R916	LYS	G777	L661	D516	GLN
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R917	LYS	R778	G666	A518	GLN
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R918	LYS	F779	G666	A518	GLN
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R919	LYS	S767	D641	V507	GLY
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R920	LYS	R769	L642	V507	GLY
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R921	LYS	P774	R656	H513	GLN
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R922	LYS	Q776	L661	D516	GLN
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R923	LYS	G777	L661	D516	GLN
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R924	LYS	R778	G666	A518	GLN
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R925	LYS	F779	G666	A518	GLN
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R926	LYS	S767	D641	V507	GLY
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R927	LYS	R769	L642	V507	GLY
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R928	LYS	P774	R656	H513	GLN
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R929	LYS	Q776	L661	D516	GLN
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R930	LYS	G777	L661	D516	GLN
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R931	LYS	R778	G666	A518	GLN
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R932	LYS	F779	G666	A518	GLN
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R933	LYS	S767	D641	V507	GLY
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R934	LYS	R769	L642	V507	GLY
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R935	LYS	P774	R656	H513	GLN
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GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R937	LYS	G777	L661	D516	GLN
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R938	LYS	R778	G666	A518	GLN
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R939	LYS	F779	G666	A518	GLN
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R940	LYS	S767	D641	V507	GLY
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R941	LYS	R769	L642	V507	GLY
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R942	LYS	P774	R656	H513	GLN
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R943	LYS	Q776	L661	D516	GLN
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R944	LYS	G777	L661	D516	GLN
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R945	LYS	R778	G666	A518	GLN
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R946	LYS	F779	G666	A518	GLN
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R947	LYS	S767	D641	V507	GLY
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R948	LYS	R769	L642	V507	GLY
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R949	LYS	P774	R656	H513	GLN
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R950	LYS	Q776	L661	D516	GLN
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R951	LYS	G777	L661	D516	GLN
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R952	LYS	R778	G666	A518	GLN
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R953	LYS	F779	G666	A518	GLN
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R954	LYS	S767	D641	V507	GLY
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GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R956	LYS	P774	R656	H513	GLN
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R957	LYS	Q776	L661	D516	GLN
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R958	LYS	G777	L661	D516	GLN
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R959	LYS	R778	G666	A518	GLN
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R960	LYS	F779	G666	A518	GLN
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R961	LYS	S767	D641	V507	GLY
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GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R970	LYS	P774	R656	H513	GLN
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GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R975	LYS	S767	D641	V507	GLY
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GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R977	LYS	P774	R656	H513	GLN
GLY	GLY	THR	C1510	GLY	E1269	D1138	E1052	R978					



SER	ALA	GLU	ALA	PHE	SER	H4048	R3938	L3802	R3659	HIS	E502	L3394	L3319	L3238
F4478	S4155	LYS	LEU	VAL	LEU	K4049	R3938	N3805	V3660	PRO	E502	F3395	P3320	P3239
K4481	R4157	GLN	THR	ALA	THR	A4050	W3940	N3805	H3664	GLN	R3505	R3396	M3322	L3241
I4482	Q4159	GLN	THR	VAL	ILE	M4051	W3940	R3810	E3677	SER	I3508	K3324	K3324	Y3244
I4483	E4160	LYS	THR	ARG	ARG	H4054	V3944	R3811	D3684	LYS	I3512	L3395	L3395	M3245
Q4486	V4164	ALA	ALA	GLY	ALA	Y4057	I3964	E3814	M3688	ALA	G3516	K3326	K3326	S3246
A4494	K4166	LYS	ASP	PHE	PHE	T4058	L3967	M3818	Y3693	THR	K3517	K3327	K3327	W3248
M4500	S4167	LYS	LEU	ILE	LEU	T4062	K3968	V3828	D3693	LYS	L3518	W3249	W3249	V3249
L4505	K4168	GLU	THR	VAL	VAL	L4066	L3970	M3971	K3696	LEU	A3522	K3331	K3331	E3250
A4508	R4169	LYS	ASN	SER	SER	A4069	M3977	D3831	S3697	SER	E3522	V3332	V3332	E3254
I4511	E4181	THR	VAL	VAL	VAL	E4075	M3977	D3832	C3698	LYS	Q3526	E3335	E3335	H3256
K4519	K4182	LYS	THR	THR	THR	T4076	M3980	F3834	H3699	ARG	W3527	K3340	K3340	M3262
V4520	K4184	GLY	LEU	GLY	LEU	L4077	M3984	R3840	GLU	ARG	Y3530	A3341	A3341	H3271
S4521	M4185	VAL	VAL	GLY	VAL	Y4079	M3984	Q3843	ASP	ALA	ASP	E3342	E3342	K3272
THR	L4187	GLU	LEU	LEU	LEU	F4082	T3993	Q3844	GLY	VAL	ASP	R3344	R3344	N3273
SER	F4188	LYS	SER	GLY	GLY	V4083	T3993	R3854	GLU	ALA	ASP	C3345	C3345	L3275
SER	T4195	ALA	LEU	ALA	ALA	E4088	K3986	N3850	GLU	CYS	P3534	D3346	D3346	L3276
SER	I4196	LYS	LYS	ALA	LYS	E4088	Q3997	S3851	GLU	PHE	R3535	M3347	M3347	L3279
VAL	M4199	GLY	SER	LYS	SER	V4099	M3998	D3852	GLU	ARG	T3537	S3348	S3348	L3280
GLU	M4199	ILE	LEU	ILE	LEU	V4099	V3999	F3853	VAL	MET	E3538	L3353	L3353	L3283
LYS	I4205	LYS	LYS	LYS	LYS	L4104	D4000	Q3854	LYS	ALA	D3539	L3353	L3353	K3286
GLU	SER	VAL	GLN	VAL	GLN	L4104	M4001	R3858	S3712	PRO	P3540	L3354	L3354	L3287
GLU	GLU	GLY	MET	ALA	ALA	M4108	V4003	T3859	E3717	TYR	K3454	L3361	L3361	L3289
PRO	ASP	GLY	LYS	LEU	LYS	D4111	E4004	T3870	Q3721	ASN	R3457	A3362	A3362	E3291
THR	LEU	LYS	MET	LEU	LEU	T4112	S4005	Q3721	Q3721	LEU	R3457	R3363	R3363	G3292
THR	ASN	ALA	LYS	ALA	LYS	R4113	M4008	V3874	Q3727	P3611	R3457	D3364	D3364	A3293
SER	GLU	ASN	LYS	ASN	LYS	R4113	V4009	D3875	A3728	H3612	L3464	L3365	L3365	W3294
SER	ARG	ILE	MET	MET	MET	I4114	E4010	L3878	R3729	R3614	I3465	F3368	F3368	M3295
ASP	LEU	PRO	THR	THR	THR	Q4115	M4011	L3879	L3730	L3618	V3466	L3372	L3372	L3298
LYS	ALA	ASP	VAL	VAL	VAL	T4116	I4012	R3879	H3731	L3618	R3470	V3376	V3376	F3301
ASN	ASN	PRO	THR	THR	THR	E4119	L4013	S3883	D3732	Y3623	L3472	S3302	S3302	Q3303
GLU	GLU	ASN	MET	GLN	GLN	L4120	L4013	S3883	R3733	Y3623	L3472	R3360	R3360	I3306
GLU	GLU	ALA	VAL	VAL	VAL	A4121	D4017	Q3900	A3736	W3627	L3473	A3381	A3381	K3307
THR	SER	GLY	GLU	GLU	GLU	V4124	L4020	R3903	P3762	E3636	P3474	K3382	K3382	K3308
ASN	GLU	VAL	ALA	VAL	ALA	L4132	T4030	N3904	M3763	E3636	I3475	W3383	W3383	V3309
LEU	GLU	GLY	ARG	ARG	ARG	L4132	F3905	F3905	V3764	P3646	L3475	L3384	L3384	K3310
THR	ARG	GLU	SER	SER	SER	I4135	E4033	I3909	T3767	C3647	C3480	K3385	K3385	L3313
SER	GLU	THR	THR	THR	THR	M4138	Y4034	D4035	Y3767	A3648	A3481	E3386	E3386	L3314
PRO	GLU	GLU	GLU	GLU	GLU	L4144	V4041	F3916	I3764	E3649	P3482	P3387	P3387	L3314
HIS	ASN	GLY	GLY	GLY	GLY	T4144	G4040	F3916	I3764	LEU	G3483	N3388	N3388	K3315
THR	GLN	VAL	VAL	VAL	VAL	L4144	V4041	T3920	N3769	PRO	D3484	P3389	P3389	T3316
PRO	PRO	ARG	ARG	ARG	ARG	Y4148	S4043	E3921	V3772	GLY	Q3485	E3390	E3390	F3318
GLU	VAL	PRO	VAL	VAL	VAL	F4149	K4044	Q3924	V3772	ASP	L3487	A3489	A3489	E3392
VAL	GLY	LEU	LEU	LEU	LEU	E4150	R4045	Q3924	K3775	GLU	T3488	L3490	L3490	E3392
VAL	PHE	LEU	LEU	LEU	LEU	T4151	D4046	L3934	M3776	ALA	SER	K3317	K3317	E3392
V4559	PHE	GLU	GLN	SER	HIS	S4152	F4047	A3935		K3658	VAL	F3491	F3491	E3393



