



wwPDB EM Validation Summary Report ⓘ

Nov 10, 2024 – 11:56 PM EST

PDB ID : 7M6L
EMDB ID : EMD-23699
Title : High resolution structure of the membrane embedded skeletal muscle ryanodine receptor
Authors : Melville, Z.; Kim, K.; Clarke, O.B.; Marks, A.R.
Deposited on : 2021-03-25
Resolution : 3.98 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.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

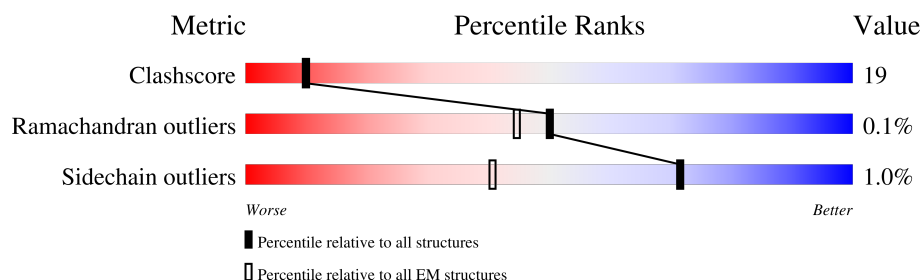
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.98 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 ≥ 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	F	108	
1	H	108	
1	J	108	
1	O	108	
2	A	5037	
2	B	5037	
2	G	5037	
2	I	5037	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 140412 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.

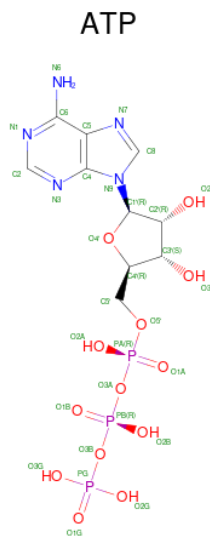
- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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

- Molecule 2 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	4299	Total	C	N	O	S	3	0
			34238	21819	5882	6302	235		
2	G	4299	Total	C	N	O	S	3	0
			34238	21819	5882	6302	235		
2	B	4299	Total	C	N	O	S	3	0
			34238	21819	5882	6302	235		
2	I	4299	Total	C	N	O	S	3	0
			34238	21819	5882	6302	235		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total 31	C 10	N 5	O 13	P 3	0
3	G	1	Total 31	C 10	N 5	O 13	P 3	0
3	B	1	Total 31	C 10	N 5	O 13	P 3	0
3	I	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total Ca 1 1	0
4	G	1	Total Ca 1 1	0
4	B	1	Total Ca 1 1	0
4	I	1	Total Ca 1 1	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

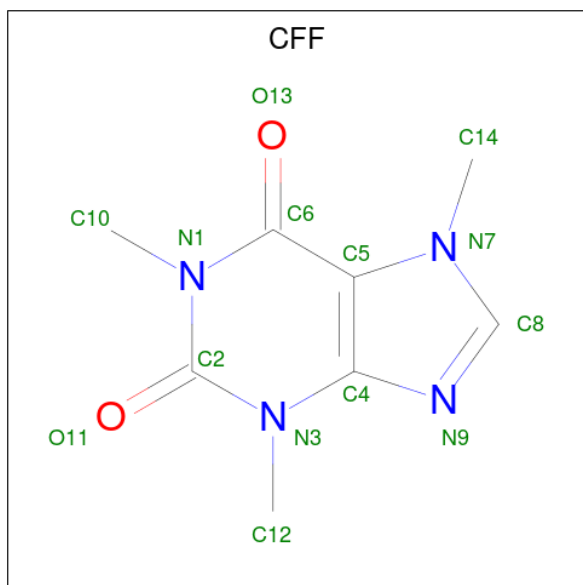
Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
5	G	1	Total	Zn	0
			1	1	
5	B	1	Total	Zn	0
			1	1	
5	I	1	Total	Zn	0
			1	1	

- Molecule 6 is CAFFEINE (three-letter code: CFF) (formula: $C_8H_{10}N_4O_2$).

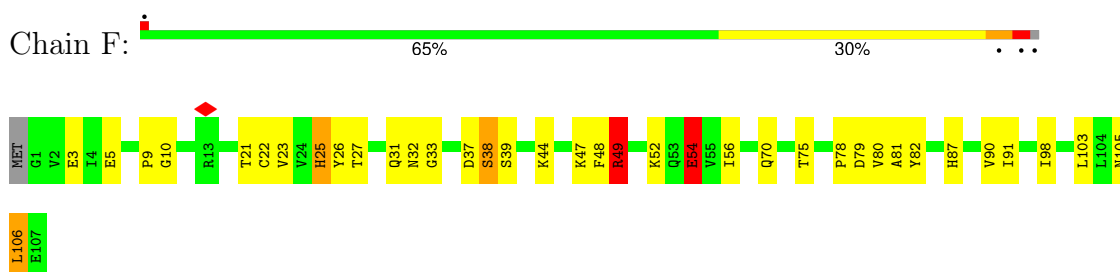


Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			14	8	4	2	
6	G	1	Total	C	N	O	0
			14	8	4	2	
6	B	1	Total	C	N	O	0
			14	8	4	2	
6	I	1	Total	C	N	O	0
			14	8	4	2	

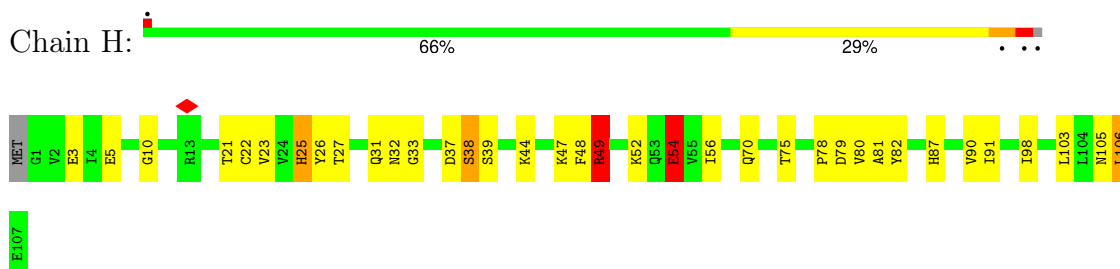
3 Residue-property plots [i](#)

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.

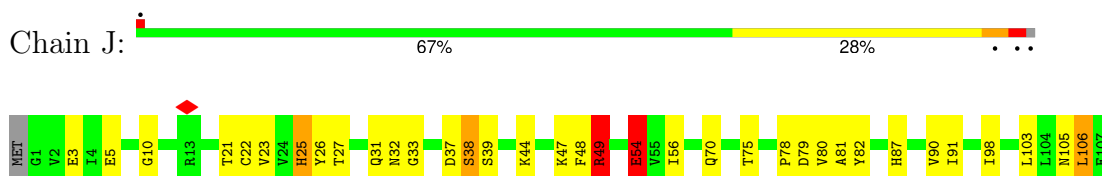
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



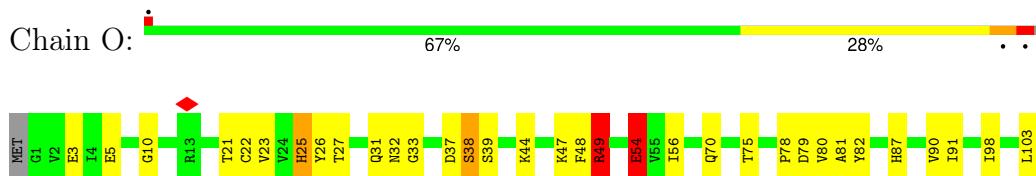
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



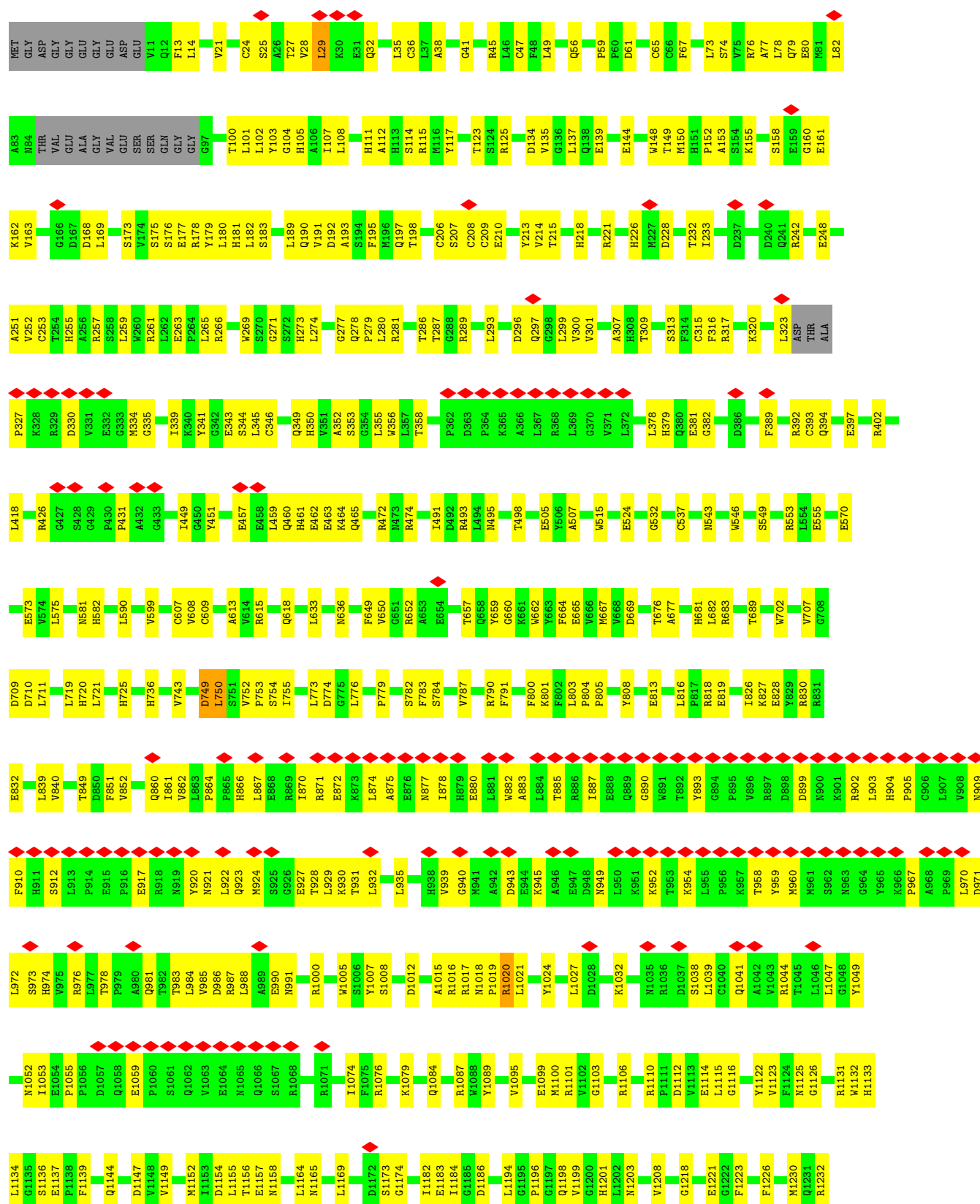
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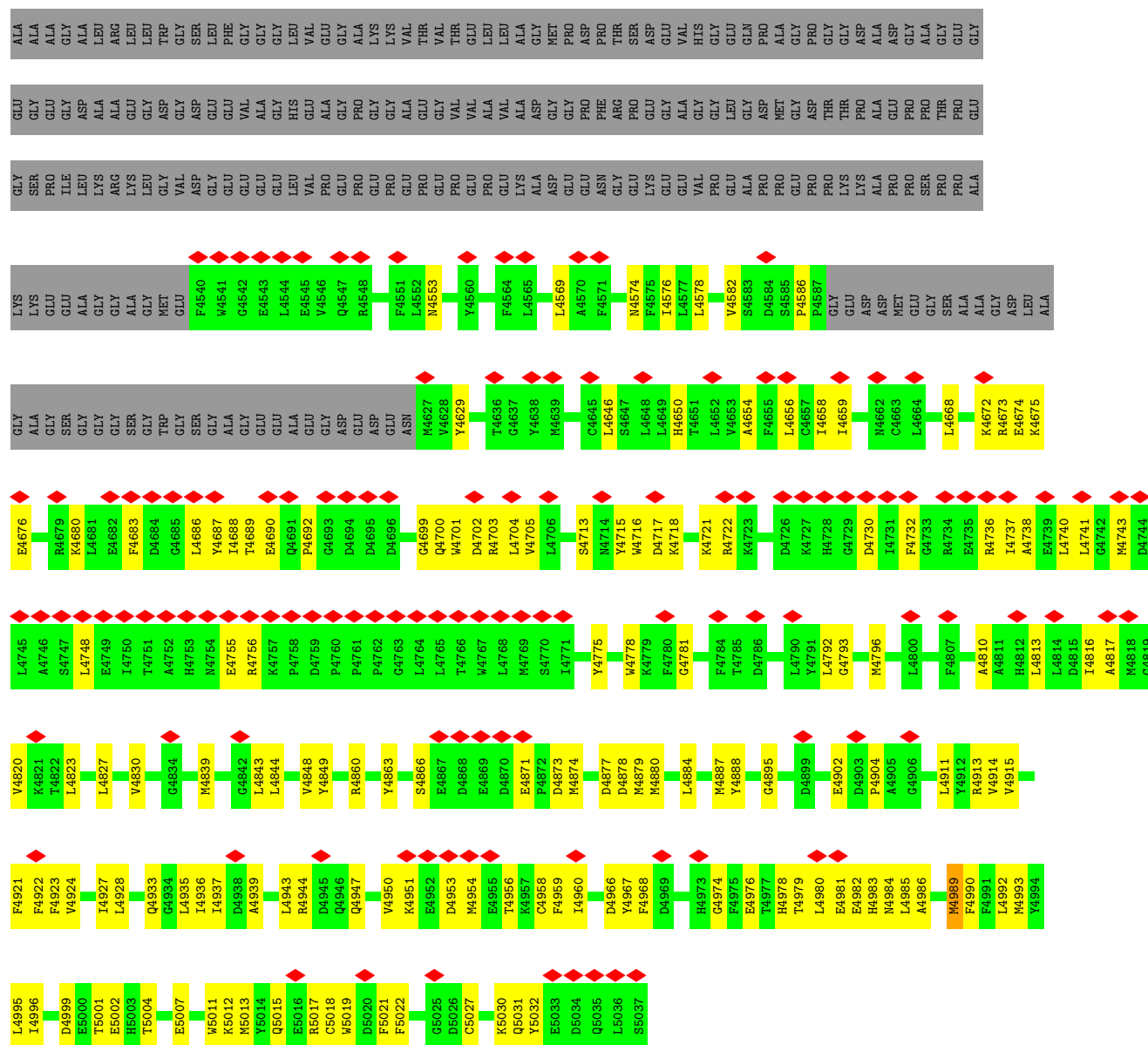
- Molecule 2: Ryanodine receptor 1



