



wwPDB EM Validation Summary Report ⓘ

Nov 5, 2024 – 01:39 AM EST

PDB ID : 8UXF
EMDB ID : EMD-42762
Title : Structure of PKA phosphorylated human RyR2-R420W in the primed state
Authors : Miotto, M.C.; Marks, A.R.
Deposited on : 2023-11-09
Resolution : 3.13 Å(reported)
Based on initial model : 7UA5

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

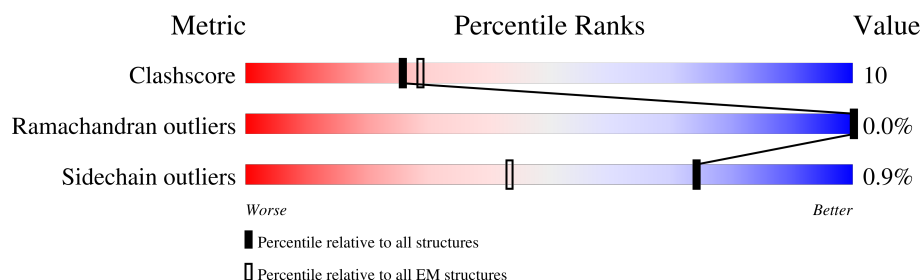
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.13 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	A	4967	<div> <div>5%</div> <div>66%</div> <div>19%</div> <div>15%</div> </div>
1	B	4967	<div> <div>5%</div> <div>66%</div> <div>19%</div> <div>15%</div> </div>
1	C	4967	<div> <div>5%</div> <div>66%</div> <div>19%</div> <div>15%</div> </div>
1	D	4967	<div> <div>5%</div> <div>65%</div> <div>19%</div> <div>15%</div> </div>
2	E	108	<div> <div>79%</div> <div>19%</div> <div>..</div> </div>
2	F	108	<div> <div>75%</div> <div>22%</div> <div>..</div> </div>
2	G	108	<div> <div>75%</div> <div>22%</div> <div>..</div> </div>
2	H	108	<div> <div>76%</div> <div>22%</div> <div>..</div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 138620 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	4224	Total 33774	C 21521	N 5743	O 6280	S 230	2	0
1	B	4224	Total 33774	C 21521	N 5743	O 6280	S 230	2	0
1	C	4224	Total 33774	C 21521	N 5743	O 6280	S 230	2	0
1	D	4224	Total 33774	C 21521	N 5743	O 6280	S 230	2	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	420	TRP	ARG	variant	UNP Q92736
B	420	TRP	ARG	variant	UNP Q92736
C	420	TRP	ARG	variant	UNP Q92736
D	420	TRP	ARG	variant	UNP Q92736

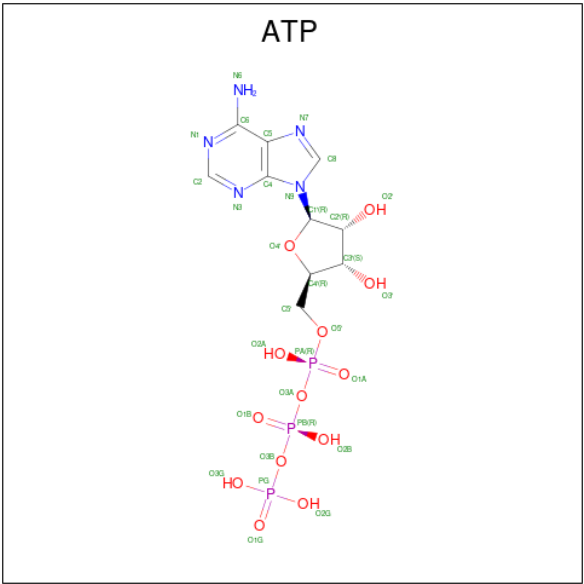
- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



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

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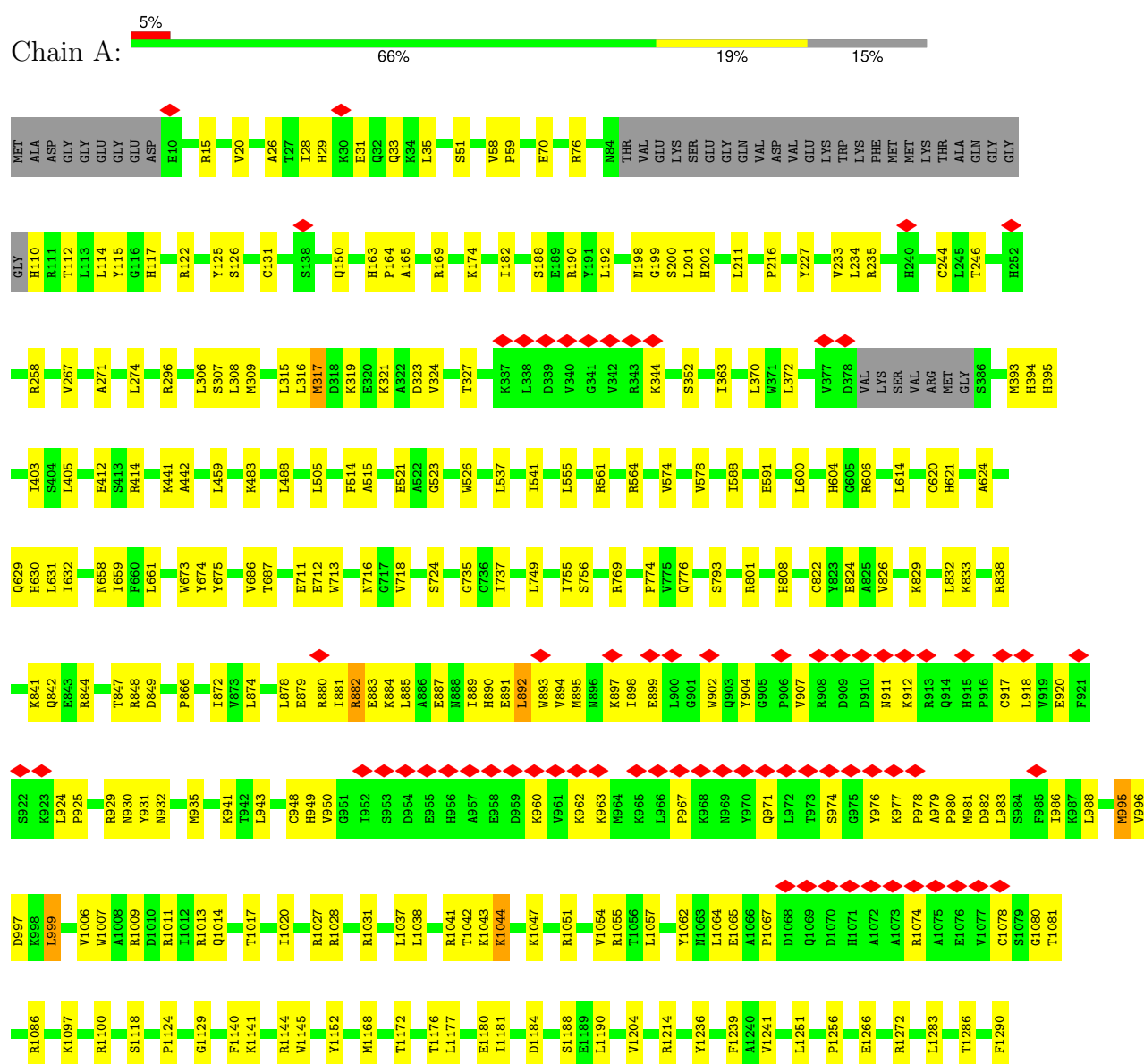
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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
4	D	1	31	10	5	13	3	0