● Molecule 1: Ryanodine receptor 2



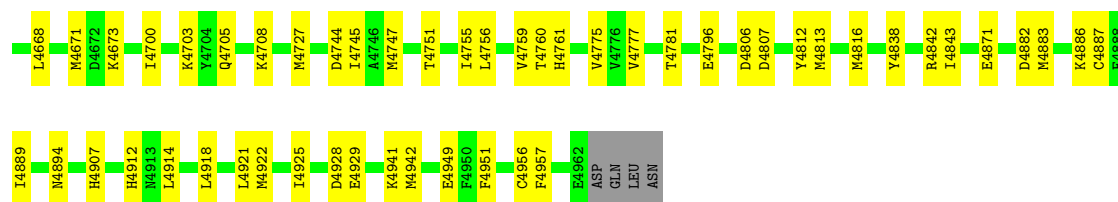
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V2592	Y2518	P2442	Y2219	Q2090	ASP	Q1845	P1750	M1600	D1458	GLY	ALA	G1218
M2604	L2519	S2224	S2224	Q2090	SER	L1846	L1754	P1601	D1459	PRO	GLY	K1219
L2608	C2520	M2233	M2233	T2094	LEU	I1847	L1754	M1602	L1460	LEU	LEU	V1221
L2609	T2521	M2233	M2233	T2094	ASP	F1852	L1758	V1609	R1461	ARG	PRO	Y1236
L2627	P2525	T2237	T2237	V2098	GLY	K1853	L1758	V1609	T1466	LEU	GLY	Y1236
Y2613	L2526	P2238	P2238	R2099	ASN	GLU	P1760	R1611	V1467	LEU	ALA	Y1236
E2614	L2527	L2239	L2239	Q1939	ASP	ALA	P1760	R1611	T1466	GLN	GLY	H1242
R2615	T2528	A2244	A2244	Q1939	LEU	VAL	F1767	G1617	T1468	ARG	PHE	H1242
L2618	R2529	E2452	E2452	T2102	THR	PRO	SER	V1620	L1469	PHE	TYR	R1245
Y2619	C2530	P2453	P2453	K2103	ILE	GLU	PHE	V1620	G1470	LEU	GLY	D1246
Y2620	L2527	L2239	L2239	T2104	ARG	GLU	VAL	Q1621	D1471	LEU	PRO	D1246
C2621	F2534	M2455	M2455	T2105	GLY	GLY	SER	C1622	E1472	ARG	LYS	T1248
L2622	A2535	S2456	D2260	S2121	ARG	GLY	ILE	L1623	H1477	THR	ASN	T1248
L2622	G2536	A2457	L2261	S1953	LEU	GLY	SER	L1623	H1477	THR	ASP	L1251
G2625	T2537	F2459	L2261	A1954	LEU	THR	ASN	E1636	I1480	LYS	LEU	L1251
H2540	H2540	D2379	V2265	L1956	SER	PRO	ASP	N1637	K1481	GLU	GLY	R1254
A2541	A2541	D2379	V2265	L1956	LEU	GLU	C1776	R1638	R1482	TYR	PHE	Q1257
S2542	S2542	H2382	R2132	R1959	VAL	LYS	D1786	D1641	S1483	SER	ASP	F1258
L2543	L2543	M2383	M2133	K1960	LYS	ILE	D1786	D1641	H1485	THR	VAL	P1262
L2544	L2544	Q2277	R2143	T1961	THR	SER	K1789	E1644	C1485	GLY	ASP	P1262
E2636	E2636	Q2277	R2143	T1961	THR	ILE	K1789	E1644	H1485	GLY	ASP	P1262
L2637	D2472	A2386	G2144	R1962	TYR	GLU	K1791	E1649	Y1486	SER	HIS	H1265
H2638	D2472	A2386	L2145	R1965	LEU	ASP	M1795	H1657	M1487	ALA	PHE	E1266
R2641	Y2474	L2387	M2149	S1967	LYS	ALA	M1795	H1657	E1507	ARG	GLU	H1267
L2642	Y2475	A2392	M2149	P1967	LYS	LYS	M1795	H1657	E1507	ARG	GLU	H1267
L2643	Q2480	M2405	F2154	P1968	LYS	LYS	M1795	H1657	E1507	ARG	GLU	H1267
F2644	D2481	H2406	P2158	P1968	LYS	LYS	M1795	H1657	E1507	ARG	GLU	H1267
L2645	F2482	L2407	R2159	Q1971	GLN	GLU	K1801	C1666	C1510	THR	LEU	E1269
G2646	L2483	L2408	L2160	I1972	GLU	GLU	E1802	C1666	C1510	THR	LEU	E1269
L2647	L2484	L2408	M2161	I1972	VAL	GLU	L1805	L1677	S1516	THR	THR	I1273
E2657	H2485	K2412	L2164	Q1971	ALA	ALA	R1808	L1686	Q1533	LEU	ALA	D1274
E2658	L2486	G2413	G2165	F1978	LYS	LYS	D1809	L1686	V1534	ALA	ALA	D1274
E2659	V2489	E2414	M2166	K1979	GLY	GLY	V1811	Y1694	E1535	ASP	GLY	THR
L2660	D2494	I2418	V2175	C1985	ARG	ARG	T1814	Y1704	V1553	PRO	PRO	R1272
F2661	L2495	R2419	P2189	C1985	LYS	PRO	T1815	D1705	F1554	ASP	ARG	I1273
K2662	R2496	R2419	P2189	P1988	CYS	LYS	E1816	L1706	E1557	ILE	ILE	THR
C2667	A2497	R2423	M2191	E1989	SER	GLU	F1817	L1707	E1557	ASP	ASP	THR
S2669	A2498	R2423	M2191	E1990	SER	GLU	L1818	L1708	E1557	ASP	ASP	THR
A2670	S2500	L2425	V2192	I1991	LYS	G1891	P1821	D1709	I1561	ASP	LYS	Q1287
V2671	L2501	L2426	A2193	R1992	LYS	M1895	Y1827	I1710	K1562	GLU	GLU	Q1287
A2672	L2502	D2430	R2197	L1995	ARG	E1899	Y1827	S1713	N1563	THR	THR	Q1283
G2673	T2503	L2343	R2197	F1998	LYS	P1900	I1831	A1718	H1576	LYS	LYS	N1294
A2674	L2506	M2346	F2198	H1999	PRO	V1901	I1834	M1721	K1577	PRO	PRO	N1295
L2680	L2507	M2346	Y2201	E2000	LYS	K1902	I1834	M1722	E1436	GLY	GLY	R1303
L2682	S2507	L2350	F2202	D2001	GLU	L1903	N1837	M1722	F1584	PHE	PHE	L1304
M2683	A2512	R2351	F2202	C2006	GLU	Q1904	E1838	Y1727	P1585	ASN	ASN	S1305
M2584	A2512	R2351	F2202	C2006	GLU	Q1904	E1838	Y1727	P1585	ASN	ASN	S1305
Q2585	L2513	I2437	I2205	I2008	LYS	L1907	L1840	P1729	H1588	HIS	HIS	C1310



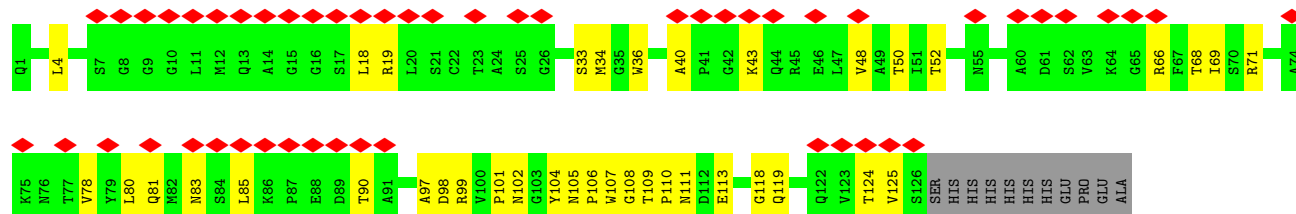
L1935	L1758	V1609	T1466	SER	LEU	K1219	Y1084	GLN	K941	ILE	L759	V610	R430
Q1939	R1759	S1610	V1467	ARG	PRO	D1220	K1097	ASP	T942	VAL	D760	L611	
R1942	P1760	R1611	T1468	LEU	GLY	V1221	A1098	VAL	L943	PRO	L761	D612	M494
M1947	P1767	G1617	L1469	LYS	ALA		A1099	ASN	L944	PRO	P764	L614	
S1953	SER	G1620	D1470	ARG	PHE	Y1236	R1099	R1027	A945		S767	R626	E500
A1954	PHE	V1620	E1471	PHE	TYR	N1242	W1101	R1028	L946		F768	L878	D503
A1955	VAL	Q1621	E1472	LEU	GLY	R1245	F1103	N1029	A953		R769	H630	R504
L1956	ILE	L1623	H1477	ARG	LYS	D1246	E1104	L1032	ASP		P774	L631	V507
R1959	THR	L1624	I1480	THR	ASN	T1247	M1113	V1033	ASP		R775	R656	
K1960	ASN	E1636	K1481	LYS	LEU	T1248	R1114	P1034	ALA		Q776	L861	A515
T1961	ASP	R1637	L1482	PRO	GLY	L1251	W1117	Y1035	GLU		G777	L666	A518
R1962	C1776	A1638	S1483	PRO	GLY	L1254	P1120	L1038	LYS		F778	G666	
R1965	D1786	D1641	N1484	TYR	PHE	R1254	P1124	D1039	VAL		F779	G666	
S1966	THR	E1644	Y1486	SER	ASP	Q1257	P1127	D1040	LYS		N781	Y670	E524
P1967	THR	E1649	M1487	GLY	ASP	F1258	E1127	K1043	LYS		F794	K671	E524
P1968	GLY	H1657	C1510	SER	SER	P1262	L1128	LYS	LEU		S795	K672	S525
Q1971	K1801	C1666	A1514	ARG	PHE	H1265	F1136	L1050	PRO		A796	M673	I529
I1972	E1802	L1677	A1515	THR	VAL	H1267	F1137	R1051	LYS		G797	Y674	A538
L1975	L1805	L1681	S1516	GLU	MET	I1268	D1138	E1052	ASN		I798	E676	
F1978	R1808	V1681	Q1533	ASP	LYS	E1269	R1144	R1055	X970		F802	L677	I541
P1979	L1809	L1686	E1534	VAL	THR	R1272	W1156	T1056	Q971		L803	M678	R542
C1985	P1810	Y1694	E1535	LEU	ALA	I1274	G1059	G1056	L972		P816	H681	K546
P1988	L1811	Y1704	T1538	ASP	GLY	D1274	C1164	Y1062	D982		Y819	H692	Q550
E1989	T1814	D1705	V1553	ARG	LEU	THR	M1165	HIS	P985		S837	P705	L555
E1990	L1815	L1706	F1554	ASP	VAL	ASP	V1166	LEU	P986		R338	Y706	D556
I1991	F1817	L1707	E1557	ARG	PRO	SER	M1167	ALA	D910		P339	P707	W557
R1992	L1818	I1708	E1557	ILE	ASP	PRO	M1173	PRO	N911		Y840	E712	L558
L1995	Y1827	D1709	R1560	ASP	LEU	CYS	M1174	ASP	K912		Y846	D720	I559
F1998	I1831	I1710	T1561	ASP	LYS	K1284	L1177	ASP	R913		L850	L732	E563
E2000	I1834	S1713	K1562	LYS	LYS	V1285	A1191	HIS	H915		L850	L732	R564
D2001	A1718	M1721	N1563	GLY	THR	T1286	F1192	ALA	P916		P853	L737	V574
C2006	N1837	M1722	C1583	PRO	PRO	Q1287	L1190	ARG	C917		L857	A738	L575
I2007	D1839	M1722	P1584	GLY	PRO	Q1293	A1191	ALA	L924		GLN	R739	V578
L1907	L1840	I1727	P1585	PHE	GLY	N1294	F1192	CYS	A1008		ALA	T741	L579
F1908	K1841	Y1728	G1444	ASN	ASN	N1295	F1201	SER	R1009		PHE	P744	A585
L1909	H1842	P1729	W1445	ASN	ASN	R1303	I1202	GLY	W1007		ALA	P744	A585
C1913	I1843	E1733	I1446	HIS	HIS	C1310	L1207	GLY	A1007		THR	H747	E591
R1920	Q1844	E1733	Q1590	LYS	LYS	S1315	G1208	GLY	Q1014		THR	L748	G592
D1929	L1846	L1739	V1595	TYR	TYR	LYS	V1209	R1084	GLY		VAL	L749	H593
V1932	I1847	P1750	W1596	ALA	ALA	SER	Q1211	F1085	TRP		PRO	R750	I594
	F1852	L1754	W1597	GLN	GLN	VAL	N1216	R1086	THR		ASP	T751	I597
	K1853		D1460	GLY	GLY	ALA	F1217	E1091	GLY		THR	S756	L601
	GLU		L1461	LYS	LYS	GLY	G1218	K1092	ILE		GLN	C757	
				PRO	PRO			T1093	GLN			C758	