P2438	A2367	S2270	F2191	ALA	D2017	GLU	V1839	E1596	N1482	LYS	LYS	ALA
E2439	L2368	L2273	P2195	GLU	E2018	GLY	P1840	V1597	V1483	LYS	ALA	ALA
I2443	R2369	G2370	G2370	GLU	E2019	GLU	M1599	Q1597	H1484	ARG	GLU	GLU
G2444	G2371	A2277	M2198	LYS	C2021	ASP	V1945	M1599	S1485	PHE	ASP	PRO
R2447	G2375	N2284	L2201	P2091	P2022	LEU	M1851	R1607	N1491	LEU	ASP	PRO
G2448	E2285	E2285	G2202	Q2092	L2023	LEU	M1851	M1608	H1262	ASP	ASP	ASP
E2449	L2286	G2203	G2203	E2096	P2024	GLU	F1854	P1609	C1492	TYR	TYR	TYR
A2450	A2378	A2287	H2204	H2100	D2025	L1926	M1865	H1611	V1501	ALA	GLU	GLU
L2451	L2288	E2205	E2205	M2101	T2007	L1927	I1866	F1612	GLY	LYS	ASN	ASN
R2452	L2289	T2206	T2206	M2101	R2028	Q1928	E1867	R1623	ALA	ARG	ARG	ARG
L2453	L2290	V2207	V2207	Y2110	L2031	M1929	E1867	R1623	ALA	ARG	ARG	ARG
E2382	E2296	M2211	M2211	Q2111	Q2032	V1935	V1870	Q1629	GLY	ALA	SER	SER
A2383	R2297	V2212	V2212	Q2111	Q2032	V1935	F1871	C1630	GLY	ALA	ALA	ALA
L2384	R2297	V2212	V2212	Q2111	Q2032	V1935	T1872	Q1631	GLY	ALA	ALA	ALA
R2385	G2216	G2216	G2216	E2115	Q2036	M1939	T1872	C1631	GLY	ALA	ALA	ALA
V2299	GLY	GLY	GLY	L2116	L2044	GLU	GLU	Q1631	GLY	ALA	ALA	ALA
L2386	L2116	L2116	L2116	L2116	L2044	GLU	GLU	Q1631	GLY	ALA	ALA	ALA
S2300	M2120	M2120	M2120	M2120	L2044	GLU	GLU	Q1631	GLY	ALA	ALA	ALA
Y2301	F2121	F2121	F2121	F2121	L2044	GLU	GLU	Q1631	GLY	ALA	ALA	ALA
L2302	GLY	GLY	GLY	GLY	L2044	GLU	GLU	Q1631	GLY	ALA	ALA	ALA
G2304	LYS	LYS	LYS	LYS	L2044	GLU	GLU	Q1631	GLY	ALA	ALA	ALA
G2304	LYS	LYS	LYS	LYS	L2044	GLU	GLU	Q1631	GLY	ALA	ALA	ALA
L2307	GLY	GLY	GLY	GLY	L2044	GLU	GLU	Q1631	GLY	ALA	ALA	ALA
Q2308	GLY	GLY	GLY	GLY	L2044	GLU	GLU	Q1631	GLY	ALA	ALA	ALA
S2309	GLY	GLY	GLY	GLY	L2044	GLU	GLU	Q1631	GLY	ALA	ALA	ALA
G2312	GLY	GLY	GLY	GLY	L2044	GLU	GLU	Q1631	GLY	ALA	ALA	ALA
P2319	GLY	GLY	GLY	GLY	L2044	GLU	GLU	Q1631	GLY	ALA	ALA	ALA
N2324	GLY	GLY	GLY	GLY	L2044	GLU	GLU	Q1631	GLY	ALA	ALA	ALA
G2328	GLY	GLY	GLY	GLY	L2044	GLU	GLU	Q1631	GLY	ALA	ALA	ALA
Y2331	GLY	GLY	GLY	GLY	L2044	GLU	GLU	Q1631	GLY	ALA	ALA	ALA
L2332	GLY	GLY	GLY	GLY	L2044	GLU	GLU	Q1631	GLY	ALA	ALA	ALA
D2333	GLY	GLY	GLY	GLY	L2044	GLU	GLU	Q1631	GLY	ALA	ALA	ALA
F2334	GLY	GLY	GLY	GLY	L2044	GLU	GLU	Q1631	GLY	ALA	ALA	ALA
L2335	GLY	GLY	GLY	GLY	L2044	GLU	GLU	Q1631	GLY	ALA	ALA	ALA
R2336	GLY	GLY	GLY	GLY	L2044	GLU	GLU	Q1631	GLY	ALA	ALA	ALA
F2337	GLY	GLY	GLY	GLY	L2044	GLU	GLU	Q1631	GLY	ALA	ALA	ALA
F2340	GLY	GLY	GLY	GLY	L2044	GLU	GLU	Q1631	GLY	ALA	ALA	ALA
V2346	GLY	GLY	GLY	GLY	L2044	GLU	GLU	Q1631	GLY	ALA	ALA	ALA
E2347	GLY	GLY	GLY	GLY	L2044	GLU	GLU	Q1631	GLY	ALA	ALA	ALA
E2348	GLY	GLY	GLY	GLY	L2044	GLU	GLU	Q1631	GLY	ALA	ALA	ALA
N2349	GLY	GLY	GLY	GLY	L2044	GLU	GLU	Q1631	GLY	ALA	ALA	ALA
R2355	GLY	GLY	GLY	GLY	L2044	GLU	GLU	Q1631	GLY	ALA	ALA	ALA
L2356	GLY	GLY	GLY	GLY	L2044	GLU	GLU	Q1631	GLY	ALA	ALA	ALA
L2357	GLY	GLY	GLY	GLY	L2044	GLU	GLU	Q1631	GLY	ALA	ALA	ALA
L2358	GLY	GLY	GLY	GLY	L2044	GLU	GLU	Q1631	GLY	ALA	ALA	ALA
R2359	GLY	GLY	GLY	GLY	L2044	GLU	GLU	Q1631	GLY	ALA	ALA	ALA
E2362	GLY	GLY	GLY	GLY	L2044	GLU	GLU	Q1631	GLY	ALA	ALA	ALA
P2366	GLY	GLY	GLY	GLY	L2044	GLU	GLU	Q1631	GLY	ALA	ALA	ALA
E2480	L2474	L2474	L2474	L2474	L2474	L2474	L2474	L2474	L2474	L2474	L2474	L2474
D2481	L2475	L2475	L2475	L2475	L2475	L2475	L2475	L2475	L2475	L2475	L2475	L2475
D2482	L2476	L2476	L2476	L2476	L2476	L2476	L2476	L2476	L2476	L2476	L2476	L2476
G2483	L2477	L2477	L2477	L2477	L2477	L2477	L2477	L2477	L2477	L2477	L2477	L2477
A2484	L2478	L2478	L2478	L2478	L2478	L2478	L2478	L2478	L2478	L2478	L2478	L2478
L2485	L2479	L2479	L2479	L2479	L2479	L2479	L2479	L2479	L2479	L2479	L2479	L2479
V2486	L2480	L2480	L2480	L2480	L2480	L2480	L2480	L2480	L2480	L2480	L2480	L2480
Q2487	L2481	L2481	L2481	L2481	L2481	L2481	L2481	L2481	L2481	L2481	L2481	L2481
P2488	L2482	L2482	L2482	L2482	L2482	L2482	L2482	L2482	L2482	L2482	L2482	L2482
S2493	L2483	L2483	L2483	L2483	L2483	L2483	L2483	L2483	L2483	L2483	L2483	L2483
F2494	L2484	L2484	L2484	L2484	L2484	L2484	L2484	L2484	L2484	L2484	L2484	L2484
V2495	L2485	L2485	L2485	L2485	L2485	L2485	L2485	L2485	L2485	L2485	L2485	L2485
H2498	L2486	L2486	L2486	L2486	L2486	L2486	L2486	L2486	L2486	L2486	L2486	L2486
A2500	L2487	L2487	L2487	L2487	L2487	L2487	L2487	L2487	L2487	L2487	L2487	L2487
S2501	L2488	L2488	L2488	L2488	L2488	L2488	L2488	L2488	L2488	L2488	L2488	L2488
L2502	L2489	L2489	L2489	L2489	L2489	L2489	L2489	L2489	L2489	L2489	L2489	L2489
L2503	L2490	L2490	L2490	L2490	L2490	L2490	L2490	L2490	L2490	L2490	L2490	L2490
L2504	L2491	L2491	L2491	L2491	L2491	L2491	L2491	L2491	L2491	L2491	L2491	L2491
F2505	L2492	L2492	L2492	L2492	L2492	L2492	L2492	L2492	L2492	L2492	L2492	L2492
L2506	L2493	L2493	L2493	L2493	L2493	L2493	L2493	L2493	L2493	L2493	L2493	L2493





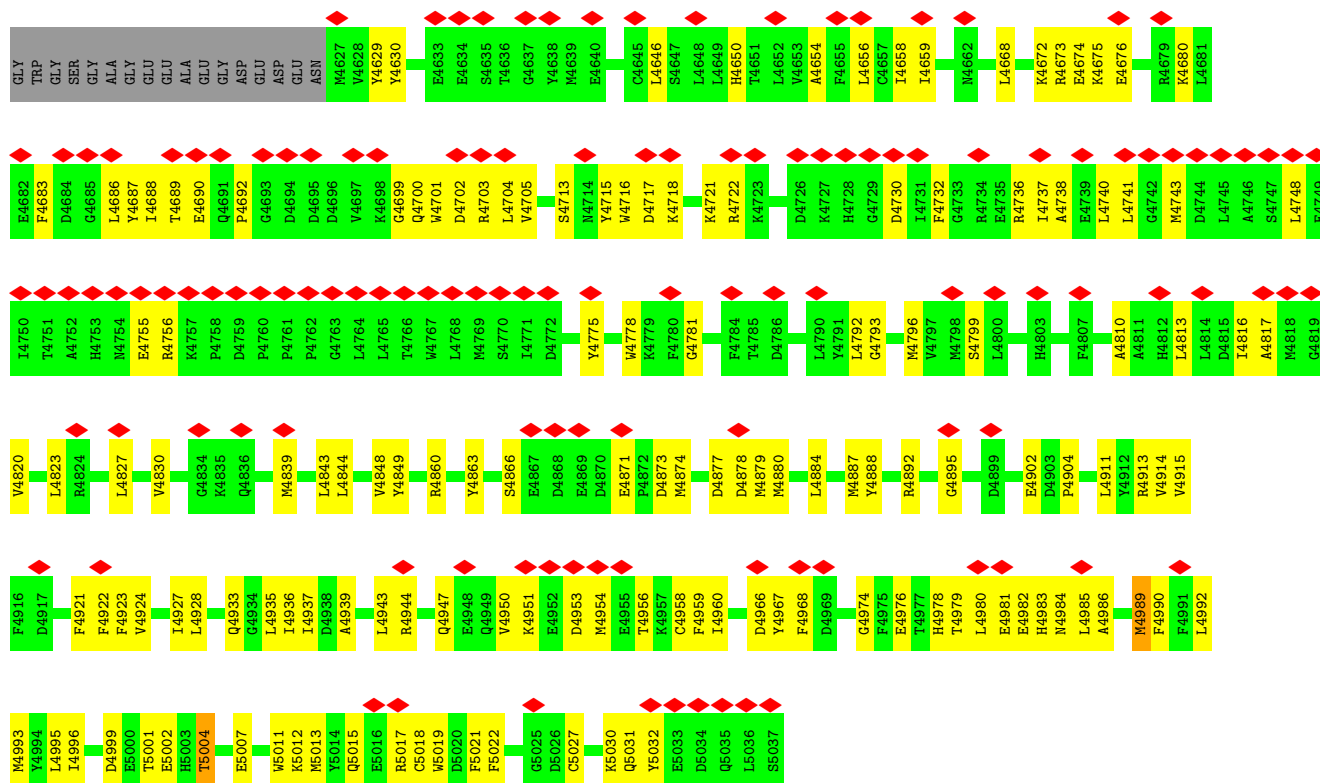




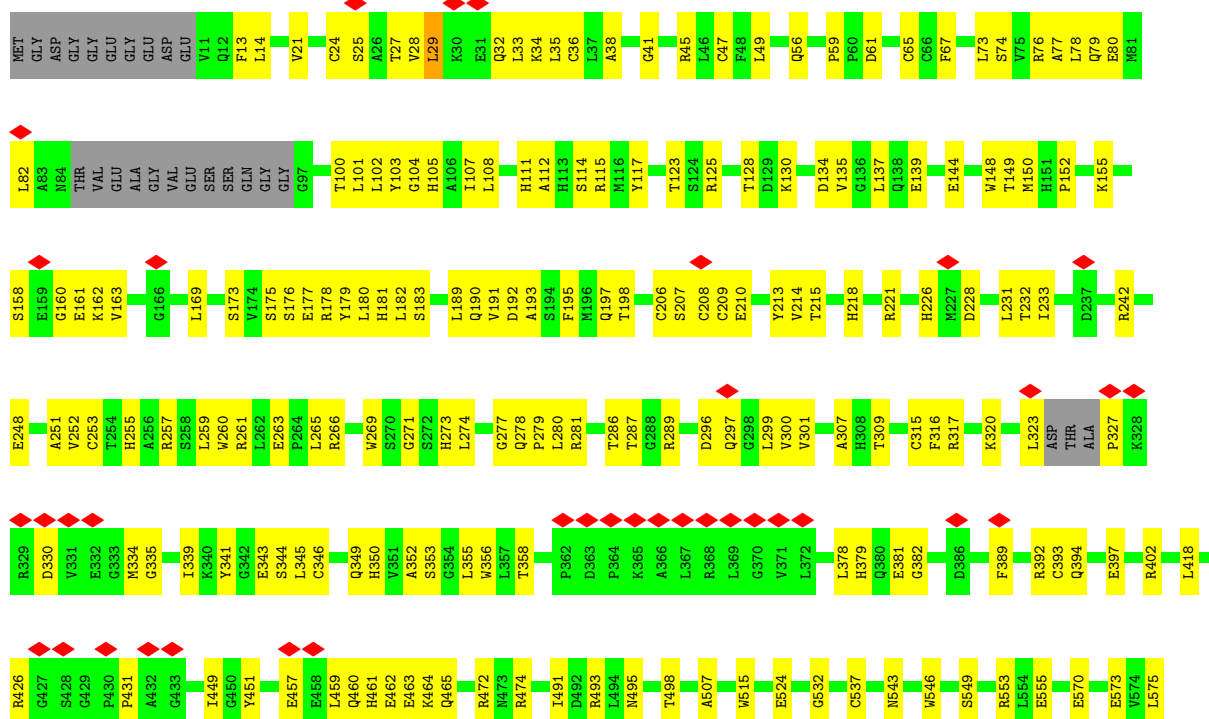








• Molecule 2: Ryanodine receptor 1

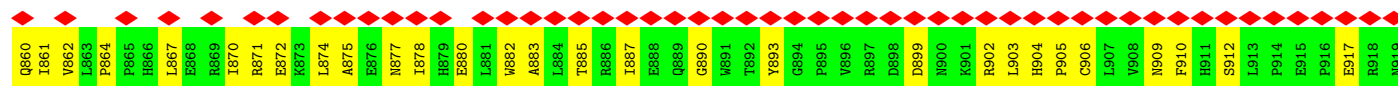




GLU	GLY	P2793	Y2794	K2795	T2796	F2797	S2798	E2799	K2800	D2801	K2802	E2803	L2804	Y2805	R2806	L2867	W2807	P2808	R2869	E2870	K2871	L2872	A2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	N2881	Y2882	H2883	W2884	T2885	W2886	G2887	R2888	K2889	K2890	K2891	GLU	GLU	ARG	THR	GLU	LYS	LYS	LYS	THR	GLU	GLU	LYS	PRO	PRO	ALA	GLU	LYS	LYS	E2016	D2017	E2018	E2019	D2020	C2021	P2022																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
L2023	P2024	E2025	D2026	L2027	R2028	L2031	Q2032	Q2036	L2044	GLN	LEU	GLU	GLY	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	