3 Residue-property plots

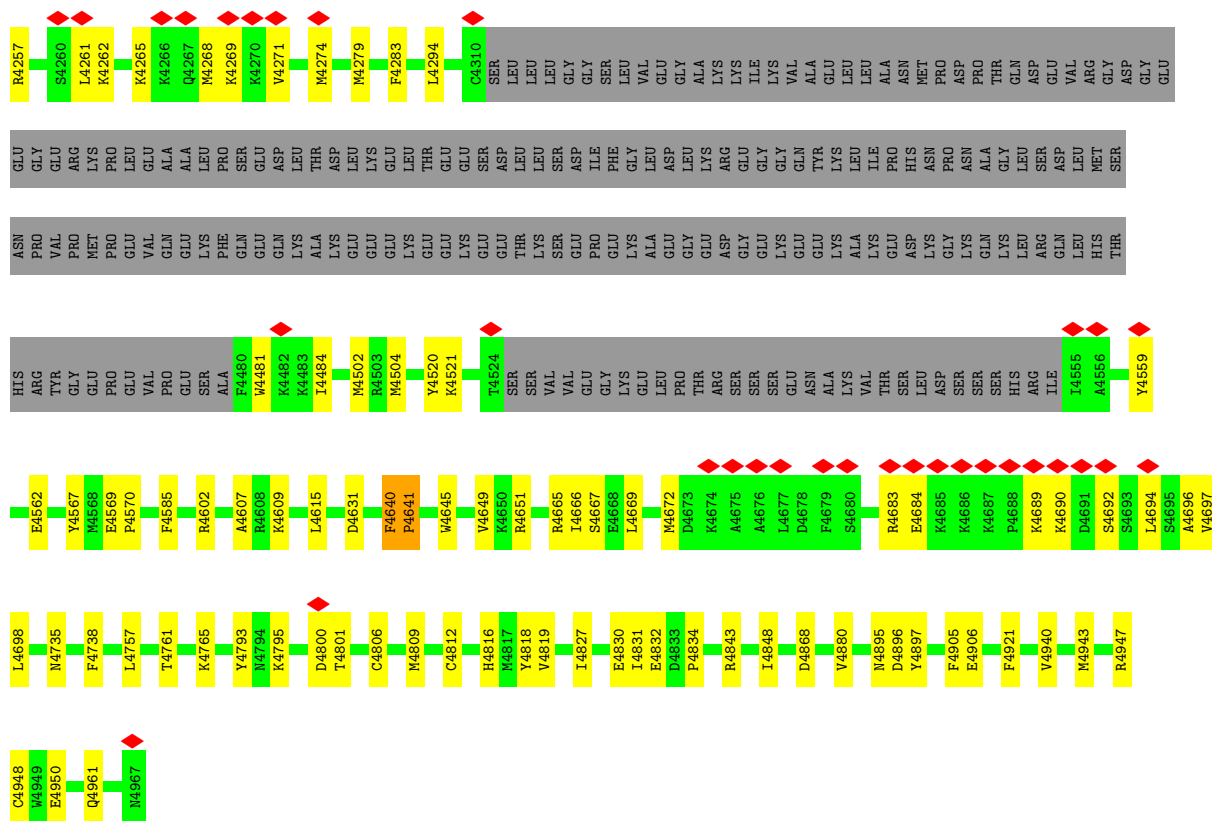
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Ryanodine receptor 2