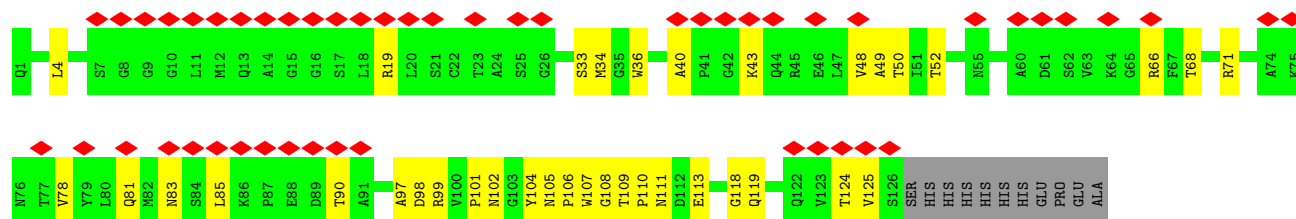




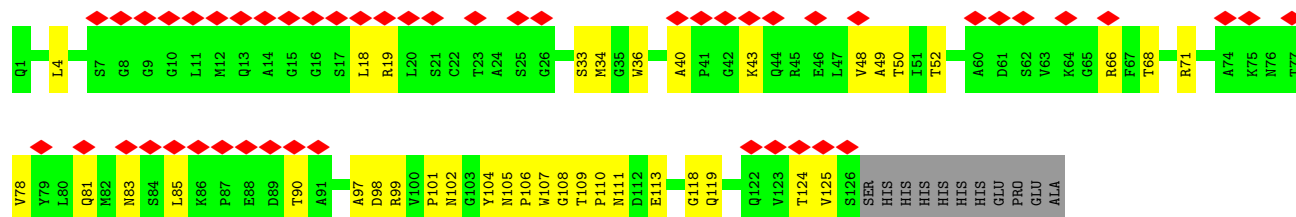
• Molecule 2: Nanobody 9657



• Molecule 2: Nanobody 9657

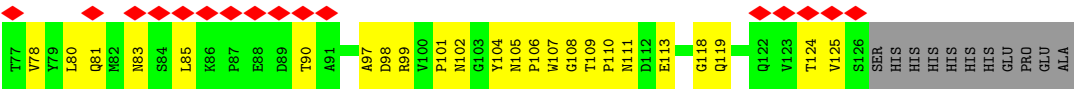


• Molecule 2: Nanobody 9657



• Molecule 2: Nanobody 9657





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	76852	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.181	Depositor
Minimum map value	-0.204	Depositor
Average map value	0.074	Depositor
Map value standard deviation	0.151	Depositor
Recommended contour level	0.35	Depositor
Map size ($\text{\AA}$)	490.56, 490.56, 490.56	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.46, 1.46, 1.46	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: ATP, CFF, CA, 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	0.13	0/33802	0.33	0/45653
1	C	0.13	0/33802	0.33	0/45653
1	E	0.13	0/33802	0.33	0/45653
1	F	0.13	0/33802	0.33	0/45653
2	B	0.11	0/984	0.28	0/1335
2	D	0.11	0/984	0.28	0/1335
2	G	0.11	0/984	0.28	0/1335
2	I	0.11	0/984	0.28	0/1335
All	All	0.13	0/139144	0.33	0/187952

There are no bond length outliers.

There are no bond angle outliers.

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	A	33088	0	32662	892	0
1	C	33088	0	32662	876	0
1	E	33088	0	32662	893	0
1	F	33088	0	32662	890	0
2	B	965	0	910	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	965	0	910	32	0
2	G	965	0	910	33	0
2	I	965	0	910	31	0
3	A	31	0	12	3	0
3	C	31	0	12	3	0
3	E	31	0	12	3	0
3	F	31	0	12	3	0
4	A	14	0	10	0	0
4	C	14	0	10	0	0
4	E	14	0	10	0	0
4	F	14	0	10	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
All	All	136400	0	134376	3636	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 13.

The worst 5 of 3636 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:3292:GLY:HA3	1:A:3295:MET:HE3	1.48	0.95
1:C:3292:GLY:HA3	1:C:3295:MET:HE3	1.48	0.93
1:E:3292:GLY:HA3	1:E:3295:MET:HE3	1.48	0.93
1:F:3292:GLY:HA3	1:F:3295:MET:HE3	1.48	0.92
1:E:2998:LYS:HG3	1:E:3002:MET:HE3	1.56	0.87

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	4094/4966 (82%)	3987 (97%)	106 (3%)	1 (0%)	100	100
1	C	4094/4966 (82%)	3986 (97%)	107 (3%)	1 (0%)	100	100
1	E	4094/4966 (82%)	3986 (97%)	107 (3%)	1 (0%)	100	100
1	F	4094/4966 (82%)	3983 (97%)	110 (3%)	1 (0%)	100	100
2	B	124/137 (90%)	118 (95%)	6 (5%)	0	100	100
2	D	124/137 (90%)	118 (95%)	6 (5%)	0	100	100
2	G	124/137 (90%)	118 (95%)	6 (5%)	0	100	100
2	I	124/137 (90%)	118 (95%)	6 (5%)	0	100	100
All	All	16872/20412 (83%)	16414 (97%)	454 (3%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2530	CYS
1	C	2530	CYS
1	E	2530	CYS
1	F	2530	CYS

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	3589/4355 (82%)	3581 (100%)	8 (0%)	87	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	3589/4355 (82%)	3582 (100%)	7 (0%)	87	85
1	E	3589/4355 (82%)	3580 (100%)	9 (0%)	86	84
1	F	3589/4355 (82%)	3581 (100%)	8 (0%)	87	85
2	B	103/114 (90%)	103 (100%)	0	100	100
2	D	103/114 (90%)	103 (100%)	0	100	100
2	G	103/114 (90%)	103 (100%)	0	100	100
2	I	103/114 (90%)	103 (100%)	0	100	100
All	All	14768/17876 (83%)	14736 (100%)	32 (0%)	85	85

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	2638	HIS
1	F	3167	ILE
1	C	3167	ILE
1	C	2638	HIS
1	F	3372	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 118 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	81	GLN
1	F	3902	GLN
1	E	2058	GLN
1	F	3881	GLN
1	F	2058	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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
4	CFF	C	5102	-	15,15,15	0.59	0	23,23,23	0.72	1 (4%)
3	ATP	A	5101	-	32,33,33	0.35	0	48,52,52	0.33	0
3	ATP	C	5101	-	32,33,33	0.35	0	48,52,52	0.33	0
4	CFF	A	5102	-	15,15,15	0.59	0	23,23,23	0.71	1 (4%)
4	CFF	F	5102	-	15,15,15	0.59	0	23,23,23	0.72	1 (4%)
3	ATP	E	5101	-	32,33,33	0.35	0	48,52,52	0.33	0
3	ATP	F	5101	-	32,33,33	0.35	0	48,52,52	0.33	0
4	CFF	E	5102	-	15,15,15	0.59	0	23,23,23	0.71	1 (4%)

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
4	CFF	C	5102	-	-	-	0/2/2/2
3	ATP	A	5101	-	-	5/22/38/38	0/3/3/3
3	ATP	C	5101	-	-	5/22/38/38	0/3/3/3
4	CFF	A	5102	-	-	-	0/2/2/2
4	CFF	F	5102	-	-	-	0/2/2/2
3	ATP	E	5101	-	-	5/22/38/38	0/3/3/3
3	ATP	F	5101	-	-	5/22/38/38	0/3/3/3
4	CFF	E	5102	-	-	-	0/2/2/2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	5102	CFF	C12-N3-C2	2.36	121.45	117.33
4	C	5102	CFF	C12-N3-C2	2.34	121.41	117.33
4	E	5102	CFF	C12-N3-C2	2.34	121.41	117.33
4	A	5102	CFF	C12-N3-C2	2.32	121.37	117.33

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

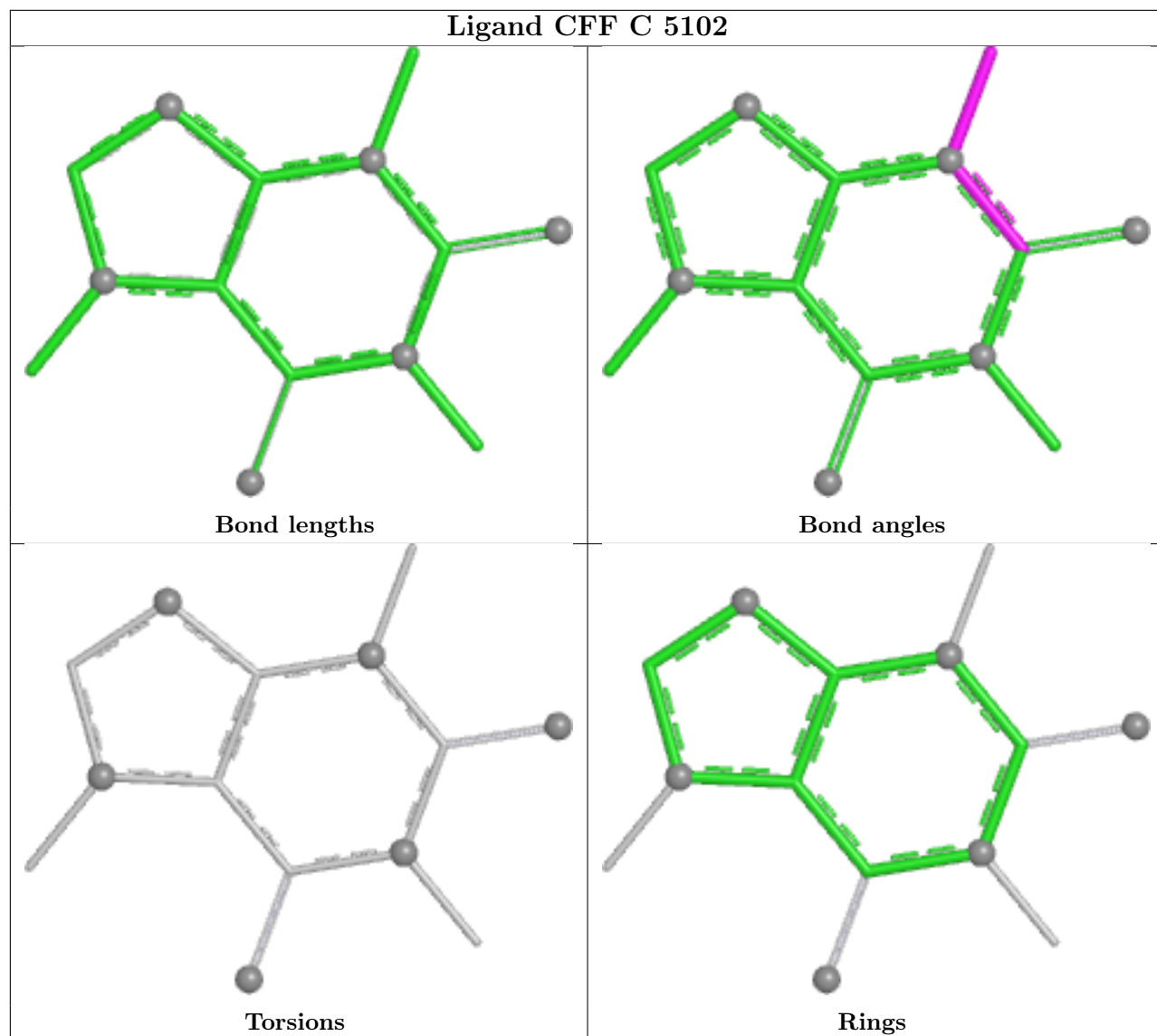
Mol	Chain	Res	Type	Atoms
3	A	5101	ATP	C5'-O5'-PA-O1A
3	A	5101	ATP	C5'-O5'-PA-O3A
3	C	5101	ATP	C5'-O5'-PA-O1A
3	C	5101	ATP	C5'-O5'-PA-O3A
3	E	5101	ATP	C5'-O5'-PA-O1A