L2116	L2031	L1927	L1866	L1766	L1668	L1562	L1427	L1304	L1194	L1099	L1012	L935	L839	L792	L731	L632	L532	L432	L332	L232	L132	L32	L22	L12	L2	L920																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
M2111	E2115	P2027	E1924	P1854	M1865	F1612	C1492	T1304	S1291	G1195	D1012	S925	H939	L970	S973	H974	P969	P967	K966	Y965	G964	N963	S962	M961	M960	Y959	T958	K957	P956	L955	K954	T953	K952	L950	K951	G940	A946	K945	E944	F943	A942	N941	G940	V939	H939	L935	L932	T931	K930	L929	T928	E927	G926	S925	M924	Q923	D986	Y985	L984	T983	Y920																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
M2100	H2100	P2022	E2025	M2001	S2000	L1927	P1851	L1714	E1692	L1690	L1572	L1562	L1561	L1557	L1554	L1553	L1548	L1547	L1546	L1543	L1539	L1538	L1537	L1536	L1535	L1534	L1533	L1532	L1531	L1530	L1529	L1528	L1527	L1526	L1525	L1524	L1523	L1522	L1521	L1520	L1519	L1518	L1517	L1516	L1515	L1514	L1513	L1512	L1511	L1510	L1509	L1508	L1507	L1506	L1505	L1504	L1503	L1502	L1501	L1500	L1499	L1498	L1497	L1496	L1495	L1494	L1493	L1492	L1491	L1490	L1489	L1488	L1487	L1486	L1485	L1484	L1483	L1482	L1481	L1480	L1479	L1478	L1477	L1476	L1475	L1474	L1473	L1472	L1471	L1470	L1469	L1468	L1467	L1466	L1465	L1464	L1463	L1462	L1461	L1460	L1459	L1458	L1457	L1456	L1455	L1454	L1453	L1452	L1451	L1450	L1449	L1448	L1447	L1446	L1445	L1444	L1443	L1442	L1441	L1440	L1439	L1438	L1437	L1436	L1435	L1434	L1433	L1432	L1431	L1430	L1429	L1428	L1427	L1426	L1425	L1424	L1423	L1422	L1421	L1420	L1419	L1418	L1417	L1416	L1415	L1414	L1413	L1412	L1411	L1410	L1409	L1408	L1407	L1406	L1405	L1404	L1403	L1402	L1401	L1400	L1399	L1398	L1397	L1396	L1395	L1394	L1393	L1392	L1391	L1390	L1389	L1388	L1387	L1386	L1385	L1384	L1383	L1382	L1381	L1380	L1379	L1378	L1377	L1376	L1375	L1374	L1373	L1372	L1371	L1370	L1369	L1368	L1367	L1366	L1365	L1364	L1363	L1362	L1361	L1360	L1359	L1358	L1357	L1356	L1355	L1354	L1353	L1352	L1351	L1350	L1349	L1348	L1347	L1346	L1345	L1344	L1343	L1342	L1341	L1340	L1339	L1338	L1337	L1336	L1335	L1334	L1333	L1332	L1331	L1330	L1329	L1328	L1327	L1326	L1325	L1324	L1323	L1322	L1321	L1320	L1319	L1318	L1317	L1316	L1315	L1314	L1313	L1312	L1311	L1310	L1309	L1308	L1307	L1306	L1305	L1304	L1303	L1302	L1301	L1300	L1299	L1298	L1297	L1296	L1295	L1294	L1293	L1292	L1291	L1290	L1289	L1288	L1287	L1286	L1285	L1284	L1283	L1282	L1281	L1280	L1279	L1278	L1277	L1276	L1275	L1274	L1273	L1272	L1271	L1270	L1269	L1268	L1267	L1266	L1265	L1264	L1263	L1262	L1261	L1260	L1259	L1258	L1257	L1256	L1255	L1254	L1253	L1252	L1251	L1250	L1249	L1248	L1247	L1246	L1245	L1244	L1243	L1242	L1241	L1240	L1239	L1238	L1237	L1236	L1235	L1234	L1233	L1232	L1231	L1230	L1229	L1228	L1227	L1226	L1225	L1224	L1223	L1222	L1221	L1220	L1219	L1218	L1217	L1216	L1215	L1214	L1213	L1212	L1211	L1210	L1209	L1208	L1207	L1206	L1205	L1204	L1203	L1202	L1201	L1200	L1199	L1198	L1197	L1196	L1195	L1194	L1193	L1192	L1191	L1190	L1189	L1188	L1187	L1186	L1185	L1184	L1183	L1182	L1181	L1180	L1179	L1178	L1177	L1176	L1175	L1174	L1173	L1172	L1171	L1170	L1169	L1168	L1167	L1166	L1165	L1164	L1163	L1162	L1161	L1160	L1159	L1158	L1157	L1156	L1155	L1154	L1153	L1152	L1151	L1150	L1149	L1148	L1147	L1146	L1145	L1144	L1143	L1142	L1141	L1140	L1139	L1138	L1137	L1136	L1135	L1134	L1133	L1132	L1131	L1130	L1129	L1128	L1127	L1126	L1125	L1124	L1123	L1122	L1121	L1120	L1119	L1118	L1117	L1116	L1115	L1114	L1113	L1112	L1111	L1110	L1109	L1108	L1107	L1106	L1105	L1104	L1103	L1102	L1101	L1100	L1099	L1098	L1097	L1096	L1095	L1094	L1093	L1092	L1091	L1090	L1089	L1088	L1087	L1086	L1085	L1084	L1083	L1082	L1081	L1080	L1079	L1078	L1077	L1076	L1075	L1074	L1073	L1072	L1071	L1070	L1069	L1068	L1067	L1066	L1065	L1064	L1063	L1062	L1061	L1060	L1059	L1058	L1057	L1056	L1055	L1054	L1053	L1052	L1051	L1050	L1049	L1048	L1047	L1046	L1045	L1044	L1043	L1042	L1041	L1040	L1039	L1038	L1037	L1036	L1035	L1034	L1033	L1032	L1031	L1030	L1029	L1028	L1027	L1026	L1025	L1024	L1023	L1022	L1021	L1020	L1019	L1018	L1017	L1016	L1015	L1014	L1013	L1012	L1011	L1010	L1009	L1008	L1007	L1006	L1005	L1004	L1003	L1002	L1001	L1000	L999	L998	L997	L996	L995	L994	L993	L992	L991	L990	L989	L988	L987	L986	L985	L984	L983	L982	L981	L980	L979	L978	L977	L976	L975	L974	L973	L972	L971	L970	L969	L968	L967	L966	L965	L964	L963	L962	L961	L960	L959	L958	L957	L956	L955	L954	L953	L952	L951	L950	L949	L948	L947	L946	L945	L944	L943	L942	L941	L940	L939	L938	L937	L936	L935	L934	L933	L932	L931	L930	L929	L928	L927	L926	L925	L924	L923	L922	L921	L920	L919	L918	L917	L916	L915	L914	L913	L912	L911	L910	L909	L908	L907	L906	L905	L904	L903	L902	L901	L900	L899	L898	L897	L896	L895	L894	L893	L892	L891	L890	L889	L888	L887	L886	L885	L884	L883	L882	L881	L880	L879	L878	L877	L876	L875	L874	L873	L872	L871	L870	L869	L868	L867	L866	L865	L864	L863	L862	L861	L860	L859	L858	L857	L856	L855	L854	L853	L852	L851	L850	L849	L848	L847	L846	L845	L844	L843	L842	L841	L840	L839	L838	L837	L836	L835	L834	L833	L832	L831	L830	L829	L828	L827	L826	L825	L824	L823	L822	L821	L820	L819	L818	L817	L816	L815	L814	L813	L812	L811	L810	L809	L808	L807	L806	L805	L804	L803	L802	L801	L800	L799	L798	L797	L796	L795	L794	L793	L792	L791	L790	L789	L788	L787	L786	L785	L784	L783	L782	L781	L780	L779	L778	L777	L776	L775	L774	L773	L772	L771	L770	L769	L768	L767	L766	L765	L764	L763	L762	L761	L760	L759	L758	L757	L756	L755	L754	L753	L752	L751	L750	L749	L748	L747	L746	L745	L744	L743	L742	L741	L740	L739	L738	L737	L736	L735	L734	L733	L732	L731	L730	L729	L728	L727	L726	L725	L724	L723	L722	L721	L720	L719	L718	L717	L716	L715	L714	L713	L712	L711	L710	L709	L708	L707	L706	L705	L704	L703	L702	L701	L700	L699	L698	L697	L696	L695	L694	L693	L692	L691	L690	L689	L688	L687	L686	L685	L684	L683	L682	L681	L680	L679	L678	L677	L676	L675	L674	L673	L672	L671	L670	L669	L668	L667	L666	L665	L664	L663	L662	L661	L660	L659	L658	L657	L656	L655	L654	L653	L652	L651	L650	L649	L648	L647	L646	L645	L644	L643	L642	L641	L640	L639	L638	L637	L636	L635	L634	L633	L632	L631	L630	L629	L628	L627	L626	L625	L624	L623	L622	L621	L620	L619	L618	L617	L616	L615	L614	L613	L612	L611	L610	L609	L608	L607	L606	L605	L604	L603	L602	L601	L600	L599	L598	L597	L596	L595	L594	L593	L592	L591	L590	L589	L588	L587	L586	L585	L584	L583	L582	L581	L580	L579	L578	L577	L576	L575	L574	L573	L572	L571	L570	L569	L568	L567	L566	L565	L564	L563	L562	L561	L560	L559	L558	L557	L556	L555	L554	L553	L552	L551	L550	L549	L548	L547	L546	L545	L544	L543	L542	L541	L540	L539	L538	L537	L536	L535	L534	L533	L532	L531	L530	L529	L528	L527	L526	L525	L524	L523	L522	L521	L520	L519	L518	L517	L516	L515	L514	L513	L512	L511	L510	L509	L508	L507	L506	L505	L504	L503	L502	L501	L500	L499	L498	L497	L496	L495	L494	L493	L492	L491	L490	L489	L488	L487	L486	L485	L484	L483	L482	L481	L480	L479	L478	L477	L476	L475	L474	L473	L472	L471	L470	L469	L468	L467	L466	L465	L464	L463	L462	L461	L460	L459	L458	L457	L456	L455	L454	L453	L452	L451	L450	L449	L448	L447	L446	L445	L444	L443	L442	L441	L440	L439	L438	L437	L436	L435	L434	L433	L432	L431	L430	L429	L428	L427	L426	L425	L424	L423	L422	L421	L420	L419	L418	L417	L416	L415	L414	L413	L412	L411	L410	L409	L408	L407	L406	L405	L404	L403	L402	L401	L400	L399	L398	L397	L396	L395	L394	L393	L392	L391	L390	L389	L388	L387	L386	L385	L384	L383	L382	L381	L380	L379	L378	L377	L376	L375	L374	L373	L372	L371	L370	L369	L368	L367	L366	L365	L364	L363	L362	L361	L360	L359	L358	L357	L356	L355	L354	L353	L352	L351	L350	L349	L348	L347	L346	L345	L344	L343	L342	L341	L340	L339	L338	L337	L336	L335	L334	L333	L332	L331	L330	L329	L328	L327	L326	L325	L324	L323	L322	L321	L320	L319	L318	L317	L316	L315	L314	L313	L312	L311	L310	L309	L308	L307	L306	L305	L304	L303	L302	L301	L300	L299	L298	L297	L296	L295	L294	L293	L292	L291	L290	L289	L288	L287	L286	L285	L284	L283	L282	L281	L280	L279	L278	L277	L276	L275	L274	L273	L272	L271	L270	L269	L268	L267	L266	L265	L264	L263	L262	L261	L260	L259	L258	L257	L256	L255	L254	L253	L252	L251	L250	L249	L248	L247	L246	L245	L244	L243	L242	L241	L240	L239	L238	L237	L236	L235	L234	L233	L232	L231	L230	L229	L228	L227	L226	L225	L224	L223	L222	L221	L220	L219	L218	L217	L216	L215	L214	L213	L212	L211	L210	L209	L208	L207	L206	L205	L204	L203	L202	L201	L200	L199	L198	L197	L196	L195	L194	L19