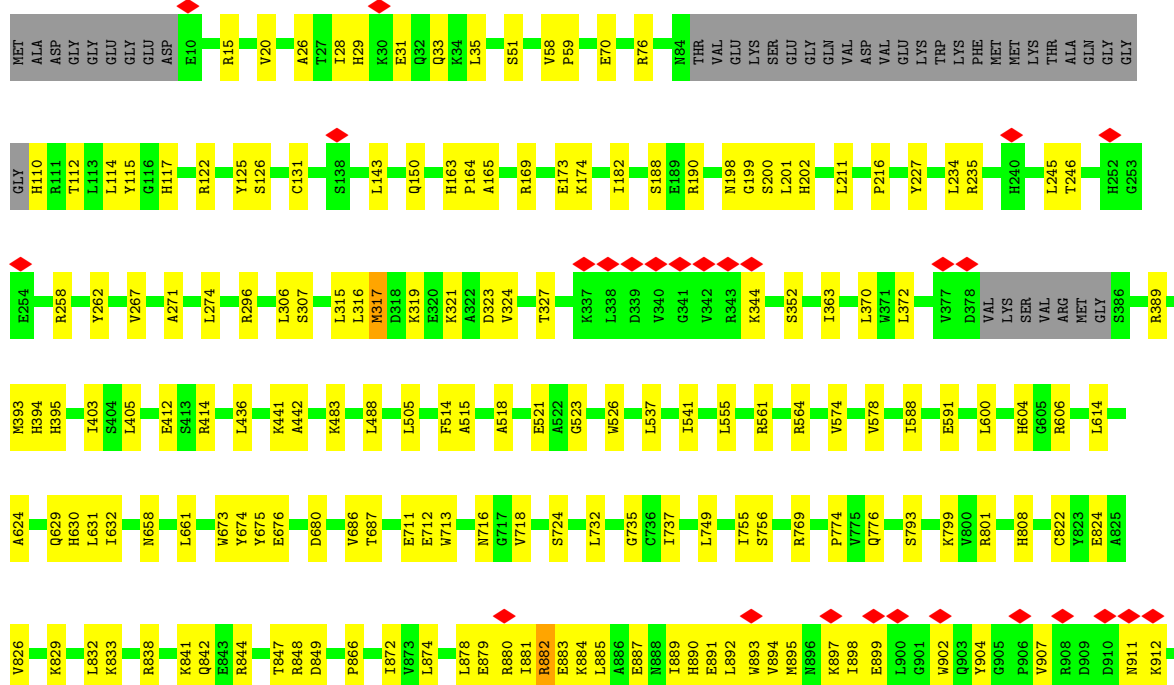


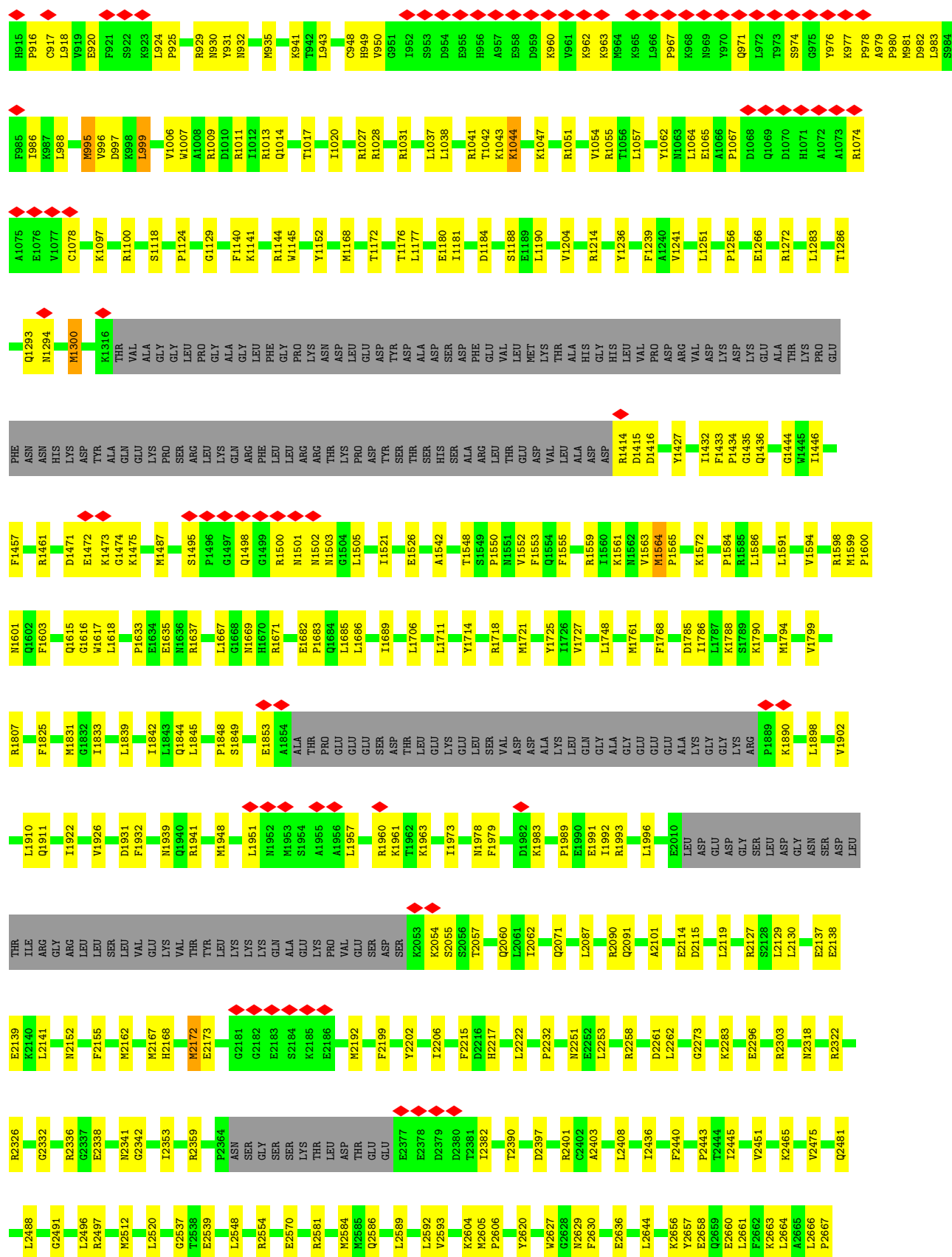


E4144	E4034	K3806	G3648	GLU	ILE	SER	PHE	K3308	M3231	G3156	E3069	H2978	D2891
S4155	Y4035	Q3811	A3649	ARG	ALA	PHE	TYR	K3311	P3232	G3157	K3070	H2978	D2891
Q4159	P4037	L3817	P3651	VAL	LEU	LEU	PRO	P3312	H3233	C3158	M3071	R2979	K2894
V4177	D4038	G3818	E3652	ASP	ASN	THR	LEU	Q3313	M3234	L3159	E3073	L2983	F2895
M4178	G4039	V3820	E3653	ALA	ARG	THR	ILE	L3314	M3235	A3160	K3074	L2987	L2896
E4179	K4040	V3821	E3654	ASN	PHE	THR	ARG	L3315	M3237	A3161	L3075	A2986	L2898
S4182	K4045	E3822	E3656	PHE	LEU	LYS	ASP	K3316	L3238	F3162	K3076	S2987	M2899
R4046	R4047	E3823	G3657	HIS	THR	ASN	TYR	T3317	L3239	F3166	Q3077	R2988	A2902
D4047	F4048	G3824	T3658	LEU	GLU	LYS	VAL	H3318	M3241	V3168	Q3078	K2999	R2905
F4049	H4049	S3825	R3659	GLN	ASP	ALA	ARG	P3321	R3248	E3172	F3080	M3002	C2906
K4050	K4050	G3826	K3659	VAL	GLU	ALA	ALA	L3322	M3249	T3173	T3081	K3010	F2907
S4054	S4054	E3827	L3664	SER	VAL	SER	LEU	K3323	W3250	H3174	THR	K3010	K2908
H4055	K4056	V3828	L3668	LEU	ASP	GLN	LYS	Q3324	N3256	L3175	ASN	V3013	D2909
H4057	H4057	V3829	L3668	VAL	ASP	GLN	LYS	K3325	E3259	D3176	GLN	L3014	E2911
S4061	Q4060	L3830	L3668	ARG	ASP	GLU	PRO	L3326	R3260	K3177	PRO	V3015	L2912
E4062	E4062	D3833	A3692	GLY	ILE	ILE	ASN	K3327	R3260	H3178	K3088	H3017	T2914
T4063	T4063	E3834	A3692	VAL	ILE	ILE	ASN	K3328	R3260	N3179	G3089	R3018	T2914
A4064	A4064	F3835	A3692	ARG	ARG	ARG	GLU	K3329	M3263	T3183	V3090	R3018	T2914
L4067	L4067	F3835	A3692	ARG	SER	LYS	GLU	A3330	T3266	Y3184	I3093	L3021	E2918
A4070	A4070	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	N3185	L3102	D3025	Y2923
E4071	E4071	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
T4072	T4072	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
E4074	E4074	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
N4076	N4076	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
T4077	T4077	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
L4078	L4078	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
E4082	E4082	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
F4084	F4084	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
K4085	K4085	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
H4088	H4088	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
D4093	D4093	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
I4094	I4094	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
S4106	S4106	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
T4113	T4113	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
Q4116	Q4116	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
T4117	T4117	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
F4118	F4118	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
L4119	L4119	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
E4120	E4120	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
L4121	L4121	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
S4237	S4237	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
T4240	T4240	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
Y4250	Y4250	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
T4254	T4254	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
L4255	L4255	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
M4256	M4256	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
L3796	L3796	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
L3778	L3778	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
M3777	M3777	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
N3770	N3770	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
K3760	K3760	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
A3756	A3756	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
L3741	L3741	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
H3732	H3732	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
L3731	L3731	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
R3730	R3730	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
A3729	A3729	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
Q3728	Q3728	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
K3717	K3717	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
L3711	L3711	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
E3710	E3710	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
GLU	GLU	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
E3702	E3702	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
L3608	L3608	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
Y3609	Y3609	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
R3604	R3604	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
F3603	F3603	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
A3601	A3601	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
V3600	V3600	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
V3599	V3599	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
ALA	ALA	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
THR	THR	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
ASP	ASP	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
ASN	ASN	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
GLY	GLY	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
LEU	LEU	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
THR	THR	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
VAL	VAL	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
GLU	GLU	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
ASP	ASP	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
THR	THR	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
ASN	ASN	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
GLY	GLY	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
LEU	LEU	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
THR	THR	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
ASN	ASN	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
GLY	GLY	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
LEU	LEU	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
THR	THR	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
ASN	ASN	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
GLY	GLY	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
LEU	LEU	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
THR	THR	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
ASN	ASN	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
GLY	GLY	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
LEU	LEU	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
THR	THR	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
ASN	ASN	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
GLY	GLY	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
LEU	LEU	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
THR	THR	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102	D3025	Y2923
ASN	ASN	F3835	A3692	ARG	ASN	MET	ALA	A3331	T3266	Y3185	L3102		