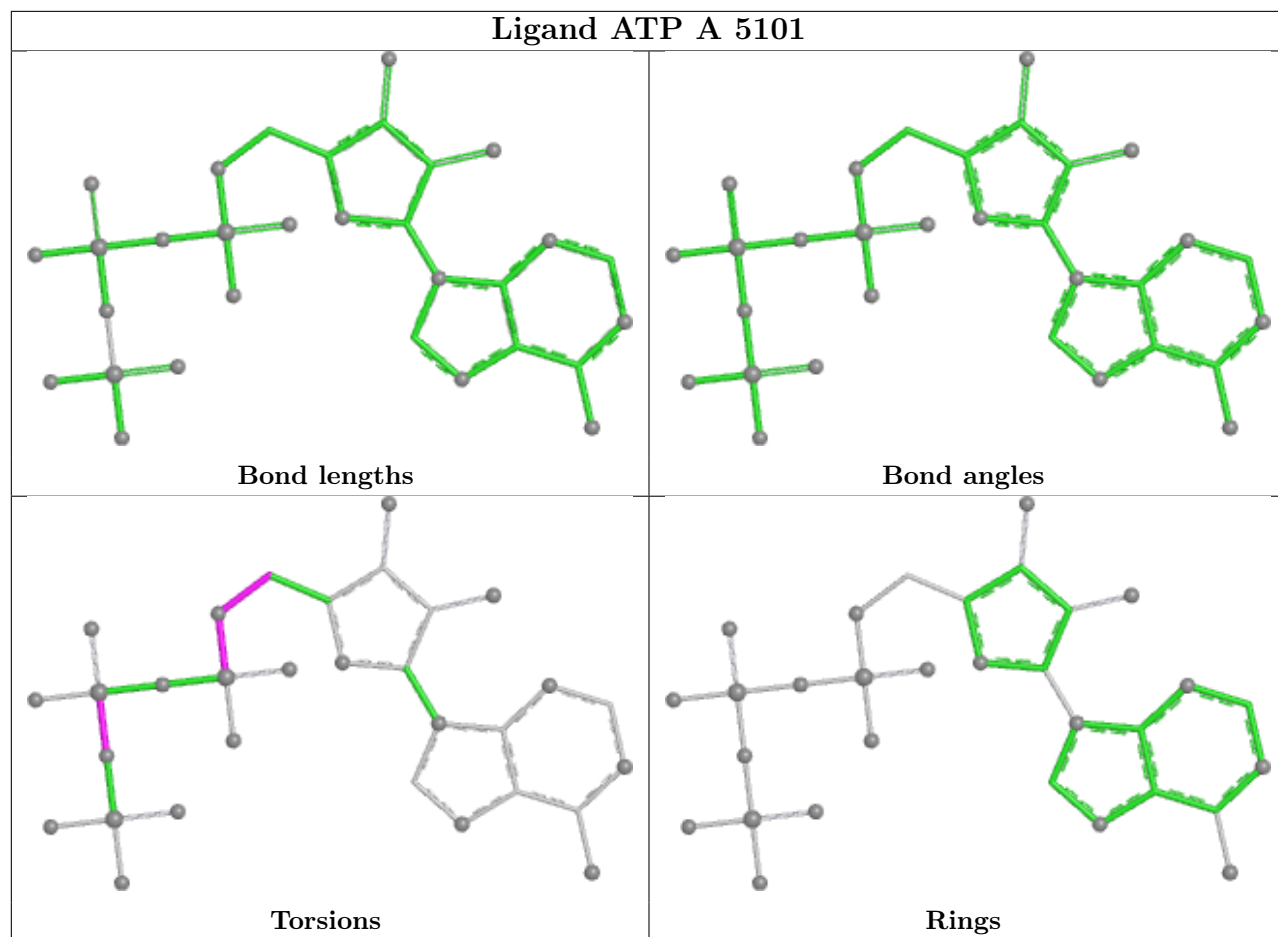
There are no ring outliers.

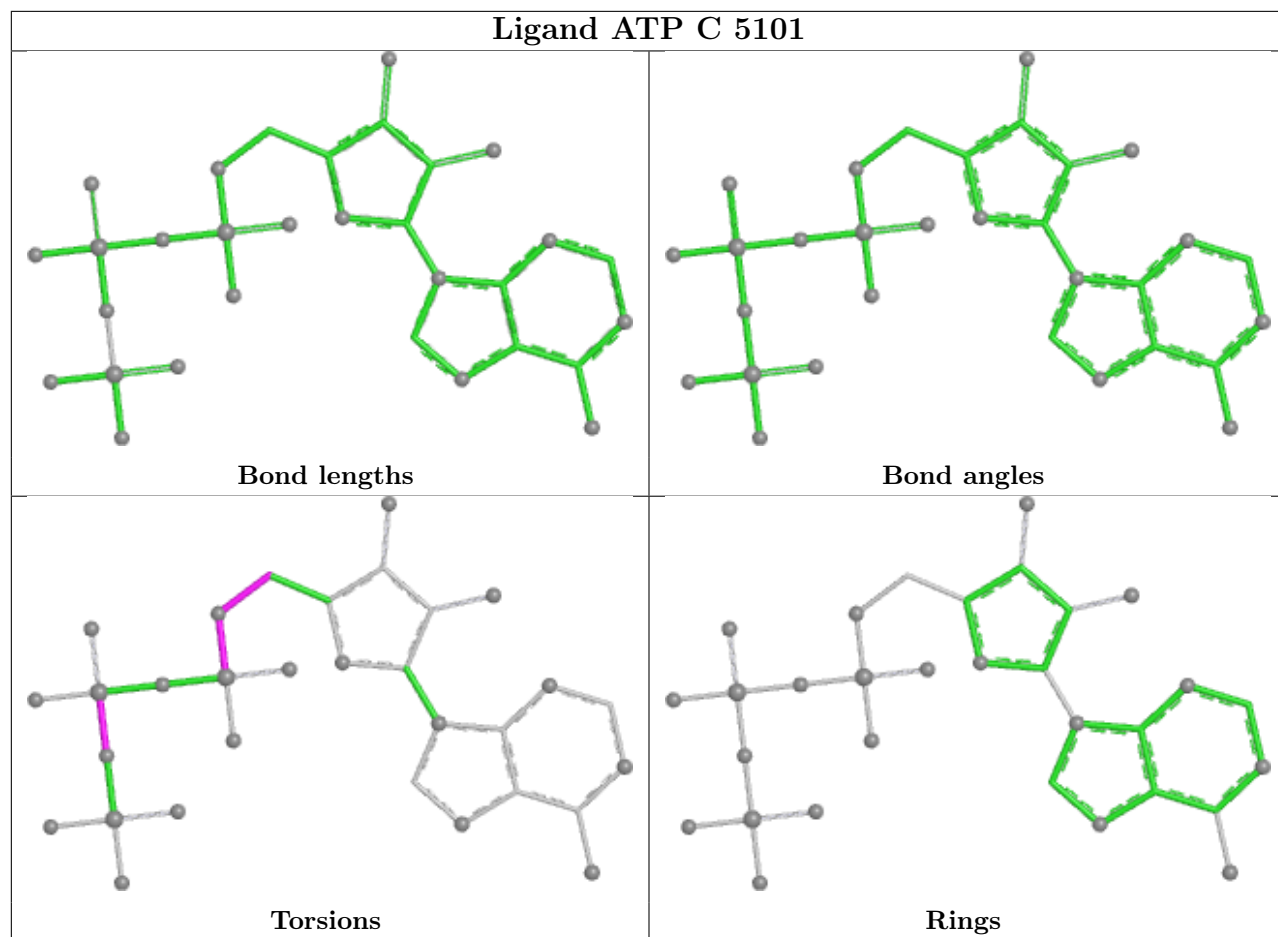
4 monomers are involved in 12 short contacts:

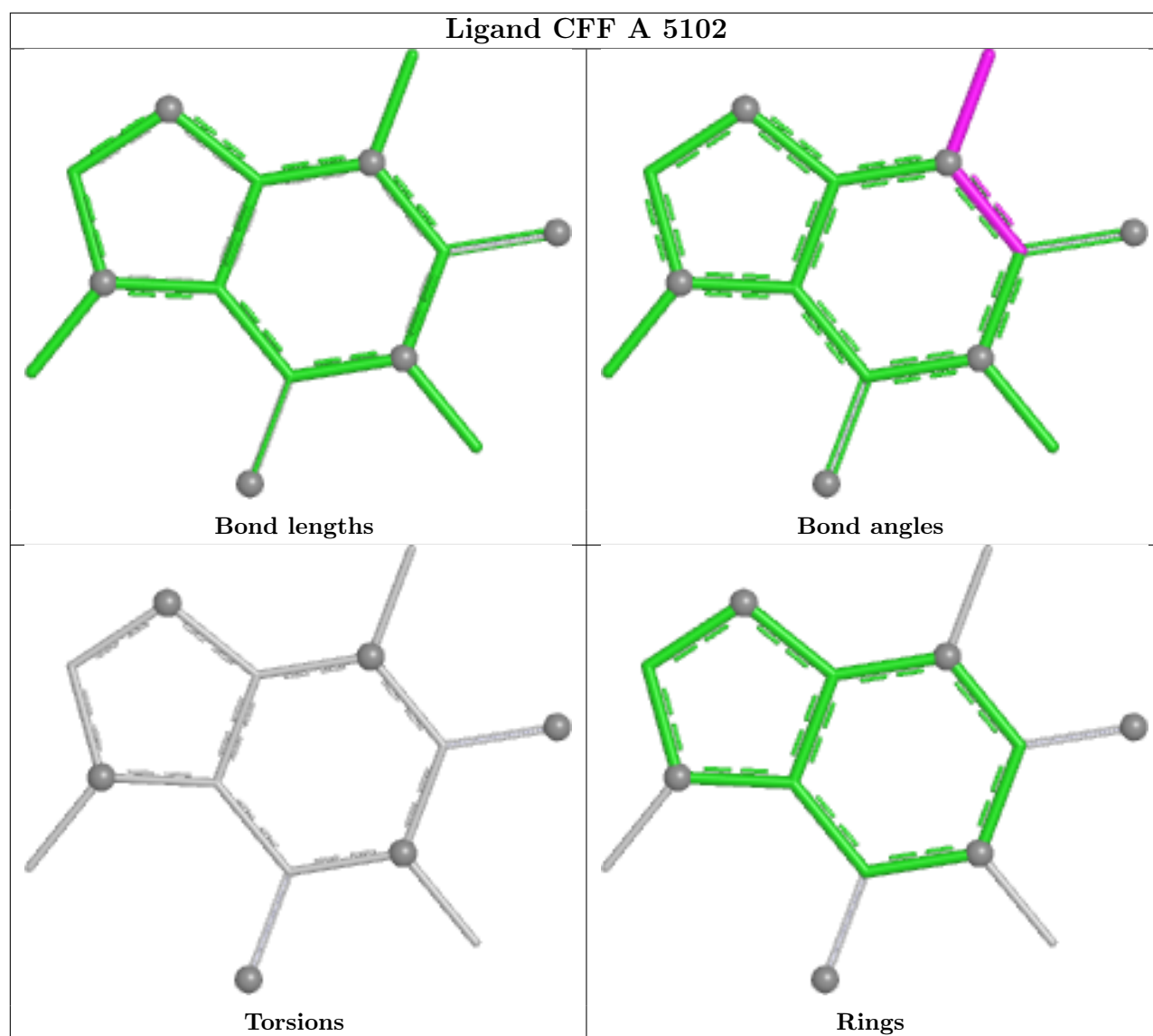
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	5101	ATP	3	0
3	C	5101	ATP	3	0
3	E	5101	ATP	3	0
3	F	5101	ATP	3	0