A3061	P3062	V3065	N3066	C3067	L3068	H3069	Q3069	L3070	L3071	A3072	R3073	S3074	L3075	N3076	A3077	T3078	T3079	V3080	K3081	K3082	S3083	G3084	K3089	A3090	R3093	F3096	E3097	S3098	E3101	D3102	I3103	E3104	K3105	M3106	V3107	E3108	N3109	L3110	R3111	L3112	G3113	VAL	SER	SER	GLN	ALA	ARG	THR	GLN	VAL	K3123	G3124	V3131	T3132						
V2986	E2987	K2988	H2991	E2992	Q2993	E2994	L2995	K2996	A2999	K3000	N3007	Q3008	V3009	F3010	T3011	N3012	H3013	C3014	L3015	V3016	F3017	L3018	S3019	V3024	L3025	G3026	S3027	G3028	G3029	I3103	N3033	K3036	E3037	M3038	L3039	L3042	F3043	G3044	K3045	L3046	A3047	A3048	L3049	V3050	R3053	V3054	L3055	L3056	F3057	G3058	T3059	D3060								
Q2924	E2925	L2926	L2927	F2928	F2929	L2930	Q2931	M2932	N2933	G2934	V2935	A2936	V2937	T2938	R2939	GLY	LEU	LYS	ASP	MET	GLU	LEU	ASP	THR	S2949	I2950	K2951	R2952	K2953	R2954	F2955	A2956	F2957	G2958	F2959	L2960	L2963	L2964	R2965	W2966	D2967	T2968	S2969	L2969	L2969	Q2970	Q2971	Q2971	E2972	F2973	L2974	A2975	H2976	L2977	V2980	V2981	S2982	S2983	G2984	R2985
G2864	V2865	T2866	L2867	S2868	R2869	E2870	L2871	A2872	Q2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	M2881	Y2882	H2883	L2884	T2885	W2886	G2887	K2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899	G2900	H2901	H2902	P2903	L2904	L2905	V2906	P2907	D2908	T2909	T2910	L2911	T2912	A2913	K2914	E2915	K2916	A2917	R2918	D2919	R2920	E2921	K2922	A2923	
Q2924	E2925	L2926	L2927	F2928	F2929	L2930	Q2931	M2932	N2933	G2934	V2935	A2936	V2937	T2938	R2939	GLY	LEU	LYS	ASP	MET	GLU	LEU	ASP	THR	S2949	I2950	K2951	R2952	K2953	R2954	F2955	A2956	F2957	G2958	F2959	L2960	L2963	L2964	R2965	W2966	D2967	T2968	S2969	L2969	L2969	Q2970	Q2971	Q2971	E2972	F2973	L2974	A2975	H2976	L2977	V2980	V2981	S2982	S2983	G2984	R2985
V2986	E2987	K2988	H2991	E2992	Q2993	E2994	L2995	K2996	A2999	K3000	N3007	Q3008	V3009	F3010	T3011	N3012	H3013	C3014	L3015	V3016	F3017	L3018	S3019	V3024	L3025	G3026	S3027	G3028	G3029	I3103	N3033	K3036	E3037	M3038	L3039	L3042	F3043	G3044	K3045	L3046	A3047	A3048	L3049	V3050	R3053	V3054	L3055	L3056	F3057	G3058	T3059	D3060								
A3061	P3062	V3065	N3066	C3067	L3068	H3069	Q3069	L3070	L3071	A3072	R3073	S3074	L3075	N3076	A3077	T3078	T3079	V3080	K3081	K3082	S3083	G3084	K3089	A3090	R3093	F3096	E3097	S3098	E3101	D3102	I3103	E3104	K3105	M3106	V3107	E3108	N3109	L3110	R3111	L3112	G3113	VAL	SER	SER	GLN	ALA	ARG	THR	GLN	VAL	K3123	G3124	V3131	T3132						
V2212	N2213	V2214	L2215	G2216	GLY	GLY	GLU	THR	LYS	GLU	T2223	K2227	H2228	C2232	C2233	R2234	F2235	L2236	C2237	Y2238	F2239	R2241	L2242	S2243	R2244	Q2245	N2246	M2250	Y2256	E2259	N2260	S2261	GLY	ILE	GLY	LEU	GLY	MET	Q2268	G2269	S2270	L2273	A2277	N2284	E2285	L2286	K2287	L2288	D2294											
L2295	E2296	K2297	V2298	V2299	S2300	Y2301	L2302	G2303	A2304	S2309	M2312	P2319	N2324	G2328	Y2331	L2332	D2333	F2334	L2335	R2336	F2337	F2340	V2346	E2347	E2348	N2349	R2355	L2356	L2357	L2358	R2359	E2362	P2366	R2369	G2375	L2376	L2377	A2378	A2379	L2380	E2381	E2382	A2383	L2384	R2385	I2386														
P2390	D2393	G2394	P2395	GLY	VAL	ARG	ASP	ARG	ARG	ARG	GLU	HIS	PHE	GLY	GLU	PRO	PRO	GLU	N2414	R2415	V2416	H2417	L2418	G2419	M2422	M2423	I2430	D2431	L2432	L2433	G2434	R2435	P2438	E2439	T2443	K2447	G2448	E2449	A2450	L2451	R2452	L2453	R2454	L2457	R2458	S2459	L2460	V2461												
P2452	L2463	D2464	D2465	L2466	V2467	G2468	T2469	L2470	L2474	Q2475	T2476	P2477	L2478	L2479	G2480	K2481	D2482	G2483	A2484	L2485	V2486	Q2487	P2488	S2493	F2494	V2495	H2498	K2499	A2500	S2501	M2502	V2503	L2504	F2505	R2508	V2509	V2510	G2511	L2512	E2513	N2514	D2515	L2516	L2517	L2518	L2519	H2520	V2521	L2522	D2523	L2524	G2525	F2526	L2527	P2528					
D2529	M2530	R2531	A2534	S2535	L2536	D2537	T2538	F2541	S2542	E2545	Y2553	A2557	V2558	L2559	P2560	L2561	L2562	T2563	R2564	C2565	F2569	A2570	R2575	A2576	L2577	M2578	V2579	D2580	S2581	M2582	L2583	H2584	T2585	R2588	L2589	S2590	G2591	G2592	R2593	S2594	L2595	T2596	Q2599	R2600	D2601	V2602	L2603	E2604	D2605	C2606										
L2607	N2608	A2609	L2610	C2611	R2612	Y2613	L2614	R2615	F2616	S2617	M2618	L2619	Q2620	H2621	L2622	L2623	R2624	R2625	L2626	V2627	F2628	D2629	V2630	N2634	A2635	F2636	A2637	K2638	M2639	P2640	L2641	K2642	L2643	L2644	T2645	N2646	H2647	E2648	R2650	C2651	V2652	K2653	Y2654	L2657	W2661	S2668	L2672	H2673	L2674	T2675	R2676	K2677	L2678							
D2684	A2687	H2688	K2689	K2690	Y2691	D2692	Q2693	E2694	L2695	Y2696	R2697	A2698	L2699	R2700	P2701	C2702	L2703	C2704	A2705	I2706	A2707	G2708	A2709	L2710	P2711	D2712	K2713	Y2714	V2715	D2716	A2717	S2718	Y2719	S2720	S2721	K2722	A2723	E2724	K2725	LYS	ALA	THR	VAL	ASP	ALA	GLY	N2734	F2735	D2736	T2737	P2738	P2739	V2740	E2741	T2742	L2743				
N2744	V2745	L2746	L2747	P2748	E2749	K2750	L2751	D2752	S2753	F2754	L2755	L2756	K2757	F2758	A2759	E2760	Y2761	T2762	H2763	E2764	K2765	W2766	A2767	F2768	D2769	K2770	L2771	Q2772	L2773	N2774	W2775	S2776	Y2777	G2778	E2779	M2780	V2781	D2782	E2783	E2784	L2785	K2786	T2787	H2788	P2789	M2790	L2791	T2792	P2793	Y2794	K2795	T2796	S2798	E2799	K2800	D2801	K2802	E2803		
L2804	Y2805	R2806	V2807	F2808	L2809	K2810	E2811	S2812	L2813	K2814	A2815	M2816	L2817	A2818	V2819	E2820	T2821	T2822	L2823	E2824	K2825	A2826	E2827	E2828	G2829	GLU	ARG	GLU	THR	GLY	LYS	LYS	THR	ARG	LYS	ILE	SER	GLN	THR	ALA	GLN	TYR	ASP	PRO	ARG	GLU	GLY	N2734	F2735	D2736	T2737	P2738	P2739	V2740	E2741	T2742	L2743			
L2804	Y2805	R2806	V2807	F2808	L2809	K2810	E2811	S2812	L2813	K2814	A2815	M2816	L2817	A2818	V2819	E2820	T2821	T2822	L2823	E2824	K2825	A2826	E2827	E2828	G2829	GLU	ARG	GLU	THR	GLY	LYS	LYS	THR	ARG	LYS	ILE	SER	GLN	THR	ALA	GLN	TYR	ASP	PRO	ARG	GLU	GLY	N2734	F2735	D2736	T2737	P2738	P2739	V2740	E2741	T2742	L2743			
G2864	V2865	T2866	L2867	S2868	R2869	E2870	L2871	A2872	Q2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	M2881	Y2882	H2883	L2884	T2885	W2886	G2887	K2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899	G2900	H2901	H2902	P2903	L2904	L2905	V2906	P2907	D2908	T2909	T2910	L2911	T2912	A2913	K2914	E2915	K2916	A2917	R2918	D2919	R2920	E2921	K2922	A2923	
Q2924	E2925	L2926	L2927	F2928	F2929	L2930	Q2931	M2932	N2933	G2934	V2935	A2936	V2937	T2938	R2939	GLY	LEU	LYS	ASP	MET	GLU	LEU	ASP	THR	S2949	I2950	K2951	R2952	K2953	R2954	F2955	A2956	F2957	G2958	F2959	L2960	L2963	L2964	R2965	W2966	D2967	T2968	S2969	L2969	L2969	Q2970	Q2971	Q2971	E2972	F2973	L2974	A2975	H2976	L2977	V2980	V2981	S2982	S2983	G2984	R2985
V2986	E2987	K2988	H2991	E2992	Q2993	E2994	L2995	K2996	A2999	K3000	N3007	Q3008	V3009	F3010	T3011	N3012	H3013	C3014	L3015	V3016	F3017	L3018	S3019	V3024	L3025	G3026	S3027	G3028	G3029	I3103	N3033	K3036	E3037	M3038	L3039	L3042	F3043	G3044	K3045	L3046	A3047	A3048	L3049	V3050	R3053	V3054	L3055	L3056	F3057	G3058	T3059	D3060								
A3061	P3062	V3065	N3066	C3067	L3068	H3069	Q3069	L3070	L3071	A3072	R3073	S3074	L3075	N3076	A3077	T3078	T3079	V3080	K3081	K3082	S3083	G3084	K3089	A3090	R3093	F3096	E3097	S3098	E3101	D3102	I3103	E3104	K3105	M3106	V3107	E3108	N3109	L3110	R3111	L3112	G3113	VAL	SER	SER	GLN	ALA	ARG	THR	GLN	VAL	K3123	G3124	V3131	T3132						
V2986	E2987	K2988	H2991	E2992	Q2993	E2994	L2995	K2996	A2999	K3000	N3007	Q3008	V3009	F3010	T3011	N3012	H3013	C3014	L3015	V3016	F3017	L3018	S3019	V3024	L3025	G3026	S3027	G3028	G3029	I3103	N3033	K3036	E3037	M3038	L3039	L3042	F3043	G3044	K3045	L3046	A3047	A3048	L3049	V3050	R3053	V3054	L3055	L3056	F3057	G3058	T3059	D3060								

R3984	S4053	R3989	T3711	L3823	N3901	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3272	A3200	L3136
L3985	M4054	V3989	L3716	F3829	N3909	R3904	L3835	F3829	F3828	K3715	ARG	N3555	GLY	T3411	P3410	L3408	F3341	T3		



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	31599	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58.34	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.771	Depositor
Minimum map value	-0.034	Depositor
Average map value	0.012	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.106	Depositor
Map size (Å)	425.472, 425.472, 425.472	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.831, 0.831, 0.831	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: CFF, ZN, CA, ATP

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	F	0.72	1/834 (0.1%)	0.76	3/1123 (0.3%)
1	H	0.73	1/834 (0.1%)	0.76	3/1123 (0.3%)
1	J	0.73	1/834 (0.1%)	0.76	3/1123 (0.3%)
1	O	0.72	1/834 (0.1%)	0.76	3/1123 (0.3%)
2	A	0.40	0/35023	0.51	6/47448 (0.0%)
2	B	0.40	0/35023	0.51	6/47448 (0.0%)
2	G	0.40	0/35023	0.51	6/47448 (0.0%)
2	I	0.40	0/35023	0.51	6/47448 (0.0%)
All	All	0.41	4/143428 (0.0%)	0.52	36/194284 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	39	SER	CA-CB	-5.12	1.45	1.52
1	J	39	SER	CA-CB	-5.11	1.45	1.52
1	F	39	SER	CA-CB	-5.08	1.45	1.52
1	O	39	SER	CA-CB	-5.06	1.45	1.52

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	752	VAL	C-N-CA	-9.43	82.41	122.00
2	G	752	VAL	C-N-CA	-9.42	82.42	122.00
2	B	752	VAL	C-N-CA	-9.42	82.42	122.00
2	I	752	VAL	C-N-CA	-9.42	82.42	122.00
2	B	752	VAL	N-CA-C	-7.32	91.23	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	818	0	824	25	0
1	H	818	0	824	24	0
1	J	818	0	824	23	0
1	O	818	0	824	23	0
2	A	34238	0	33844	1330	0
2	B	34238	0	33844	1337	0
2	G	34238	0	33844	1326	0
2	I	34238	0	33844	1329	0
3	A	31	0	12	5	0
3	B	31	0	12	5	0
3	G	31	0	12	6	0
3	I	31	0	12	6	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	G	1	0	0	0	0
5	I	1	0	0	0	0
6	A	14	0	10	2	0
6	B	14	0	10	2	0
6	G	14	0	10	2	0
6	I	14	0	10	2	0
All	All	140412	0	138760	5318	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 19.

The worst 5 of 5318 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)
2:G:4983:HIS:HB2	3:G:5301:ATP:HN62	1.25	1.01
2:A:4880:MET:SD	2:G:4578:LEU:O	2.19	1.00
2:A:4983:HIS:HB2	3:A:5301:ATP:HN62	1.25	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4983:HIS:HB2	3:I:5301:ATP:HN62	1.25	0.99
2:A:4935:LEU:CD2	2:G:4944:ARG:NH2	2.27	0.98

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	F	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
1	H	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
1	J	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
1	O	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
2	A	4256/5037 (84%)	3938 (92%)	314 (7%)	4 (0%)	48	81
2	B	4256/5037 (84%)	3936 (92%)	316 (7%)	4 (0%)	48	81
2	G	4256/5037 (84%)	3939 (93%)	313 (7%)	4 (0%)	48	81
2	I	4256/5037 (84%)	3940 (93%)	312 (7%)	4 (0%)	48	81
All	All	17444/20580 (85%)	16137 (92%)	1291 (7%)	16 (0%)	50	81

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	3876	ALA
2	G	3876	ALA
2	B	3876	ALA
2	I	3876	ALA
2	A	1783	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	88/89 (99%)	79 (90%)	9 (10%)	6	22
1	H	88/89 (99%)	79 (90%)	9 (10%)	6	22
1	J	88/89 (99%)	79 (90%)	9 (10%)	6	22
1	O	88/89 (99%)	79 (90%)	9 (10%)	6	22
2	A	3732/4276 (87%)	3702 (99%)	30 (1%)	79	84
2	B	3732/4276 (87%)	3702 (99%)	30 (1%)	79	84
2	G	3732/4276 (87%)	3702 (99%)	30 (1%)	79	84
2	I	3732/4276 (87%)	3702 (99%)	30 (1%)	79	84
All	All	15280/17460 (88%)	15124 (99%)	156 (1%)	71	81

5 of 156 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	3904	ARG
2	I	3874	VAL
2	B	3967	GLU
2	I	877	ASN
2	I	3969	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	495	ASN
2	I	4946	GLN
2	B	3313	ASN
2	I	4109	GLN
2	I	3313	ASN

5.3.3 RNA ⓘ

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 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$
6	CFF	G	5304	-	8,15,15	2.20	4 (50%)	8,23,23	1.58	1 (12%)
6	CFF	A	5304	-	8,15,15	2.20	4 (50%)	8,23,23	1.57	1 (12%)
3	ATP	G	5301	-	28,33,33	0.86	0	34,52,52	1.16	2 (5%)
6	CFF	I	5304	-	8,15,15	2.20	4 (50%)	8,23,23	1.57	1 (12%)
3	ATP	B	5301	-	28,33,33	0.86	0	34,52,52	1.15	2 (5%)
3	ATP	I	5301	-	28,33,33	0.85	0	34,52,52	1.16	2 (5%)
3	ATP	A	5301	-	28,33,33	0.86	0	34,52,52	1.16	2 (5%)
6	CFF	B	5304	-	8,15,15	2.20	4 (50%)	8,23,23	1.58	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CFF	G	5304	-	-	-	0/2/2/2
6	CFF	A	5304	-	-	-	0/2/2/2
3	ATP	G	5301	-	-	5/18/38/38	0/3/3/3
6	CFF	I	5304	-	-	-	0/2/2/2
3	ATP	B	5301	-	-	5/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	I	5301	-	-	5/18/38/38	0/3/3/3
3	ATP	A	5301	-	-	5/18/38/38	0/3/3/3
6	CFF	B	5304	-	-	-	0/2/2/2

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	5304	CFF	C6-N1	-3.58	1.32	1.38
6	I	5304	CFF	C6-N1	-3.55	1.32	1.38
6	A	5304	CFF	C6-N1	-3.53	1.32	1.38
6	B	5304	CFF	C5-C4	-3.52	1.33	1.39
6	B	5304	CFF	C6-N1	-3.50	1.32	1.38

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	5301	ATP	N3-C2-N1	-3.93	123.33	128.67
3	G	5301	ATP	N3-C2-N1	-3.92	123.35	128.67
3	A	5301	ATP	N3-C2-N1	-3.90	123.38	128.67
3	B	5301	ATP	N3-C2-N1	-3.85	123.45	128.67
6	B	5304	CFF	C14-N7-C8	-3.18	110.12	125.43

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	5301	ATP	C5'-O5'-PA-O3A
3	G	5301	ATP	C5'-O5'-PA-O3A
3	B	5301	ATP	C5'-O5'-PA-O3A
3	I	5301	ATP	C5'-O5'-PA-O3A
3	A	5301	ATP	C3'-C4'-C5'-O5'

There are no ring outliers.