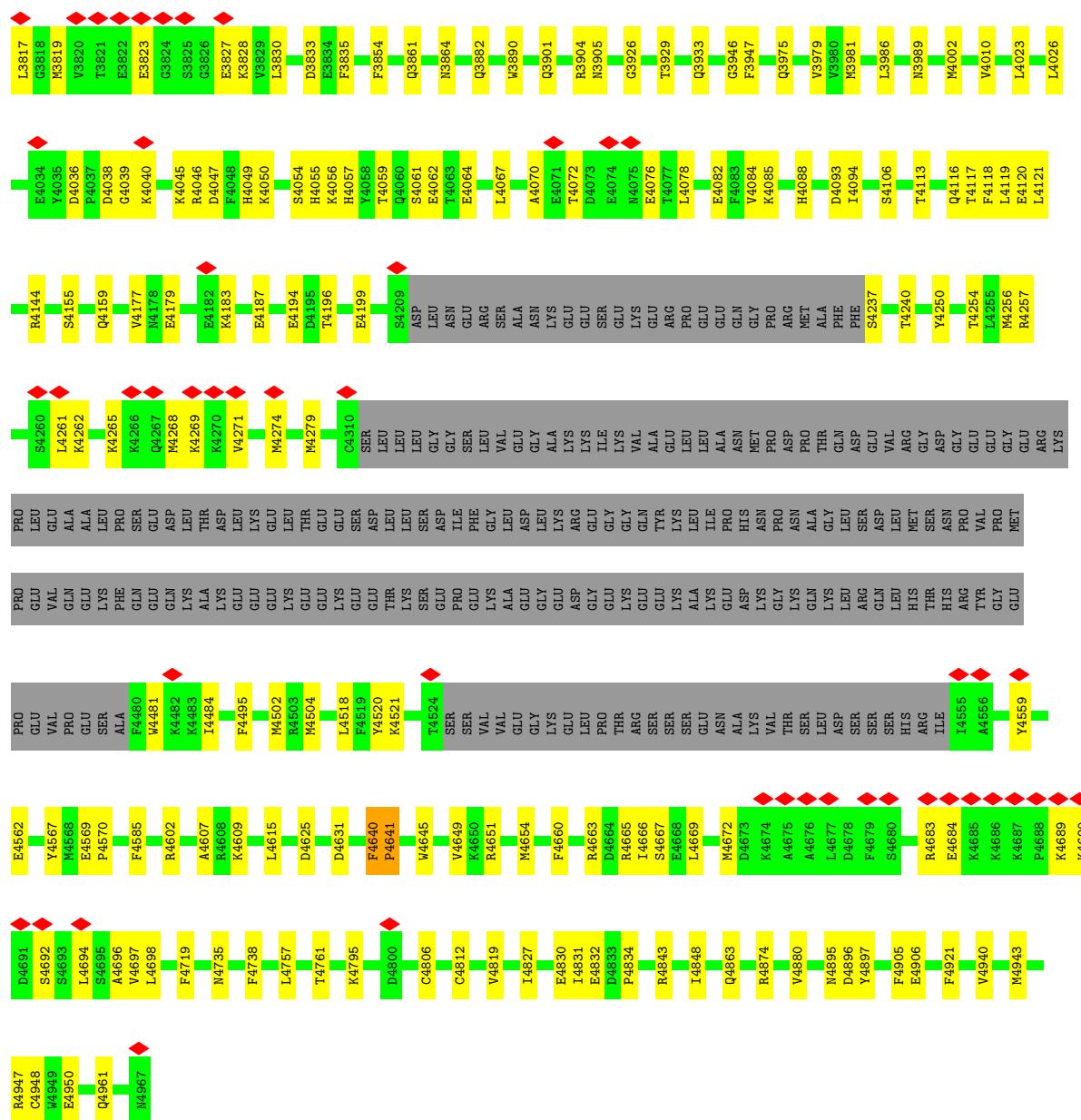


● Molecule 1: Ryanodine receptor 2

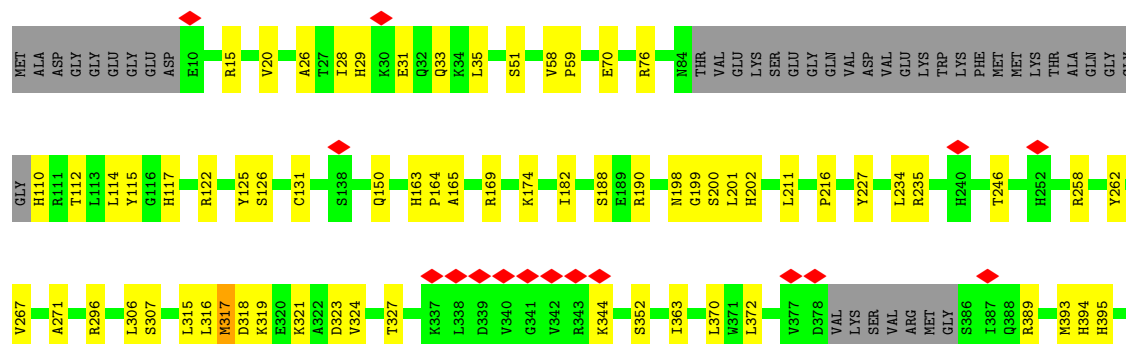








• Molecule 1: Ryanodine receptor 2









V3228	E3149	E3066	H2978	A2889	L2737	E2660	V2475	N2318	E2137	V1902
T3229	R3152	D3067	R2979	Q2890	A2738	L2661	Q2481	R2322	E2138	L1910
N3230	S3153	L3068	R2979	D2891	N2739	K2663	L2488	R2332	E2139	Q1911
P3232	E3069	E3069	L2983	K2894	G2740	A2665	G2491	R2326	L2141	I1922
H3233	T3071	K3070	A2986	F2895	W2741	A2666	L2496	G2332	L2146	V1926
K3235	G3158	M3072	S2987	L2896	I2742	P2667	R2497	G2336	N2152	D1931
E3236	E3073	N3074	R2988	I2898	Y2743	S2670	M2512	E2337	F2155	F1932
V3237	N3074	N3074	P2989	VAL	G2744	G2674	L2520	E2338	VAL	N1939
L3238	L3075	L3075	L2990	ALA	E2745	N2681	G2537	E2342	GLU	Q1940
L3239	A3161	K3076	K2999	ALA	I2746	Y2685	E2539	L2353	THR	R1941
P3240	F3162	Q3077	K2999	HIS	Y2747	M2688	L2548	R2359	LEU	M1948
K3241	F3166	F2907	E3002	G2906	S2748	E2689	R2554	P2364	L1951	L1951
R3248	P3167	K2908	M3003	F2908	D2749	E2690	E2570	ASN	M1952	M1952
V3249	V3168	D2909	K3010	D2909	S2750	K2691	L2581	GLY	M1953	S1954
K3250	F3172	L2910	V3013	L2910	S2751	E2692	R2581	THR	A1955	A1955
N3256	H3173	E2911	L3014	E2911	K2752	E2693	R2581	ASP	A1956	L1957
E3259	H3174	D2913	V3015	D2913	Q2753	S2694	M2584	THR	R1960	R1960
R3260	L3175	T2914	R3016	T2914	P2755	S2694	Q2585	GLU	K1961	K1961
A3261	D3176	T2914	R3017	T2914	P2756	M2695	Q2586	GLU	T1962	T1962
F3262	K3177	E2918	R3018	E2918	W2757	D2696	L2589	GLU	K1963	K1963
K3263	N3179	Y2923	I3019	Y2923	K2758	S2697	L2589	GLU	I1973	I1973
T3266	I3183	S2924	S3020	S2924	Y2760	E2698	M2584	ASP	N1978	N1978
A3267	N3185	L2926	L3021	L2926	K2761	G2699	Q2586	THR	F1979	F1979
L3268	K3186	L2929	D3025	L2929	L2762	N2700	L2589	GLU	D1982	D1982
N3269	K3187	I2930	T3027	I2930	S2764	F2701	L2589	GLU	K1983	K1983
S3270	K3188	H2937	S3028	H2937	E2765	N2702	L2589	GLU	C1988	C1988
E3271	S3189	V3030	V3030	V3030	K2766	Q2704	L2592	GLU	P1989	P1989
H3272	R3190	L3033	L3033	L3033	E2767	P2705	V2593	GLU	E1990	E1990
K3273	E3191	L3036	L3036	L3036	K2768	N2706	K2604	GLU	E1991	E1991
N3274	R3192	L3036	L3036	L3036	L2770	P2707	M2605	GLU	I1992	I1992
T3276	L3195	L3036	L3036	L3036	Y2771	S2709	P2606	GLU	R1993	R1993
L3277	S3196	L3036	L3036	L3036	R2772	N2710	Y2620	GLU	L1996	L1996
L3277	L3197	L3036	L3036	L3036	R2773	I2711	L2620	GLU	E2010	E2010
G3278	P3198	L3036	L3036	L3036	P2774	K2716	W2627	GLU	ASP	ASP
N3279	T3199	L3036	L3036	L3036	L2775	L2717	G2528	GLU	GLU	GLU
L3280	N3200	L3036	L3036	L3036	K2776	E2718	N2629	GLU	ASP	ASP
L3281	D3125	L3036	L3036	L3036	K2780	F2719	F2630	GLU	GLY	GLY
K3282	E3202	L3036	L3036	L3036	L2781	N2720	E2636	GLU	LEU	LEU
L3283	D3203	L3036	L3036	L3036	M2782	K2723	L2644	GLU	ASP	ASP
L3284	V3204	L3036	L3036	L3036	L2783	Y2724	A2651	GLU	GLY	GLY
Y3285	P3209	L3036	L3036	L3036	W2787	Y2724	K2655	GLU	ASN	ASN
L3288	K3213	L3036	L3036	L3036	R2788	S2728	K2655	GLU		
G3289	L3214	L3036	L3036	L3036	R2791	K2731	K2655	GLU		
D3291	K3215	L3036	L3036	L3036	L2792	W2732	Y2657	GLU		
E3292	E3216	L3036	L3036	L3036	R2793	N2733	E2658	GLU		
G3293	E3217	L3036	L3036	L3036	E2794	S2734	K2659	GLU		
A3294	L3218	L3036	L3036	L3036	G2795	D2735	Q2659	GLU		
V3295	V3219	L3036	L3036	L3036	D2796	K2736		GLU		
K3296	R3227	L3036	L3036	L3036	N2802	K2736		GLU		
K3297		L3036	L3036	L3036	ARG			GLU		
R3298		L3036	L3036	L3036	THR			GLU		
L3299		L3036	L3036	L3036	ARG			GLU		





- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E: 79% 19% ..



- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F: 75% 22% ..



- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain G: 75% 22% ..



- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H: 76% 22% ..



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	102478	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	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.646	Depositor
Minimum map value	-0.013	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	430.848, 430.848, 430.848	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8415, 0.8415, 0.8415	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	A	0.29	0/34516	0.49	2/46623 (0.0%)
1	B	0.29	0/34516	0.49	1/46623 (0.0%)
1	C	0.29	0/34516	0.49	2/46623 (0.0%)
1	D	0.29	0/34516	0.49	1/46623 (0.0%)
2	E	0.31	0/834	0.55	0/1123
2	F	0.31	0/834	0.55	0/1123
2	G	0.31	0/834	0.55	0/1123
2	H	0.31	0/834	0.55	0/1123
All	All	0.29	0/141400	0.49	6/190984 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
All	All	0	8

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3215	MET	CB-CG-SD	5.58	129.15	112.40
1	C	3215	MET	CB-CG-SD	5.58	129.14	112.40
1	B	3215	MET	CB-CG-SD	5.58	129.12	112.40
1	D	3215	MET	CB-CG-SD	5.57	129.12	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	892	LEU	CB-CG-CD2	-5.03	102.45	111.00

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3926	GLY	Peptide
1	A	4640	PHE	Peptide
1	B	3926	GLY	Peptide
1	B	4640	PHE	Peptide
1	C	3926	GLY	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	33774	0	33452	689	0
1	B	33774	0	33452	685	0
1	C	33774	0	33452	679	0
1	D	33774	0	33452	694	0
2	E	818	0	821	14	0
2	F	818	0	821	17	0
2	G	818	0	821	17	0
2	H	818	0	821	16	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	62	0	24	0	0
4	B	62	0	24	0	0
4	C	62	0	24	0	0
4	D	62	0	24	0	0
All	All	138620	0	137188	2751	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 10.

The worst 5 of 2751 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:B:3235:MET:HA	1:B:3239:LEU:HD13	1.41	1.03
1:D:3235:MET:HA	1:D:3239:LEU:HD13	1.41	1.02
1:C:3235:MET:HA	1:C:3239:LEU:HD13	1.41	1.02
1:A:3235:MET:HA	1:A:3239:LEU:HD13	1.41	1.02
1:B:3152:ARG:HH21	1:B:3236:GLU:HB3	1.39	0.88

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	4198/4967 (84%)	4097 (98%)	99 (2%)	2 (0%)	100	100
1	B	4198/4967 (84%)	4099 (98%)	97 (2%)	2 (0%)	100	100
1	C	4198/4967 (84%)	4099 (98%)	97 (2%)	2 (0%)	100	100
1	D	4198/4967 (84%)	4098 (98%)	98 (2%)	2 (0%)	100	100
2	E	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	F	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	G	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
2	H	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
All	All	17212/20300 (85%)	16802 (98%)	402 (2%)	8 (0%)	100	100

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2988	ARG
1	A	4641	PRO
1	B	2988	ARG
1	B	4641	PRO

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Mol	Chain	Res	Type
1	C	2988	ARG

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	3708/4358 (85%)	3676 (99%)	32 (1%)	75	86
1	B	3708/4358 (85%)	3676 (99%)	32 (1%)	75	86
1	C	3708/4358 (85%)	3676 (99%)	32 (1%)	75	86
1	D	3708/4358 (85%)	3676 (99%)	32 (1%)	75	86
2	E	88/89 (99%)	86 (98%)	2 (2%)	45	67
2	F	88/89 (99%)	86 (98%)	2 (2%)	45	67
2	G	88/89 (99%)	86 (98%)	2 (2%)	45	67
2	H	88/89 (99%)	86 (98%)	2 (2%)	45	67
All	All	15184/17788 (85%)	15048 (99%)	136 (1%)	74	86

5 of 136 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	2884	LYS
1	D	3057	LEU
2	F	18	LYS
1	B	2766	LYS
1	B	2695	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	604	HIS
1	D	4055	HIS
1	D	658	ASN
1	D	3114	GLN

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Mol	Chain	Res	Type
2	G	26	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 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	ATP	B	5003	-	28,33,33	0.63	0	34,52,52	0.59	1 (2%)
4	ATP	A	5002	-	28,33,33	0.68	0	34,52,52	0.69	1 (2%)
4	ATP	B	5002	-	28,33,33	0.67	0	34,52,52	0.69	1 (2%)
4	ATP	A	5003	-	28,33,33	0.63	0	34,52,52	0.58	1 (2%)
4	ATP	D	5002	-	28,33,33	0.68	0	34,52,52	0.70	2 (5%)
4	ATP	C	5003	-	28,33,33	0.62	0	34,52,52	0.59	1 (2%)
4	ATP	D	5003	-	28,33,33	0.63	0	34,52,52	0.59	1 (2%)
4	ATP	C	5002	-	28,33,33	0.68	0	34,52,52	0.69	1 (2%)

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	ATP	B	5003	-	-	7/18/38/38	0/3/3/3
4	ATP	A	5002	-	-	8/18/38/38	0/3/3/3
4	ATP	B	5002	-	-	8/18/38/38	0/3/3/3
4	ATP	A	5003	-	-	7/18/38/38	0/3/3/3
4	ATP	D	5002	-	-	8/18/38/38	0/3/3/3
4	ATP	C	5003	-	-	7/18/38/38	0/3/3/3
4	ATP	D	5003	-	-	7/18/38/38	0/3/3/3
4	ATP	C	5002	-	-	8/18/38/38	0/3/3/3

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	5003	ATP	C5-C6-N6	2.34	123.87	120.31
4	B	5003	ATP	C5-C6-N6	2.32	123.84	120.31
4	C	5002	ATP	C5-C6-N6	2.31	123.84	120.31
4	A	5002	ATP	C5-C6-N6	2.31	123.82	120.31
4	D	5002	ATP	C5-C6-N6	2.30	123.81	120.31

There are no chirality outliers.