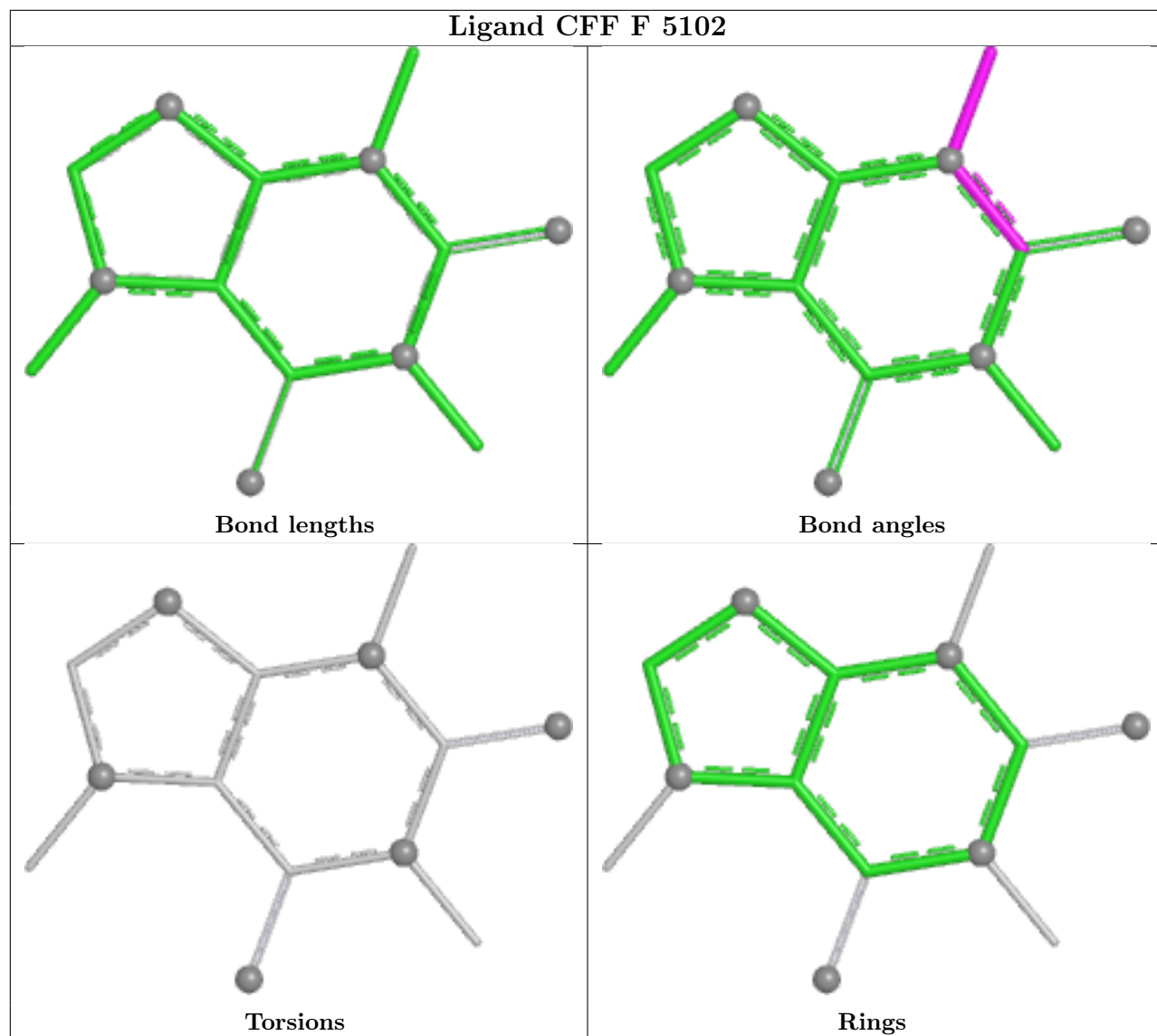
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