8 monomers are involved in 30 short contacts:

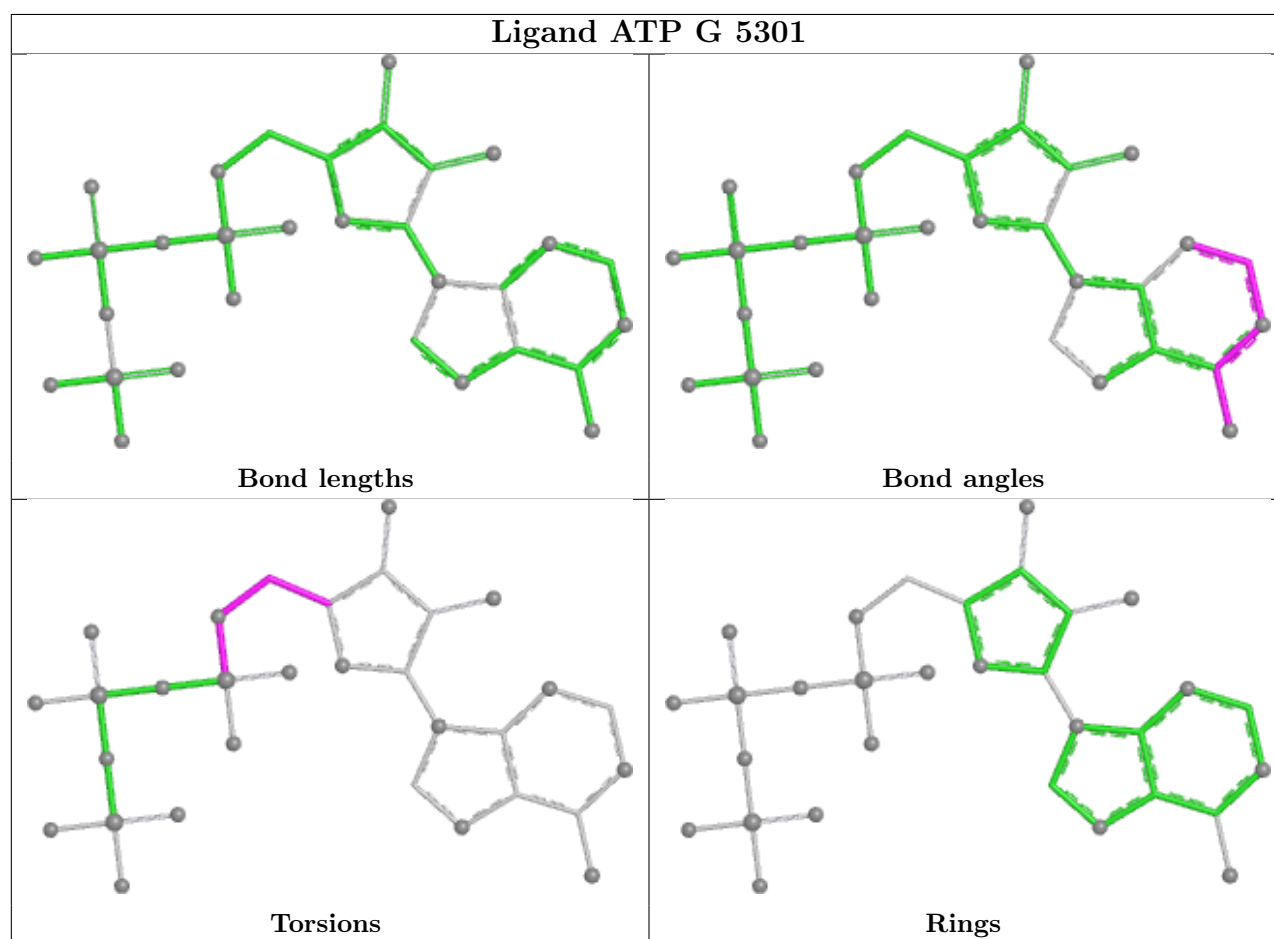
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	5304	CFF	2	0
6	A	5304	CFF	2	0
3	G	5301	ATP	6	0
6	I	5304	CFF	2	0

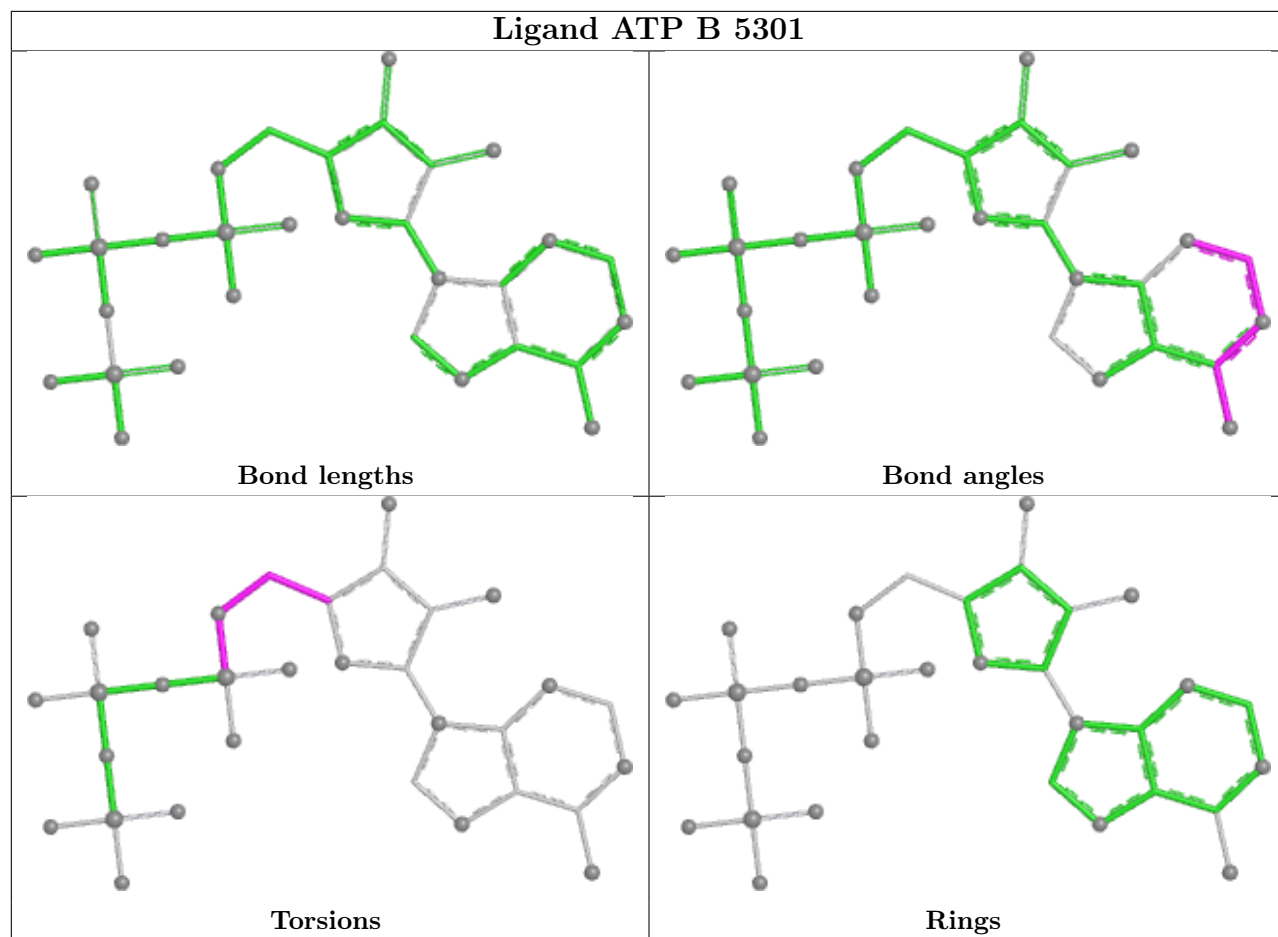
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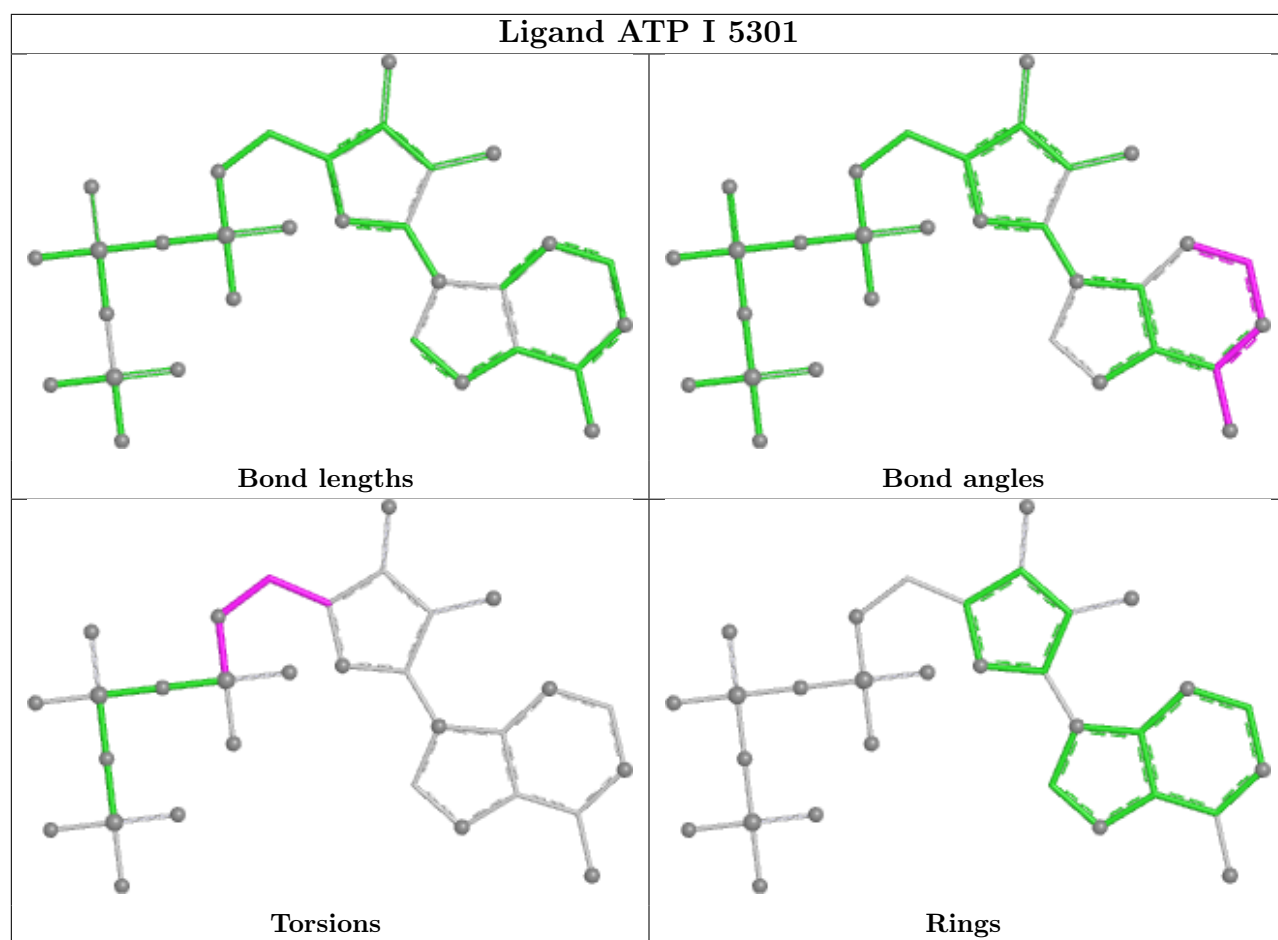
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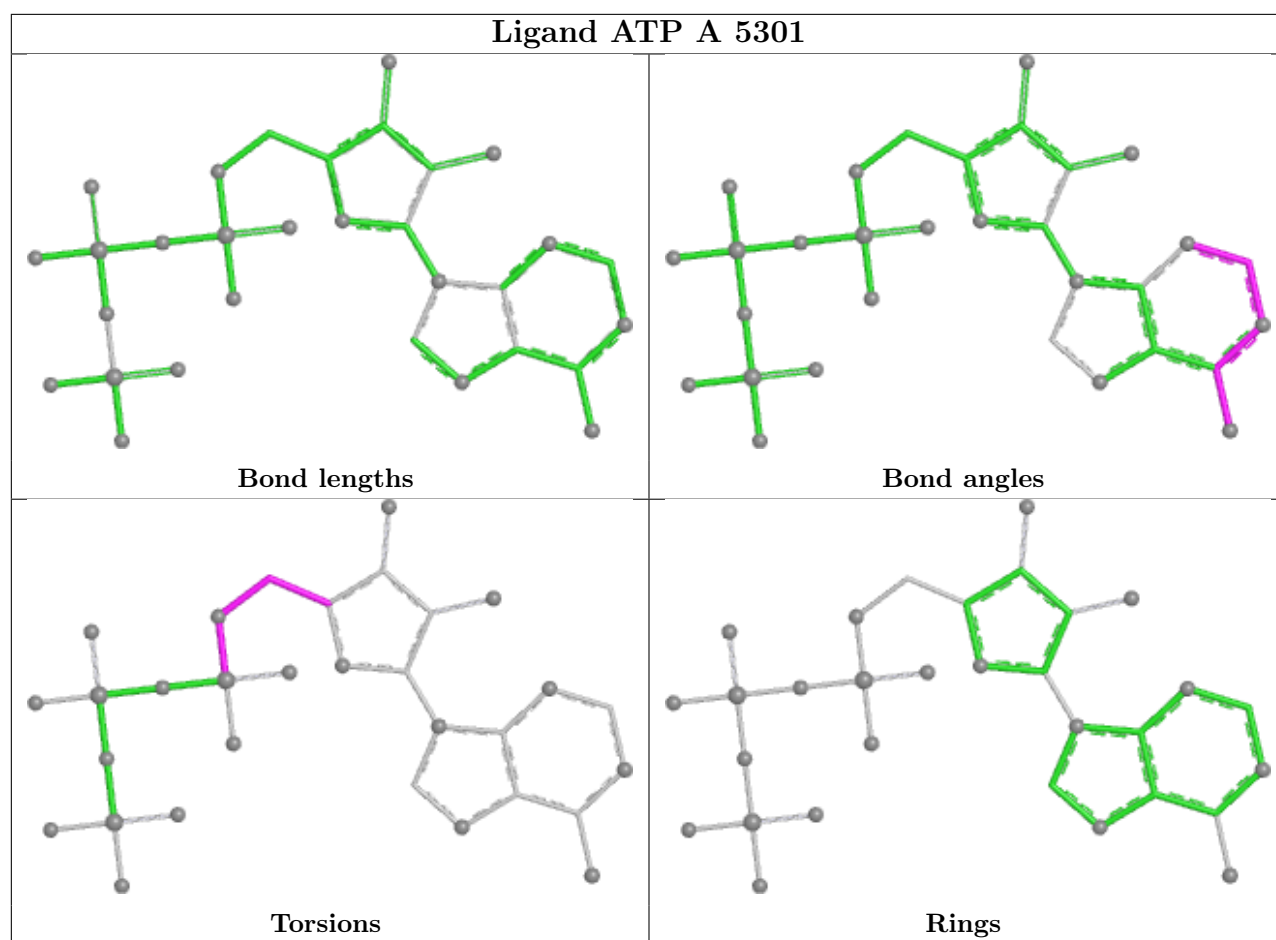
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5301	ATP	5	0
3	I	5301	ATP	6	0
3	A	5301	ATP	5	0
6	B	5304	CFF	2	0