5 of 60 torsion outliers are listed below:

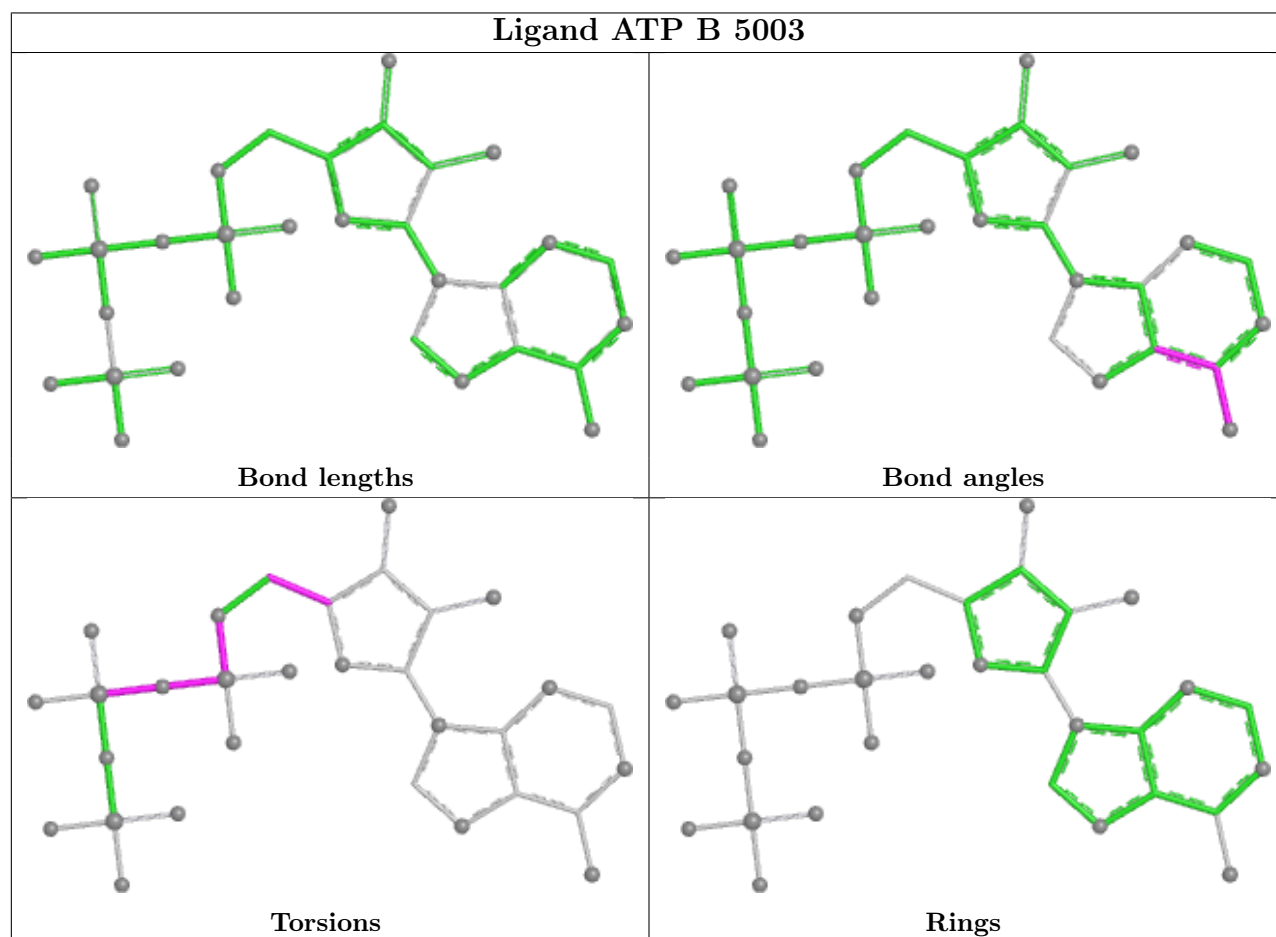
Mol	Chain	Res	Type	Atoms
4	A	5002	ATP	C5'-O5'-PA-O1A
4	A	5002	ATP	C5'-O5'-PA-O3A
4	A	5003	ATP	C5'-O5'-PA-O1A
4	A	5003	ATP	C5'-O5'-PA-O2A
4	A	5003	ATP	C5'-O5'-PA-O3A

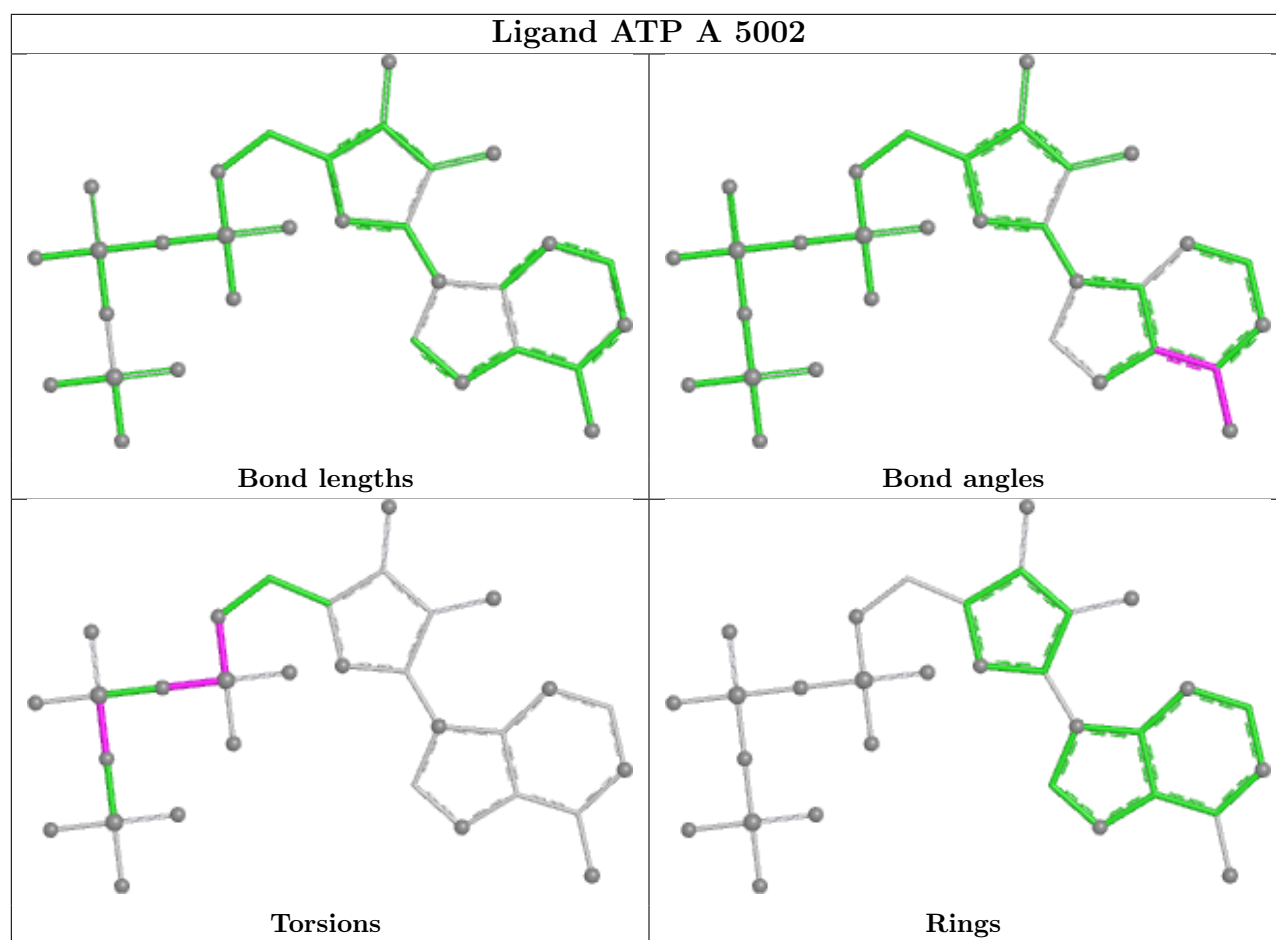
There are no ring outliers.