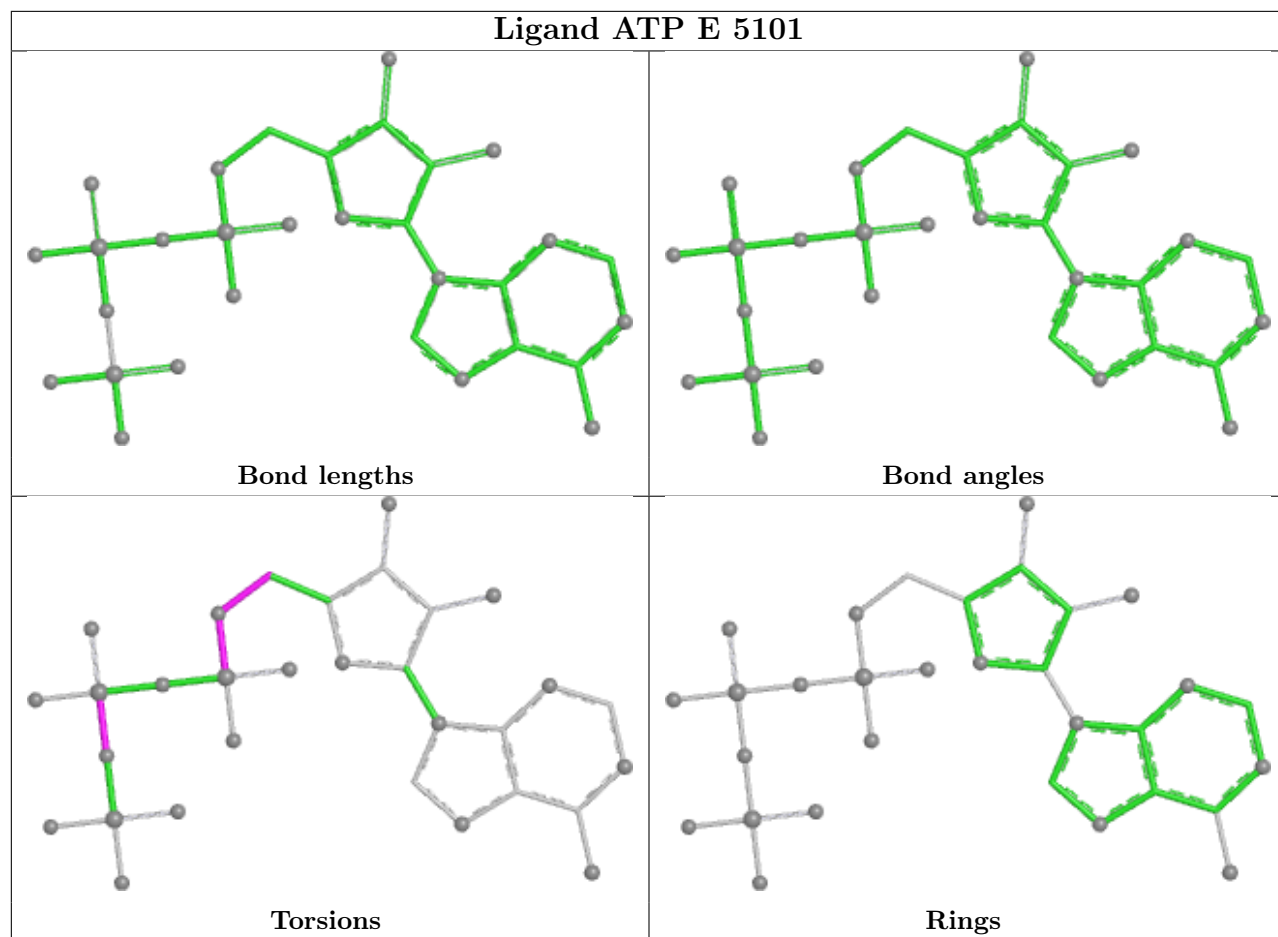


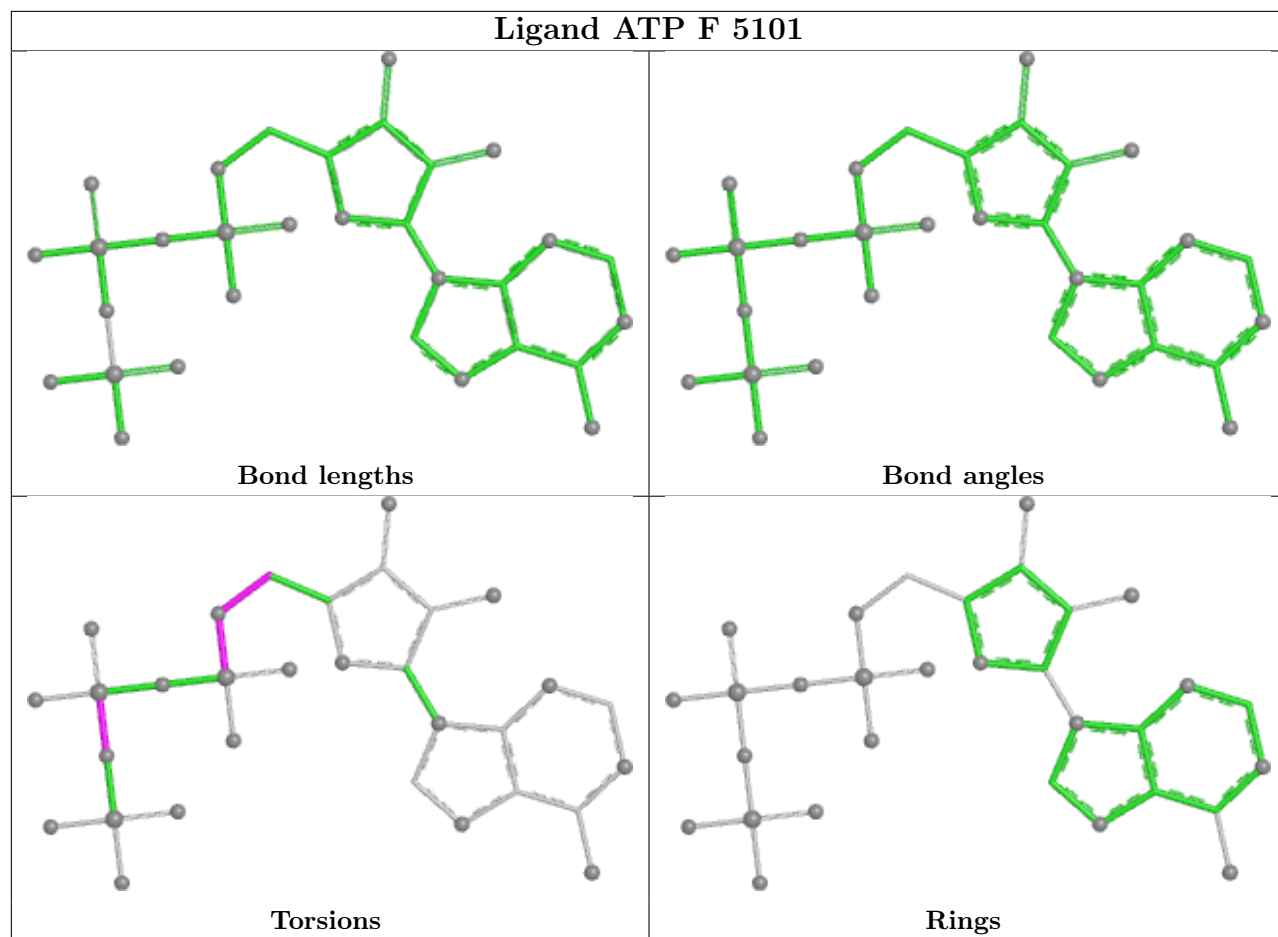


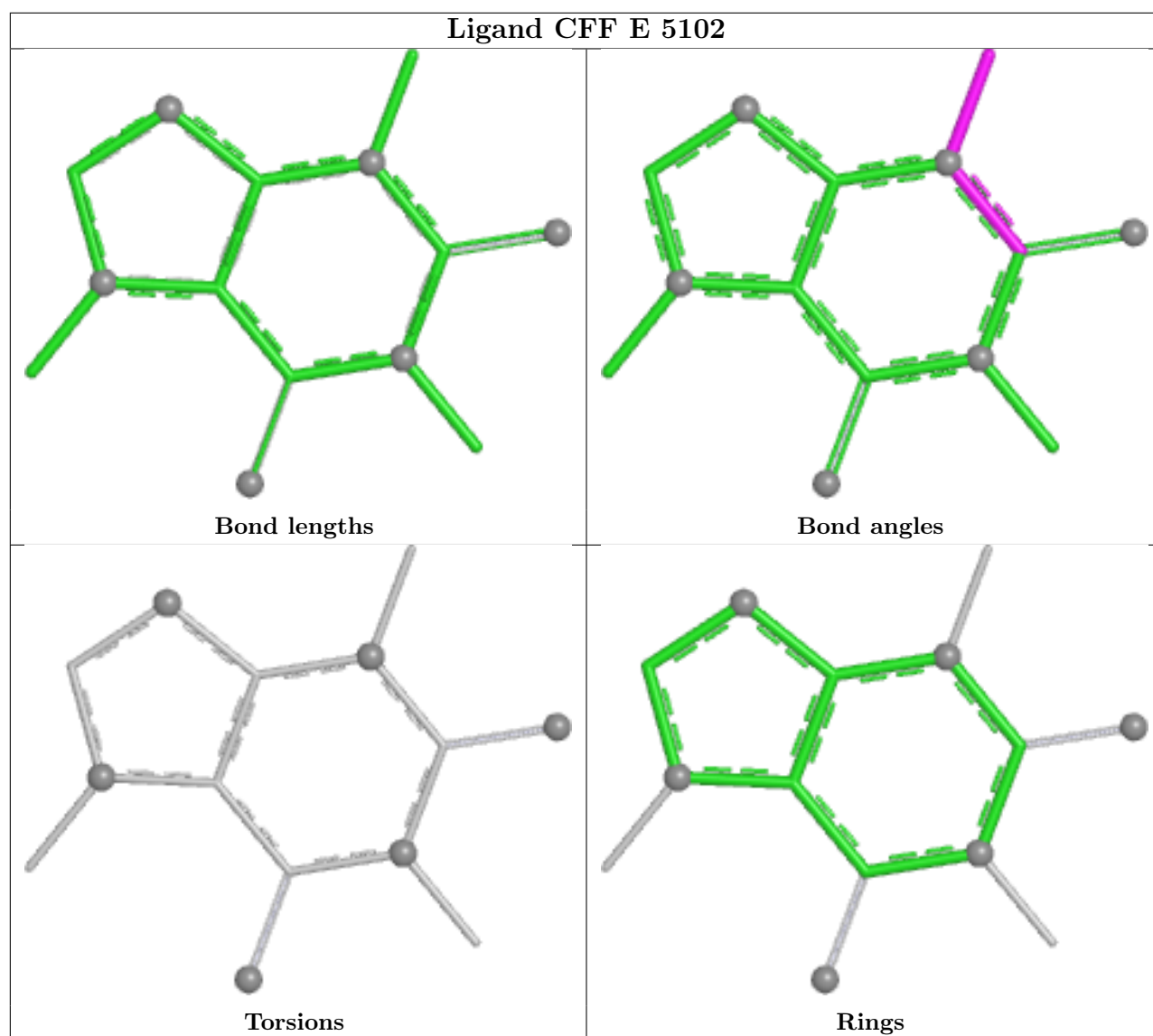












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

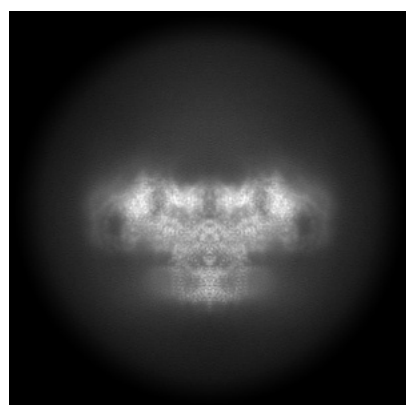
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19463. These allow visual inspection of the internal detail of the map and identification of artifacts.

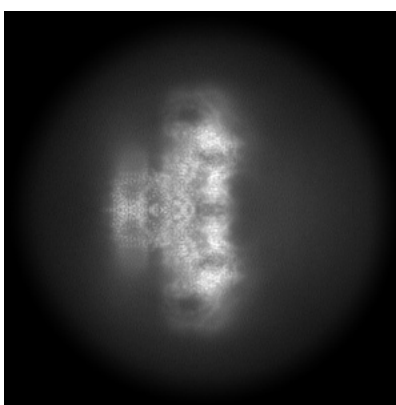
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

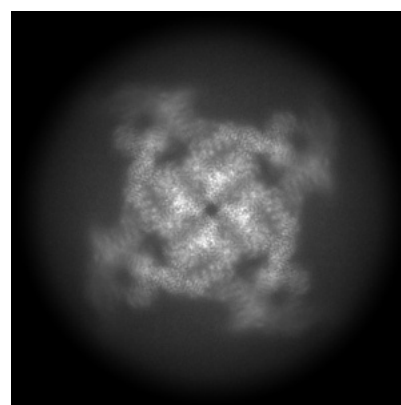
6.1.1 Primary map



X



Y

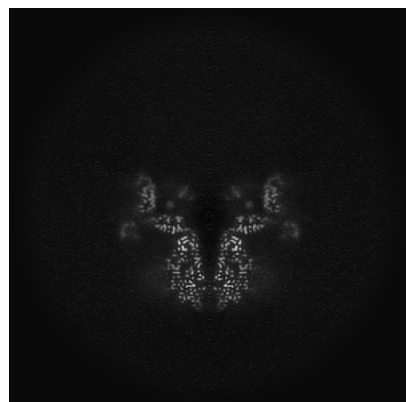


Z

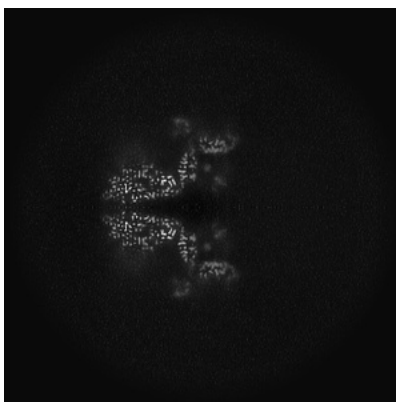
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

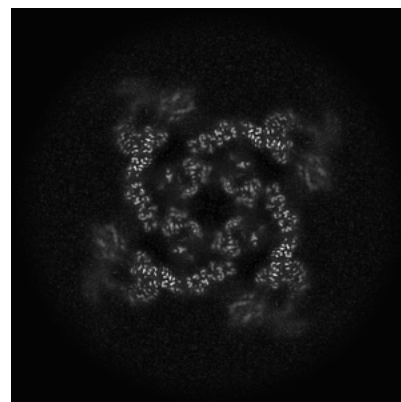
6.2.1 Primary map



X Index: 168



Y Index: 168

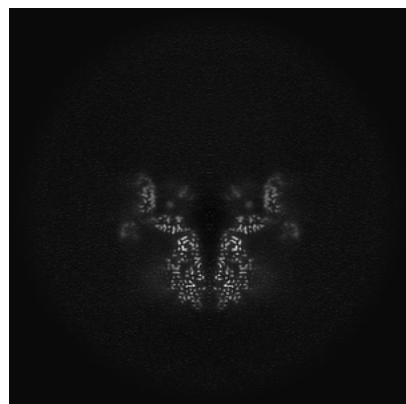


Z Index: 168

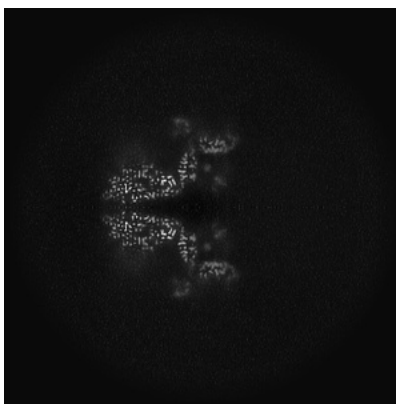
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

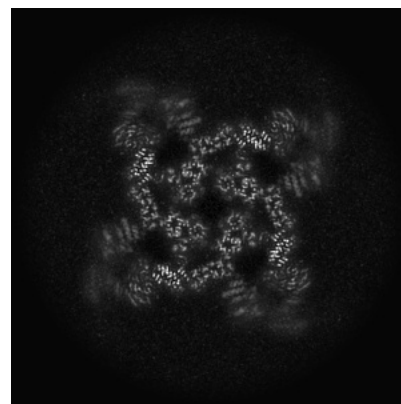
6.3.1 Primary map



X Index: 168



Y Index: 168

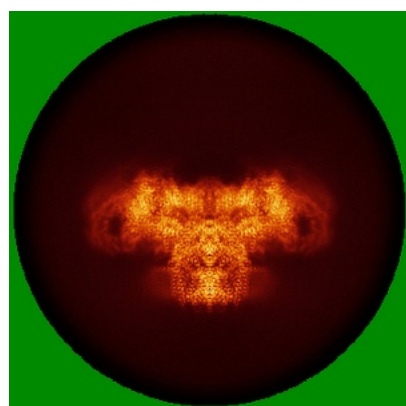


Z Index: 173

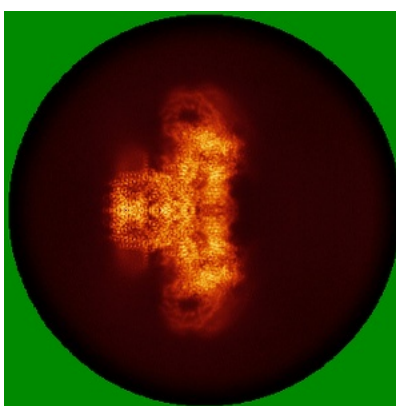
The images above show the largest variance slices of the map in three orthogonal directions.

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

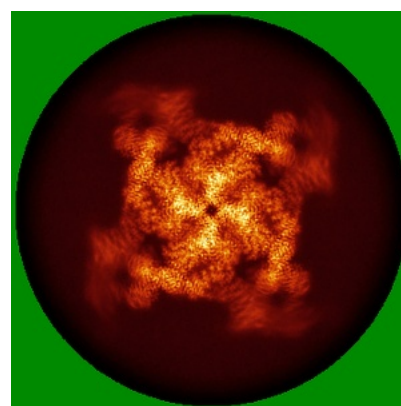
6.4.1 Primary map



X



Y

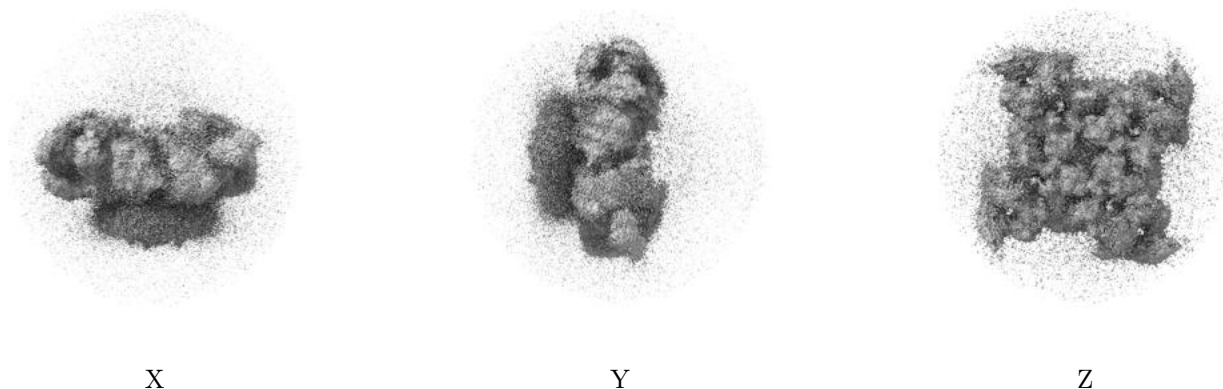


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.35. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