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.

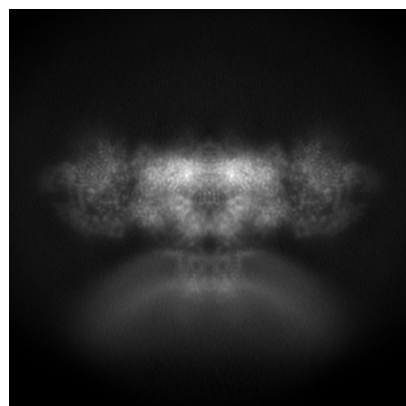
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23699. These allow visual inspection of the internal detail of the map and identification of artifacts.

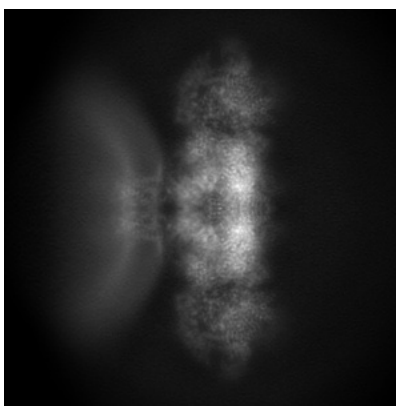
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

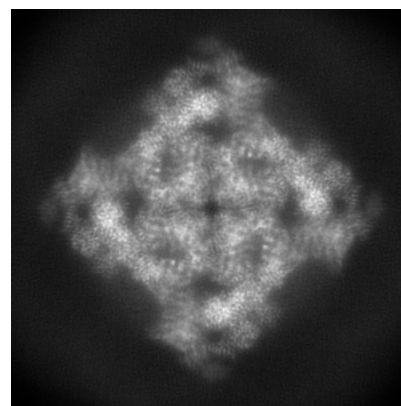
6.1.1 Primary map



X

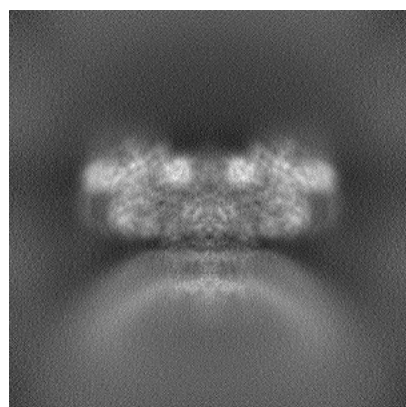


Y

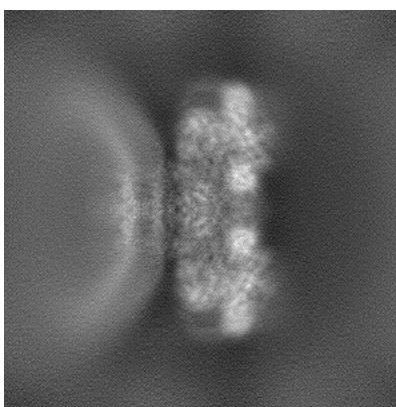


Z

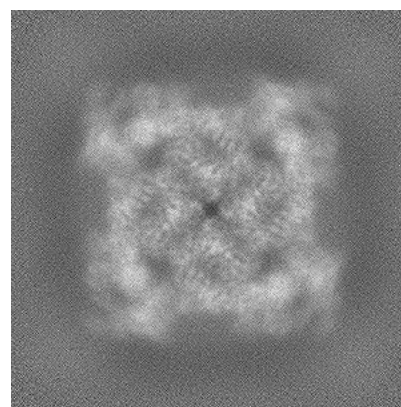
6.1.2 Raw map



X



Y

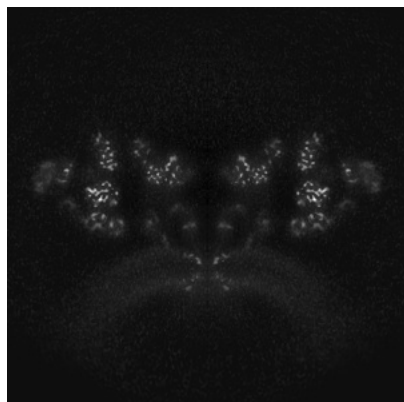


Z

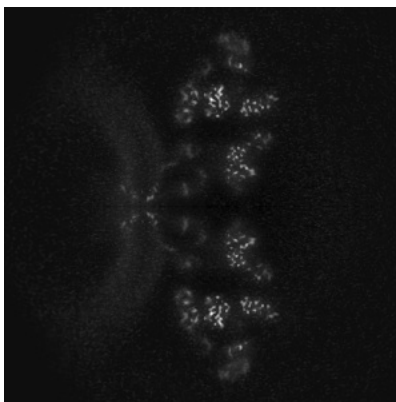
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

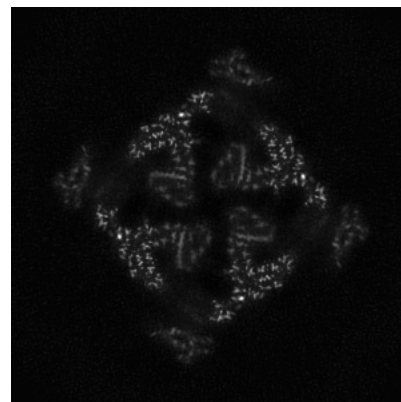
6.2.1 Primary map



X Index: 256



Y Index: 256

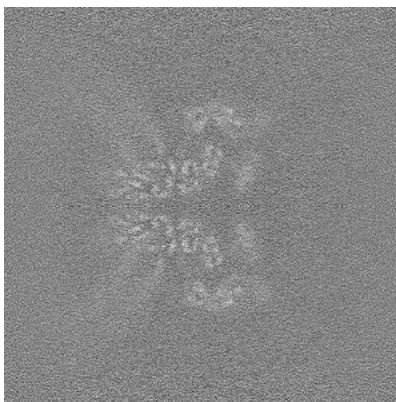


Z Index: 256

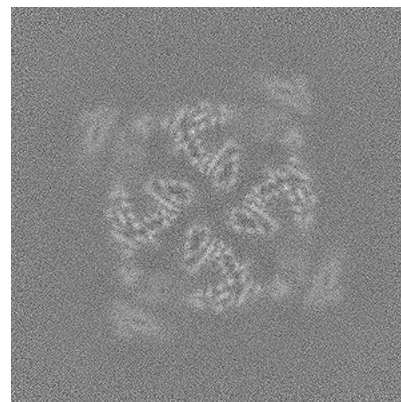
6.2.2 Raw map



X Index: 256



Y Index: 256

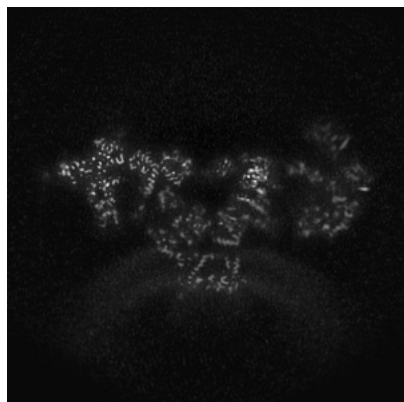


Z Index: 256

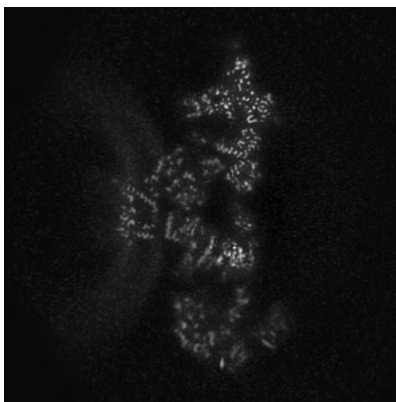
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

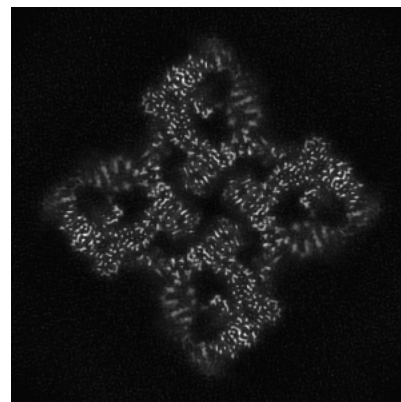
6.3.1 Primary map



X Index: 279

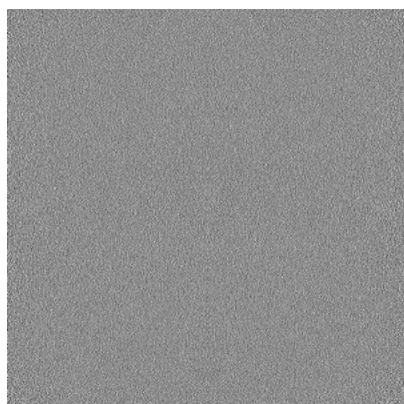


Y Index: 279

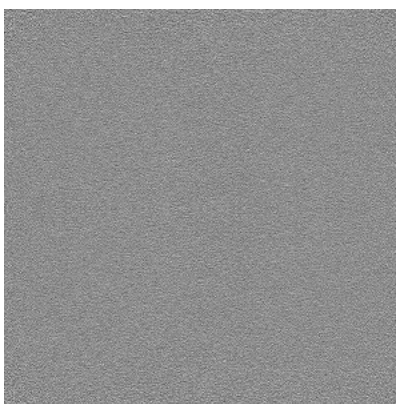


Z Index: 304

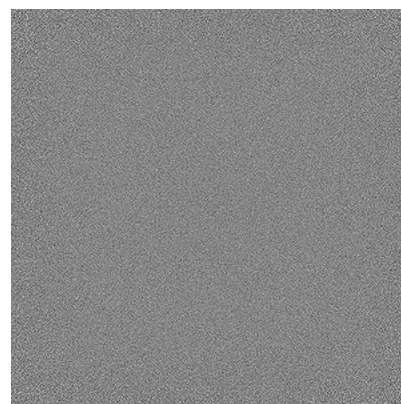
6.3.2 Raw map



X Index: 0



Y Index: 0

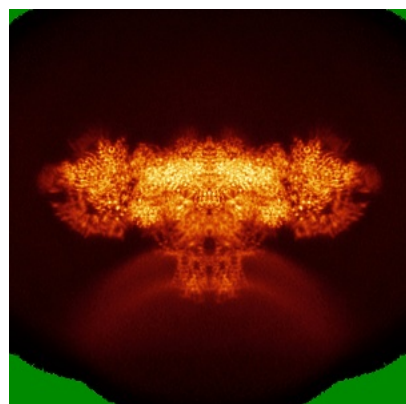


Z Index: 0

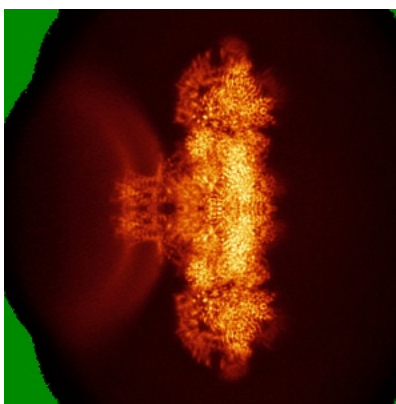
The images above show the largest variance slices of the map in three orthogonal directions.

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

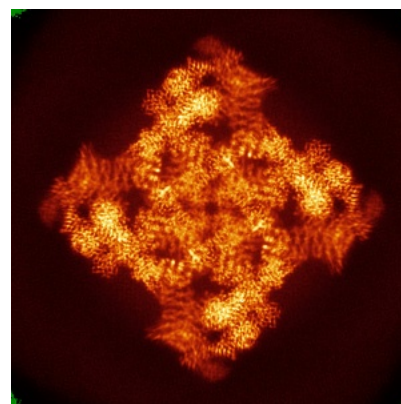
6.4.1 Primary map



X

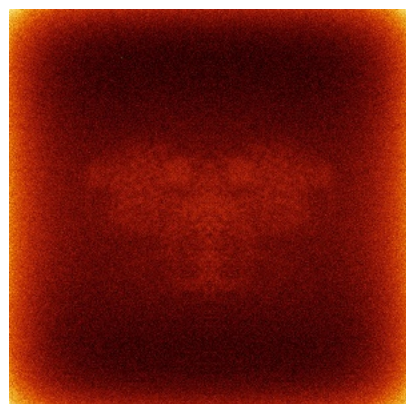


Y

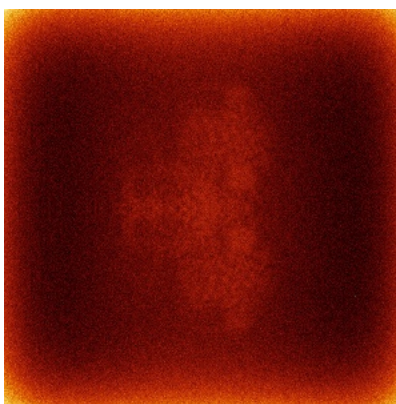


Z

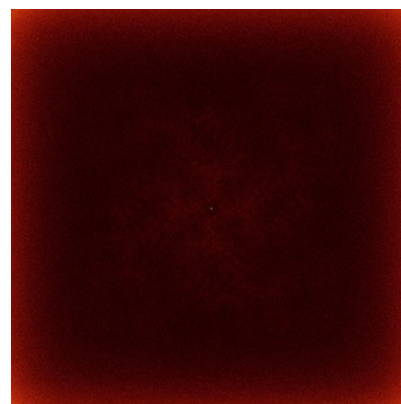
6.4.2 Raw map



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.