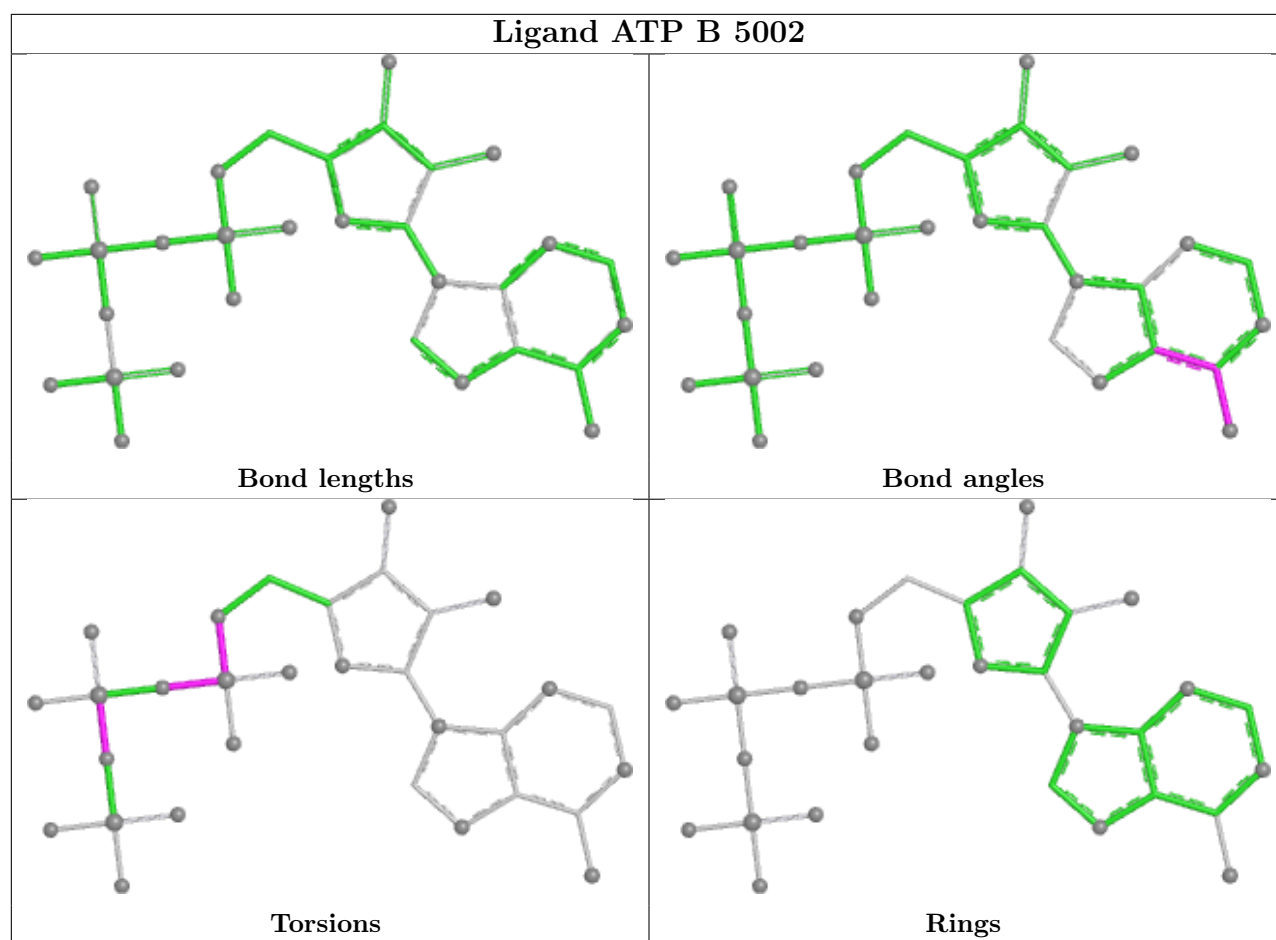
No monomer is involved in short contacts.

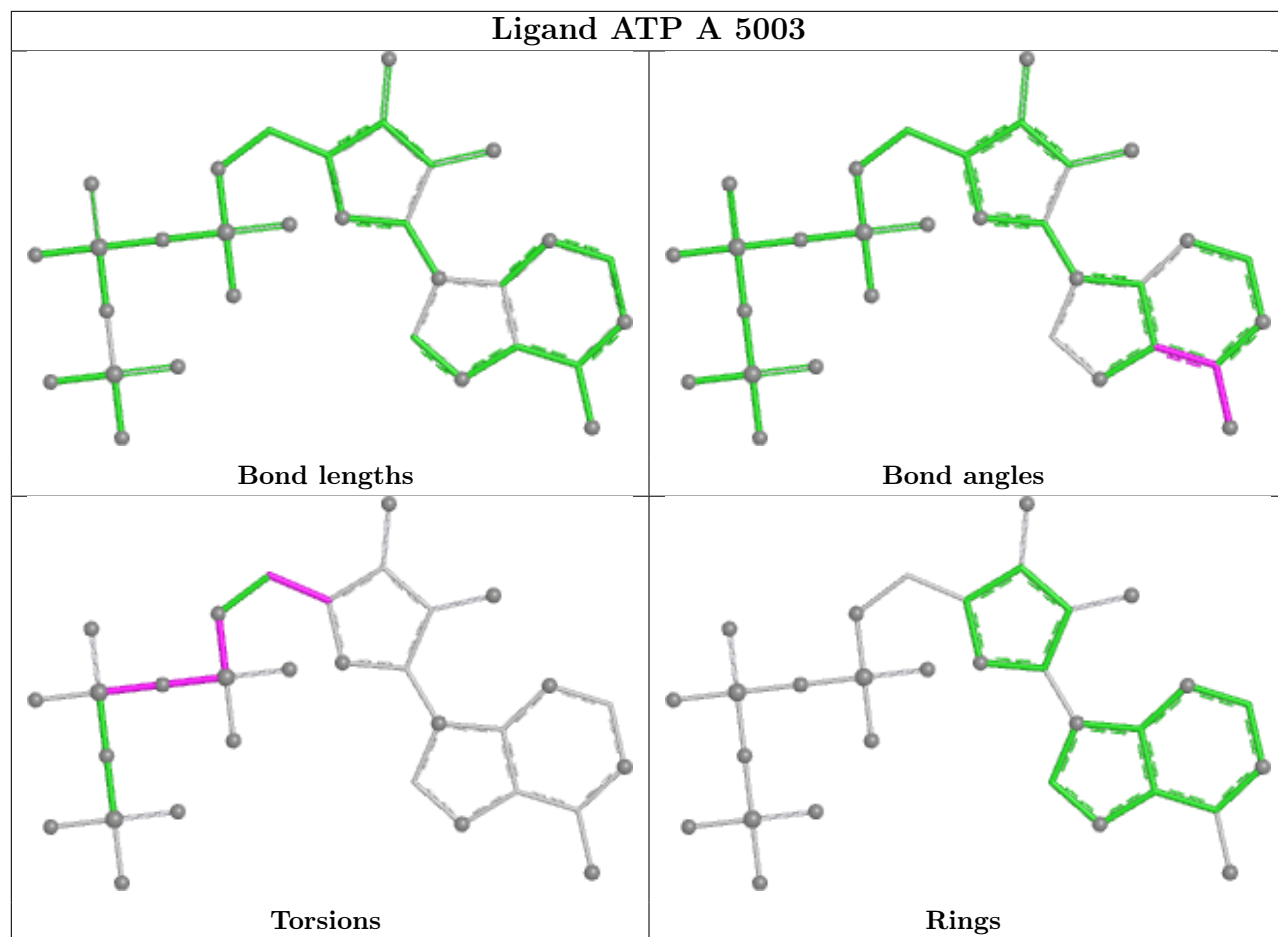
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