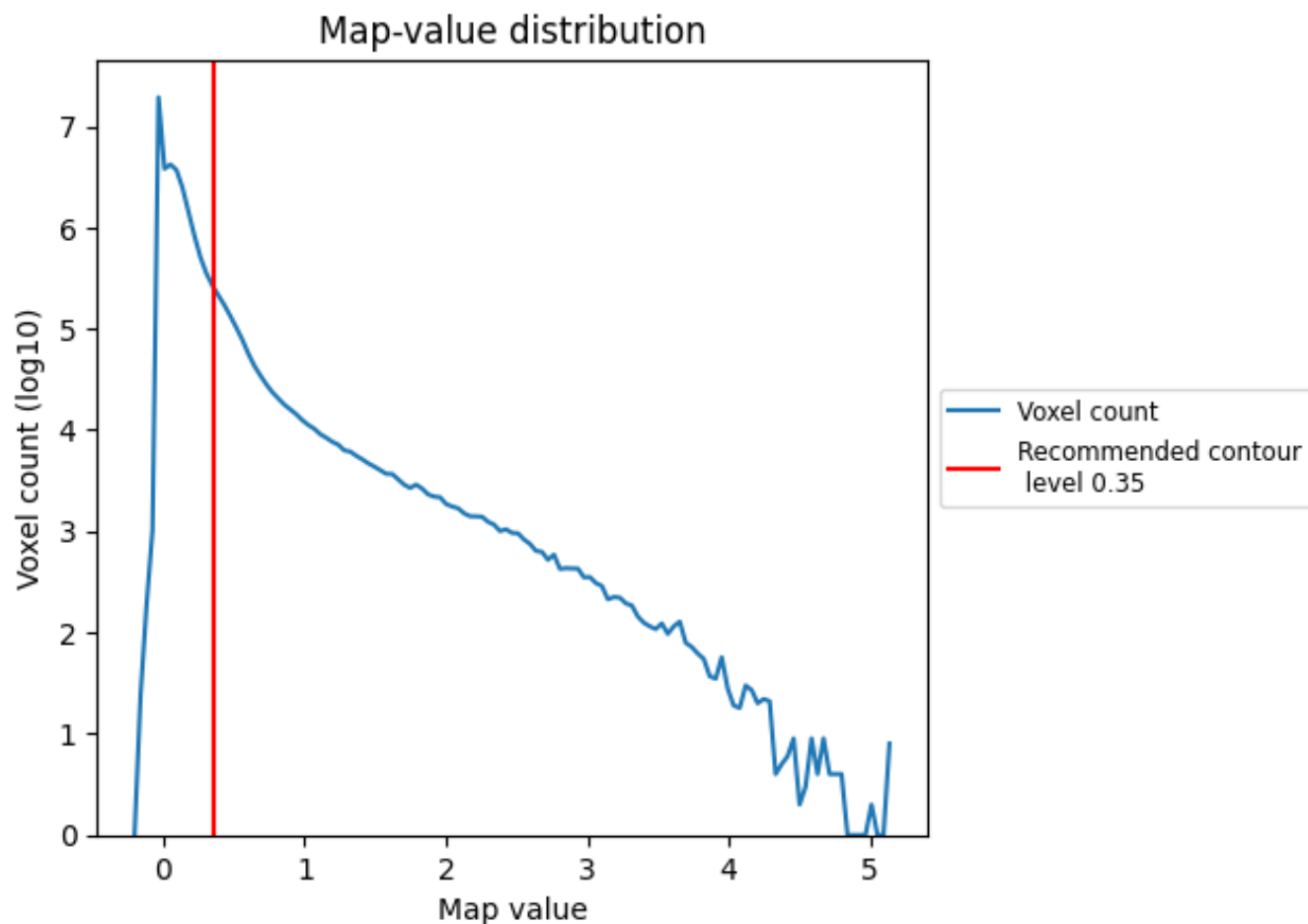
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

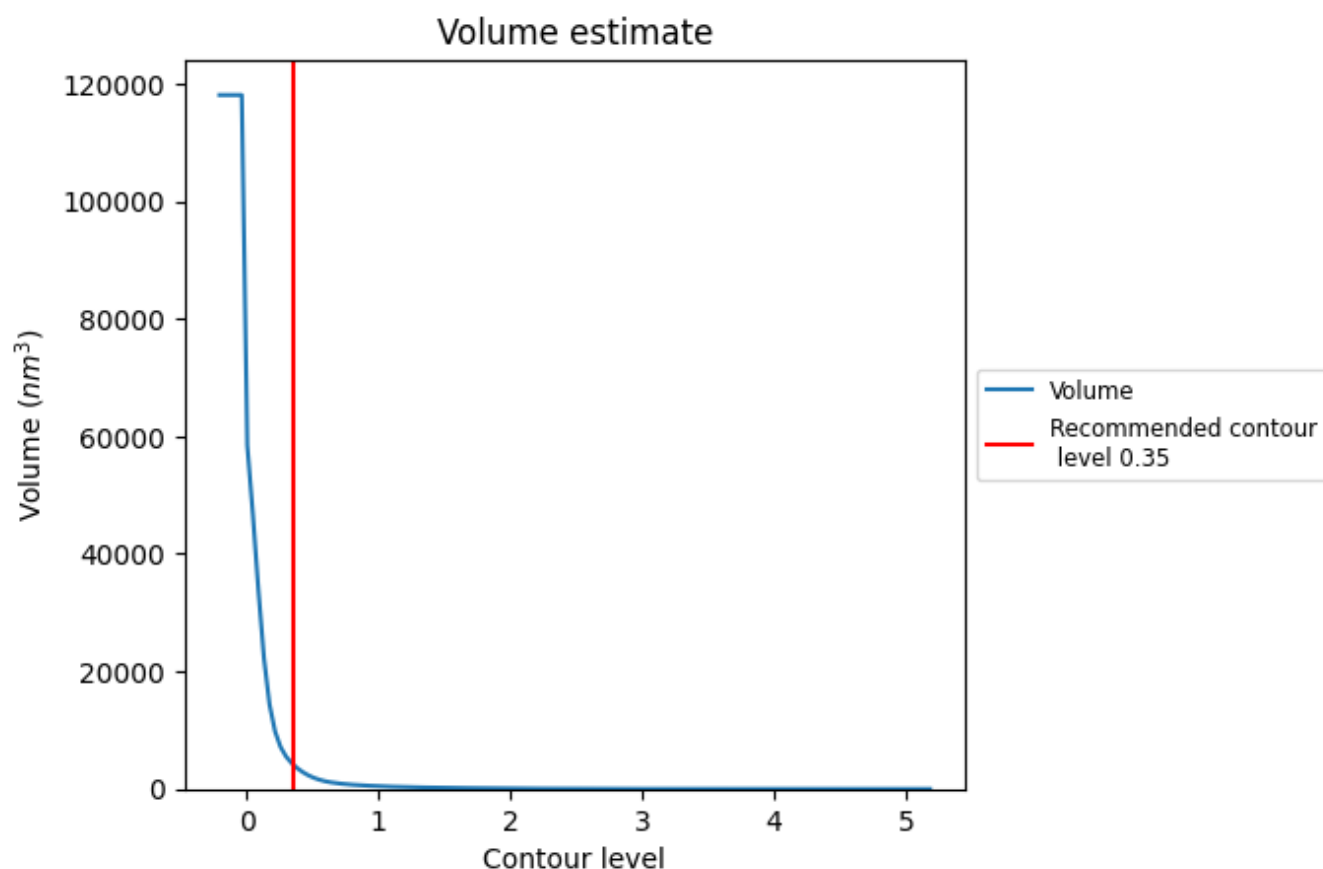
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

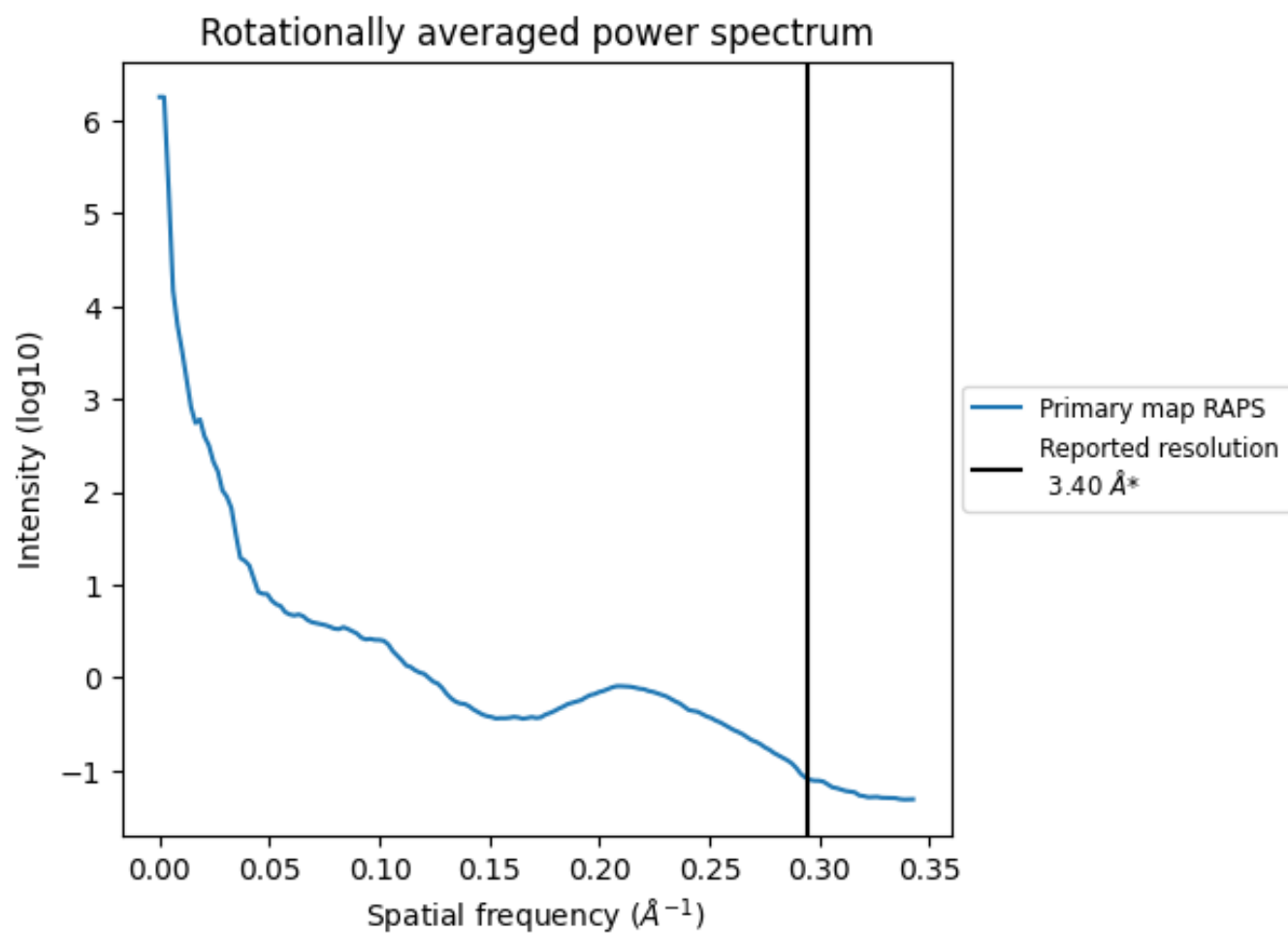
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4230 nm³; this corresponds to an approximate mass of 3821 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 ⓘ