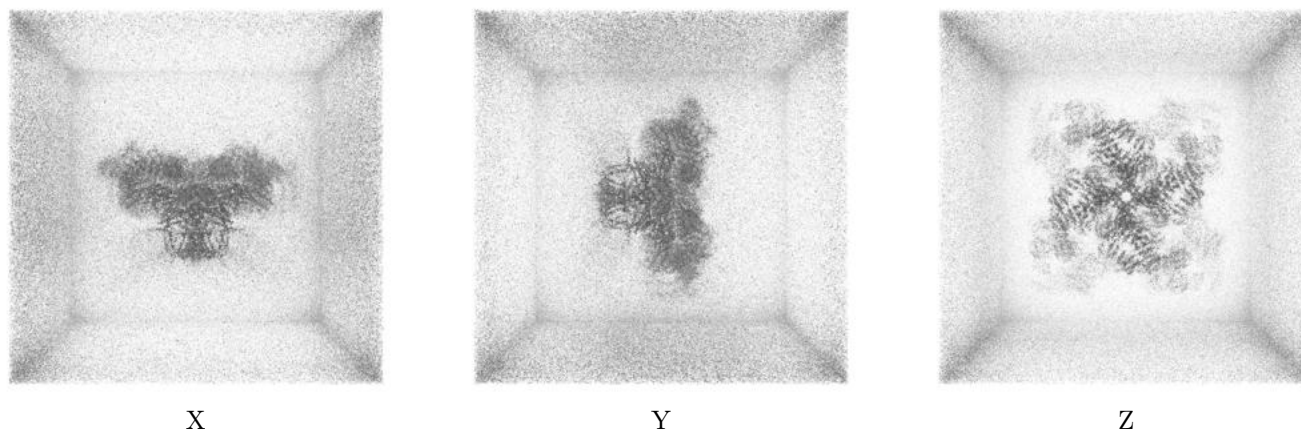
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.106. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

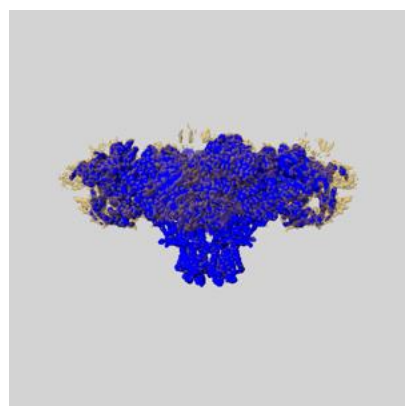
6.6 Mask visualisation [i](#)

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

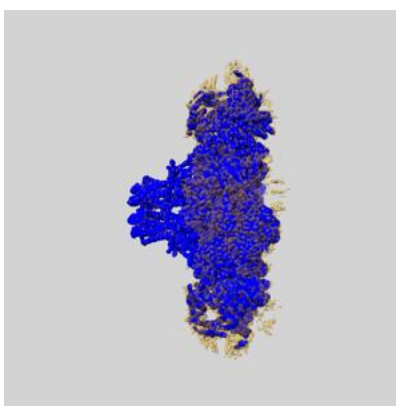
A mask typically either:

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

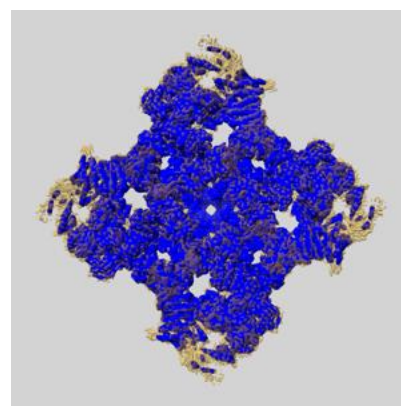
6.6.1 emd_23699_msk_1.map [i](#)



X



Y

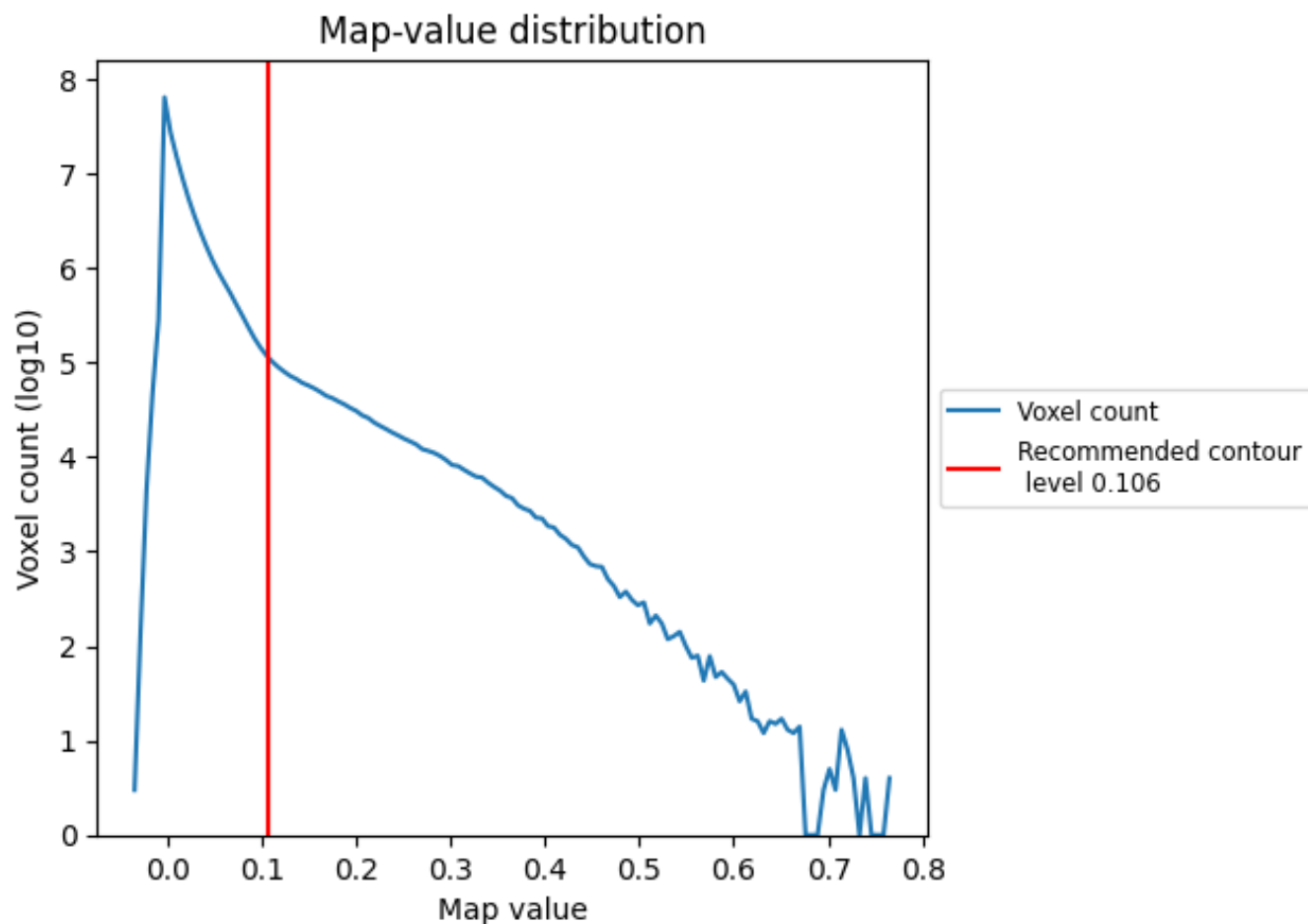


Z

7 Map analysis [i](#)

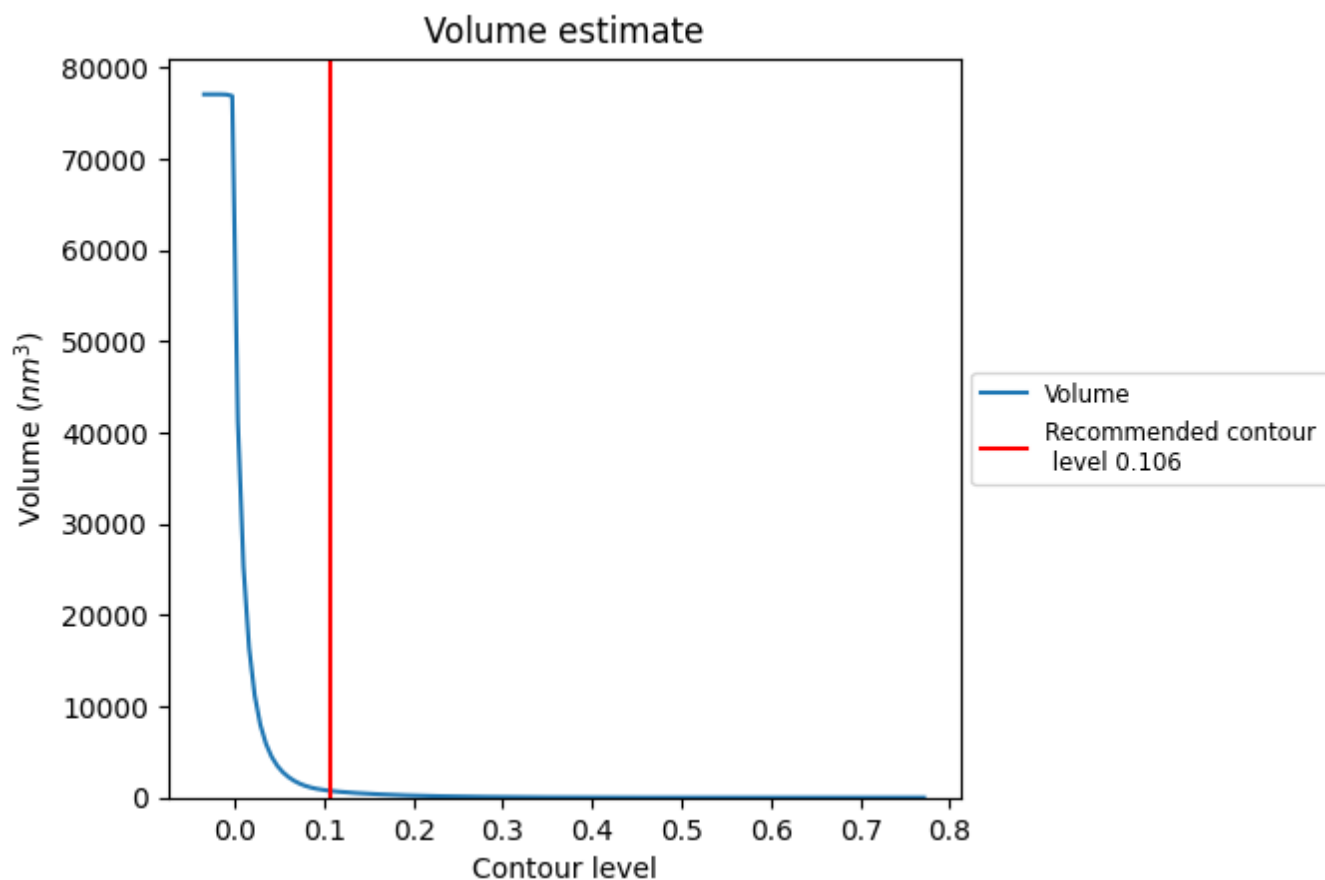
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

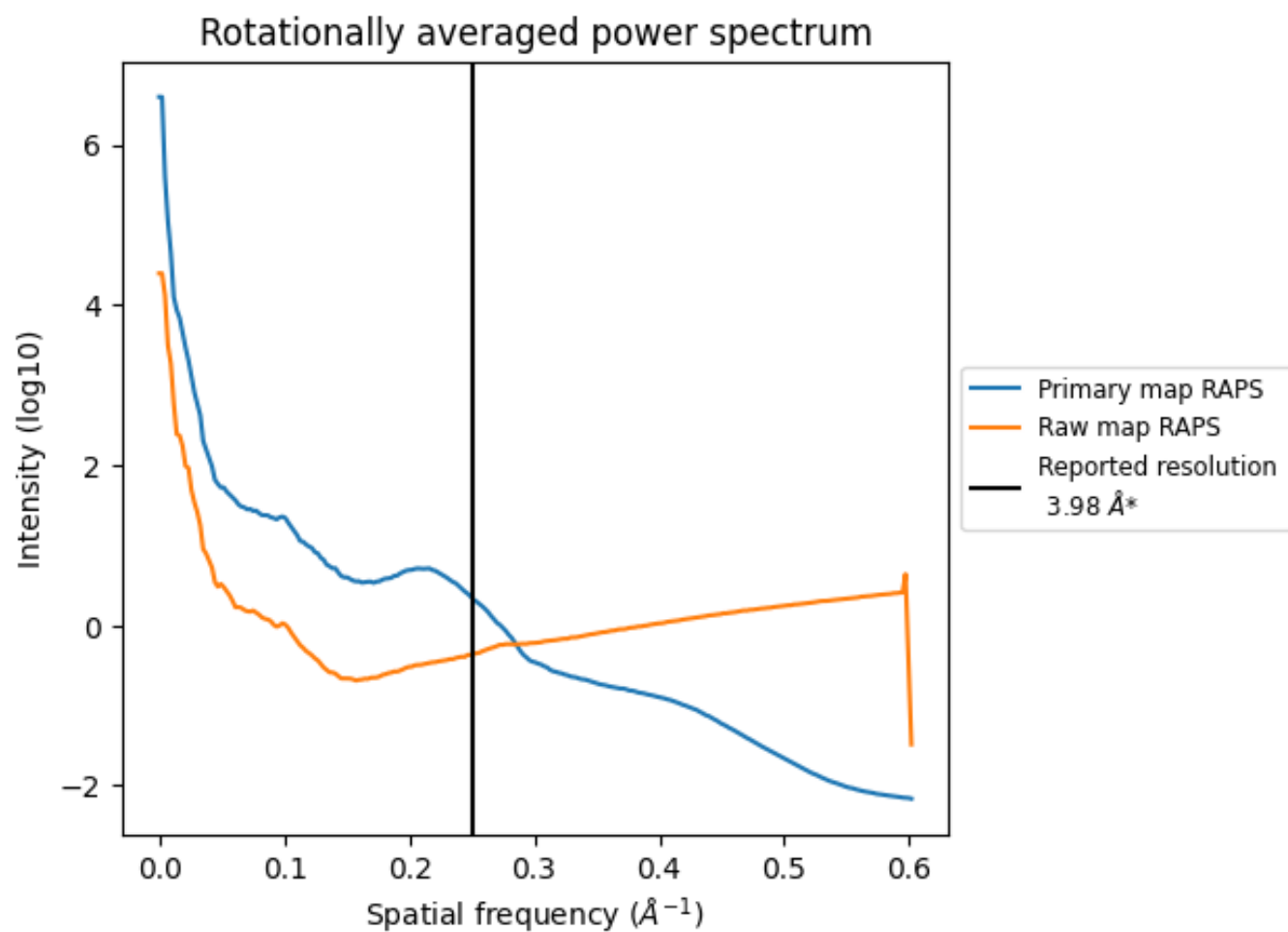
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 747 nm³; this corresponds to an approximate mass of 675 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 ⓘ