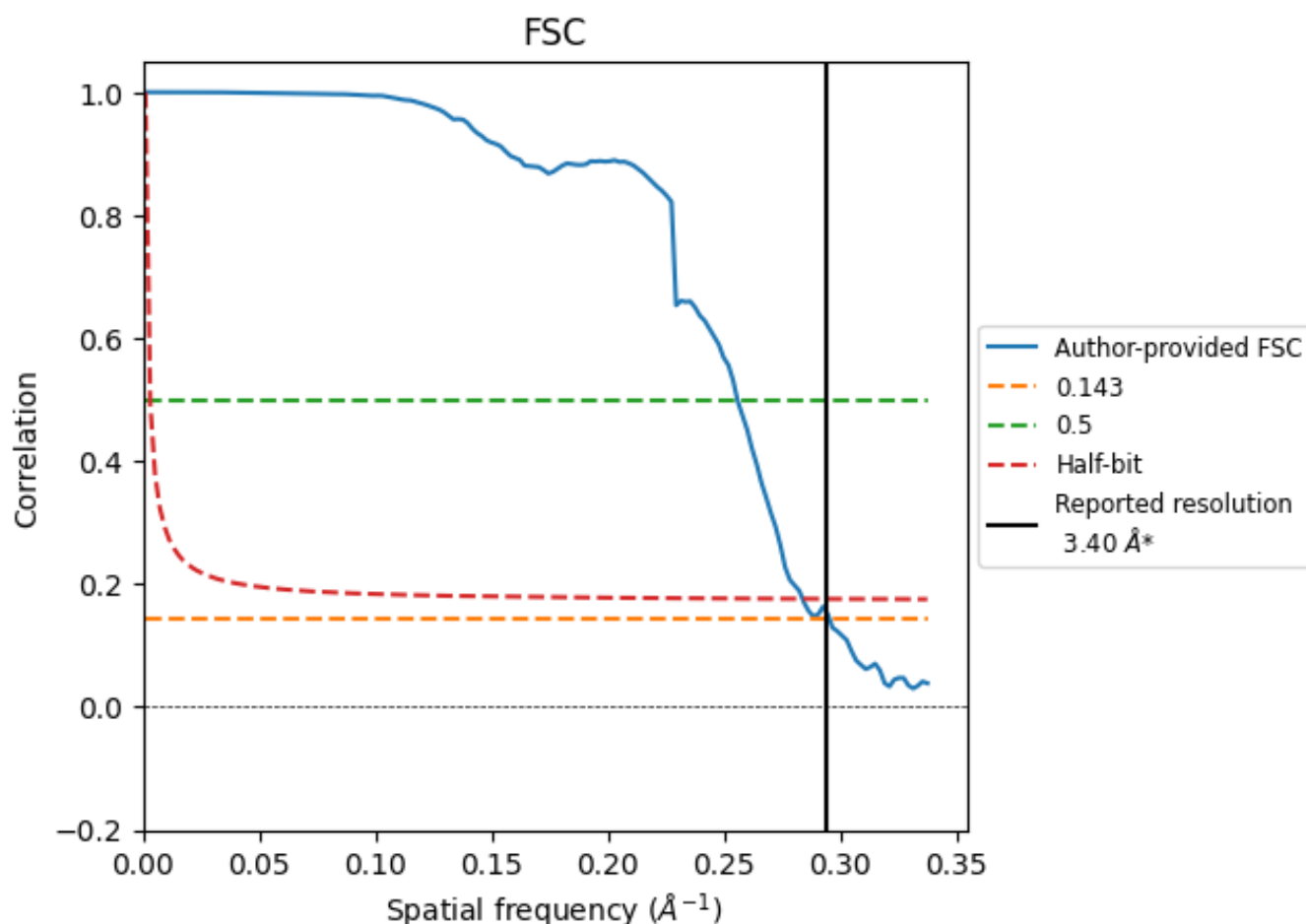


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

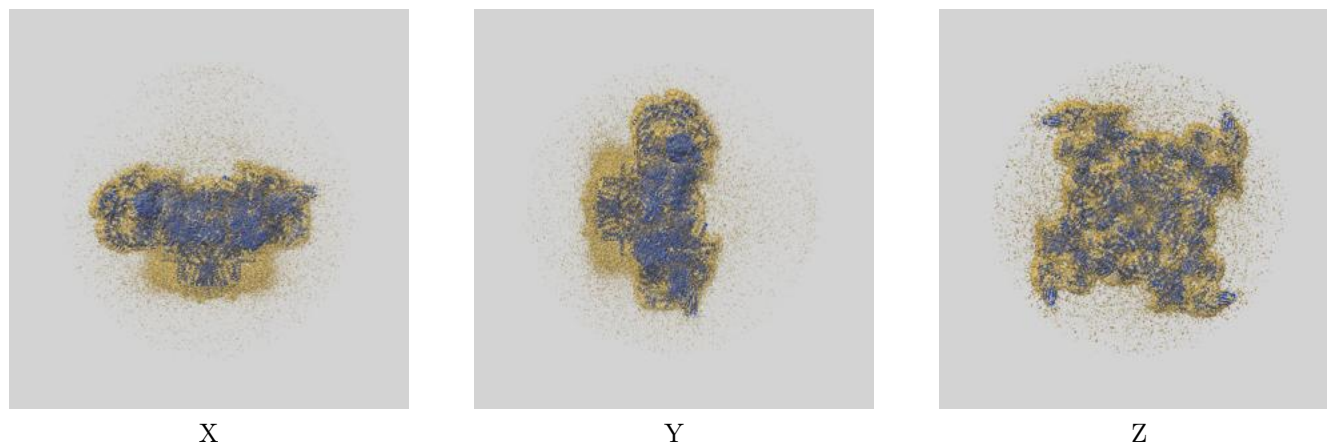
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.39	3.91	3.52
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

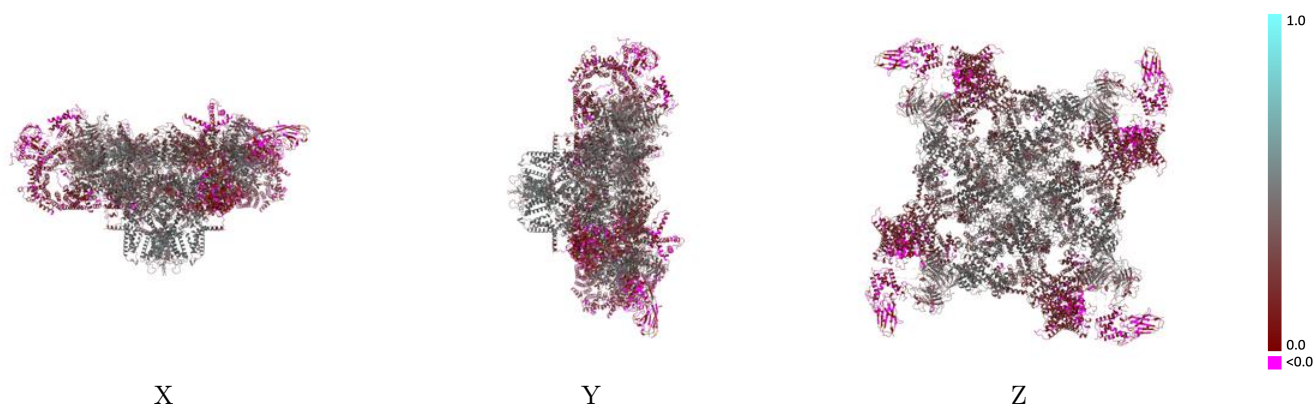
This section contains information regarding the fit between EMDB map EMD-19463 and PDB model 8RRS. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



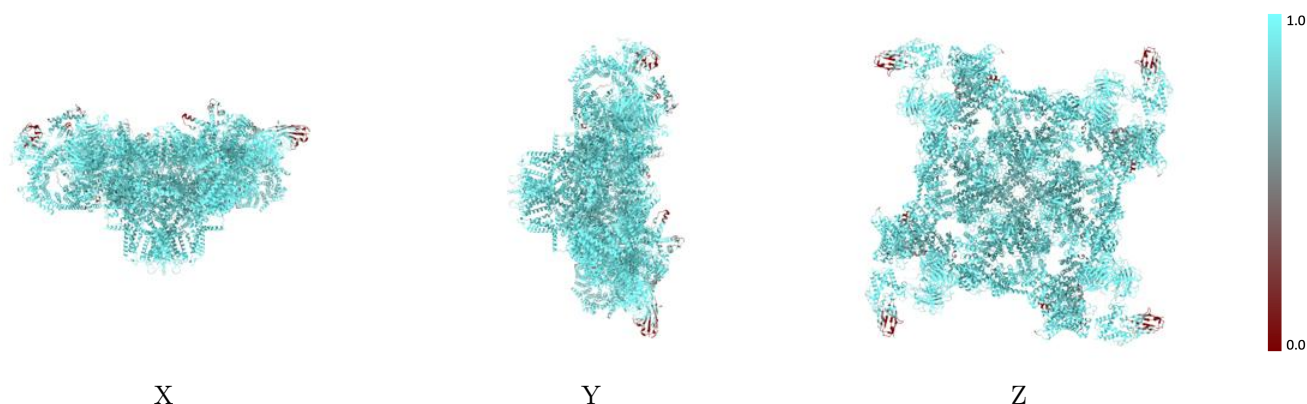
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



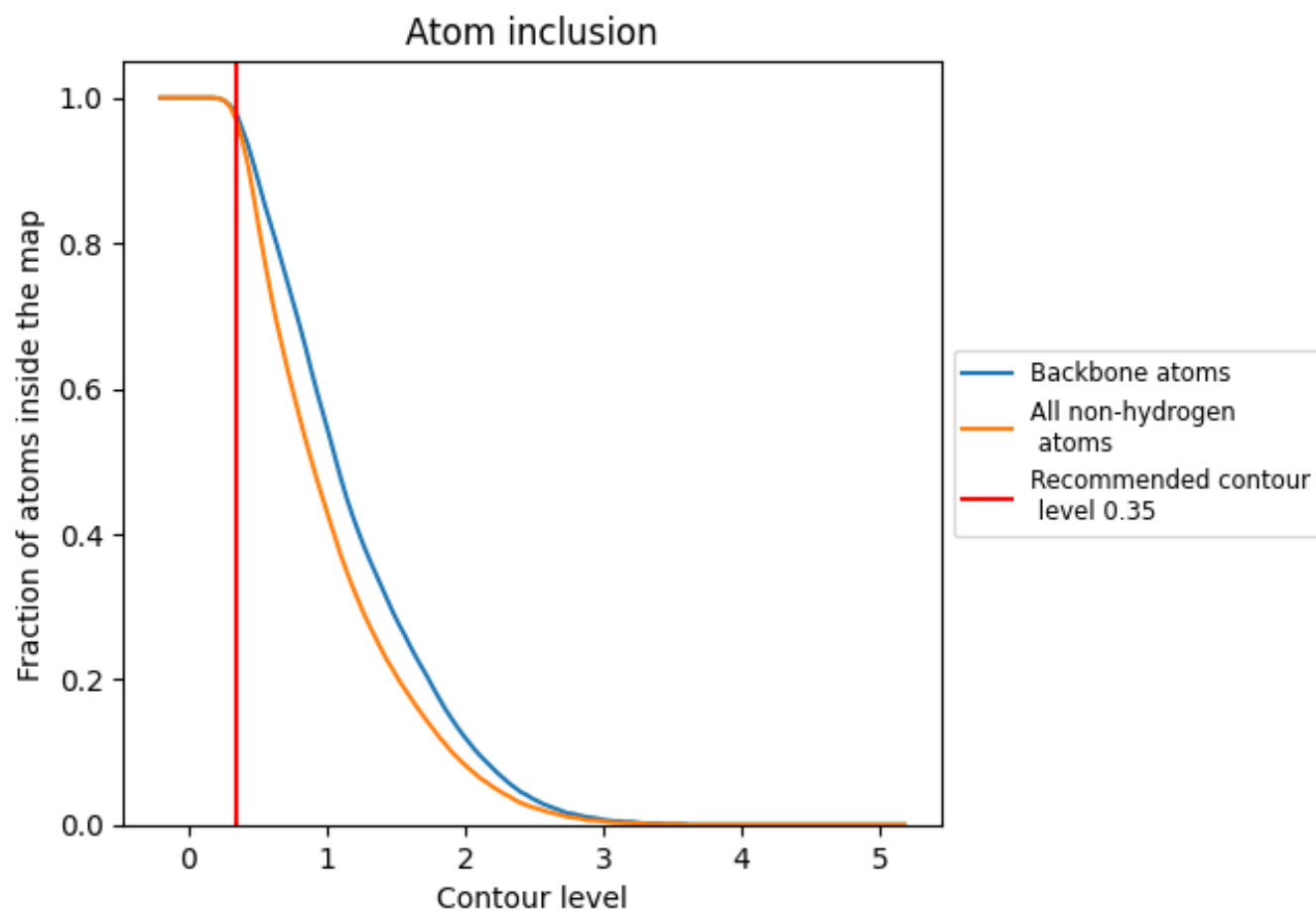
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.35).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 97% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9670	0.3070
A	0.9780	0.3140
B	0.5750	0.0800
C	0.9780	0.3140
D	0.5720	0.0810
E	0.9780	0.3130
F	0.9780	0.3130
G	0.5750	0.0790
I	0.5750	0.0790

1.0

0.0

<0.0