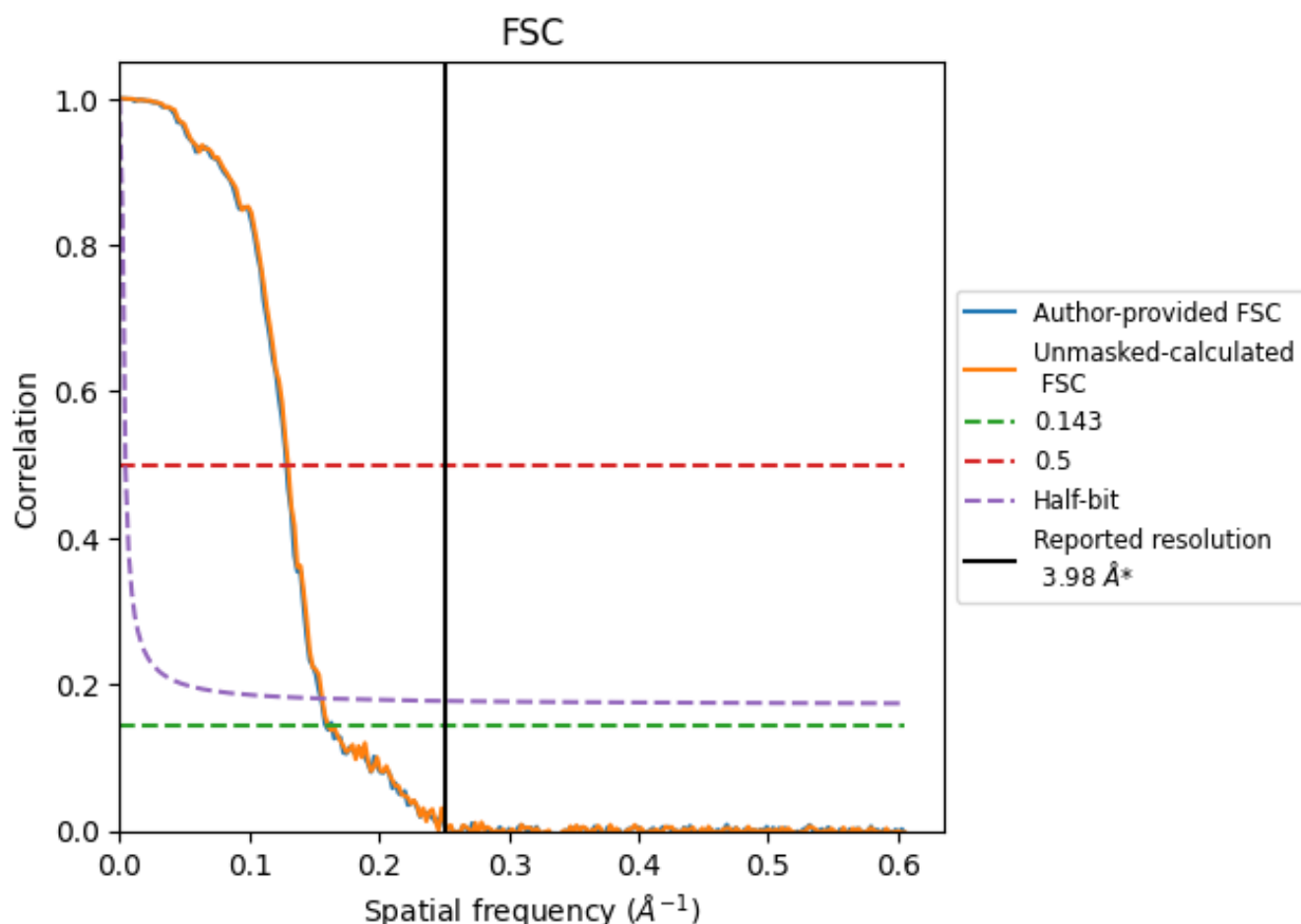


*Reported resolution corresponds to spatial frequency of 0.251 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.251 Å⁻¹

8.2 Resolution estimates

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.98	-	-
Author-provided FSC curve	6.28	7.78	6.44
Unmasked-calculated*	6.22	7.70	6.40

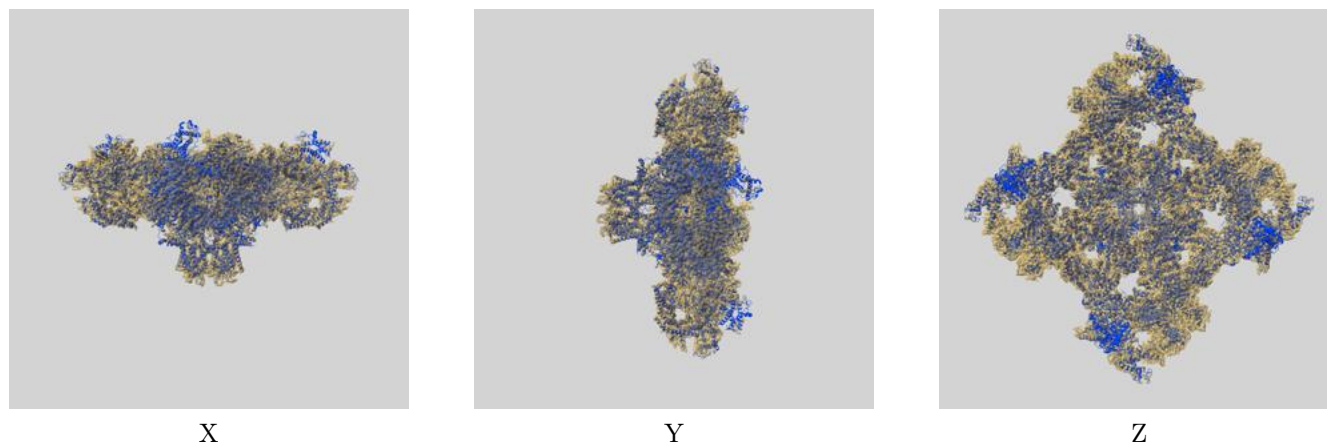
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 6.28 differs from the reported value 3.98 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.22 differs from the reported value 3.98 by more than 10 %

9 Map-model fit [i](#)

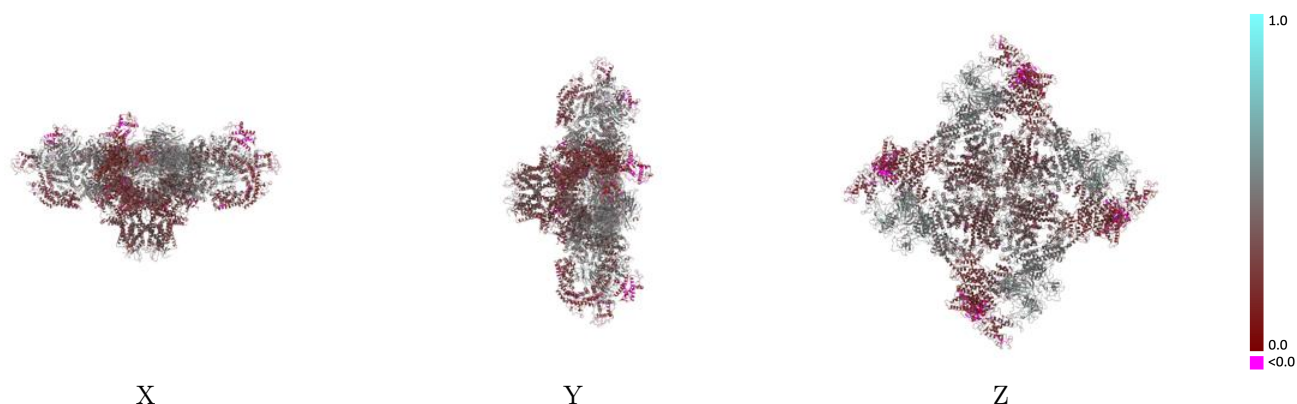
This section contains information regarding the fit between EMDB map EMD-23699 and PDB model 7M6L. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



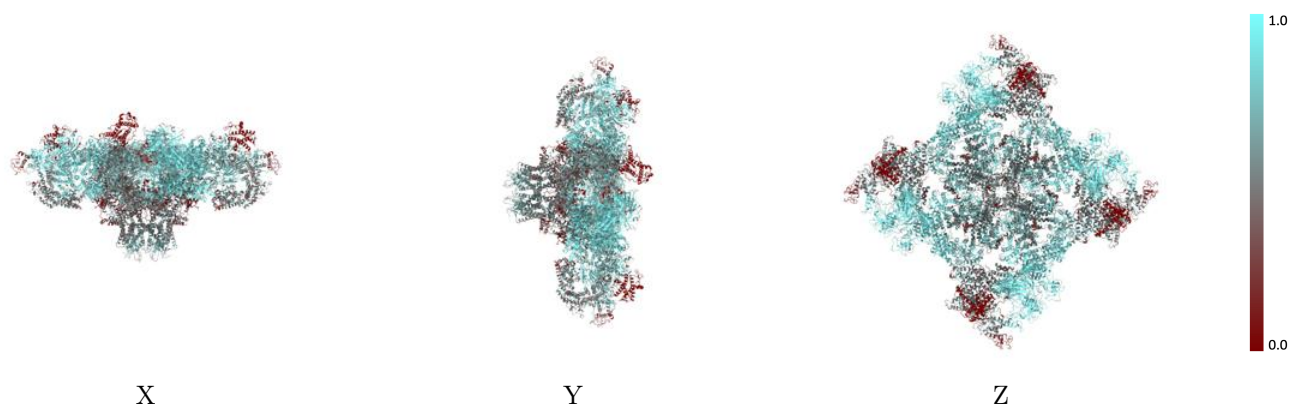
The images above show the 3D surface view of the map at the recommended contour level 0.106 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



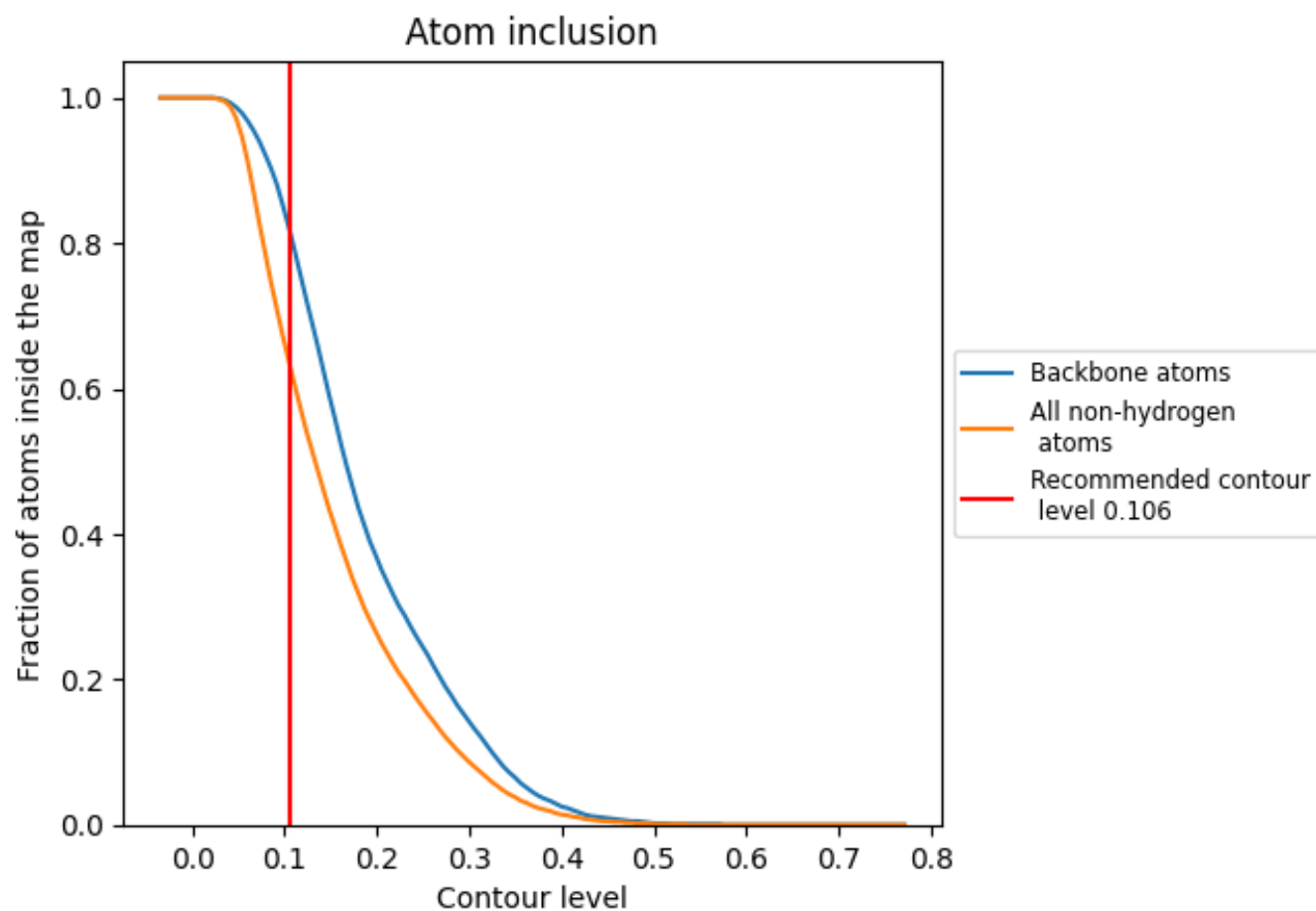
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.106).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 63% 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 (0.106) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6300	<div></div> 0.3560
A	<div></div> 0.6280	<div></div> 0.3600
B	<div></div> 0.6240	<div></div> 0.3500
F	<div></div> 0.8110	<div></div> 0.4790
G	<div></div> 0.6250	<div></div> 0.3500
H	<div></div> 0.8000	<div></div> 0.4790
I	<div></div> 0.6260	<div></div> 0.3500
J	<div></div> 0.8100	<div></div> 0.4780
O	<div></div> 0.8090	<div></div> 0.4800