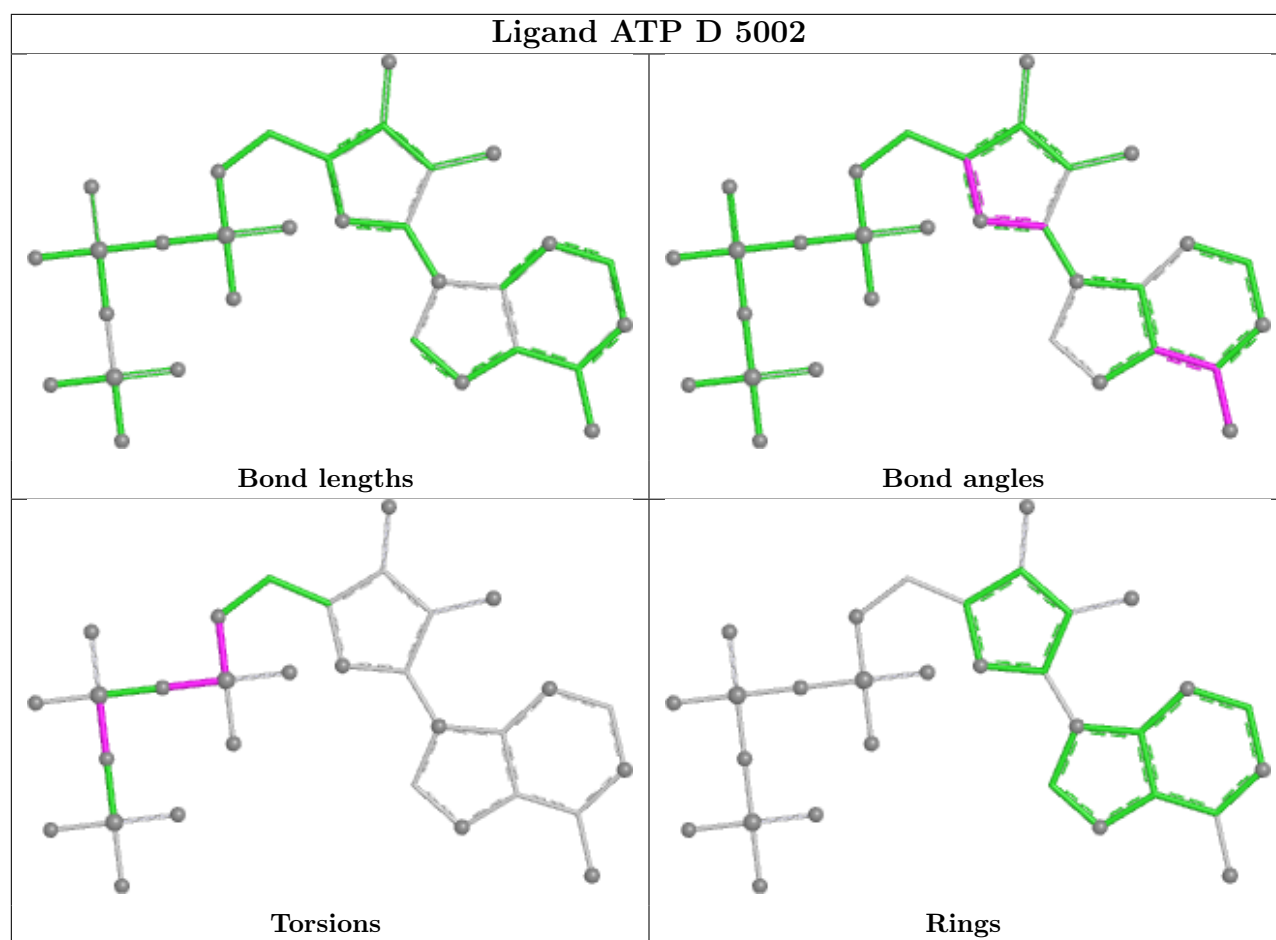
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

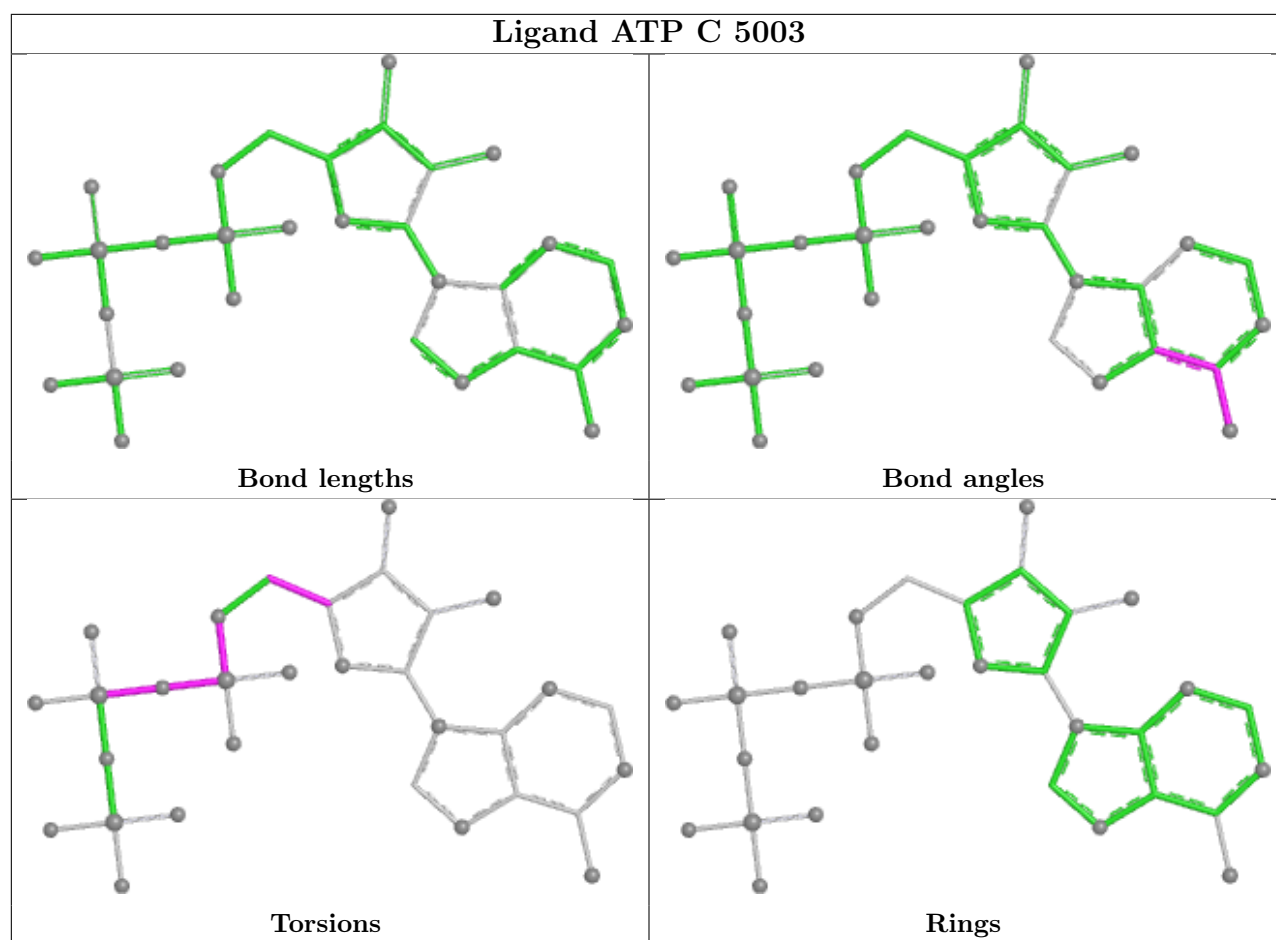


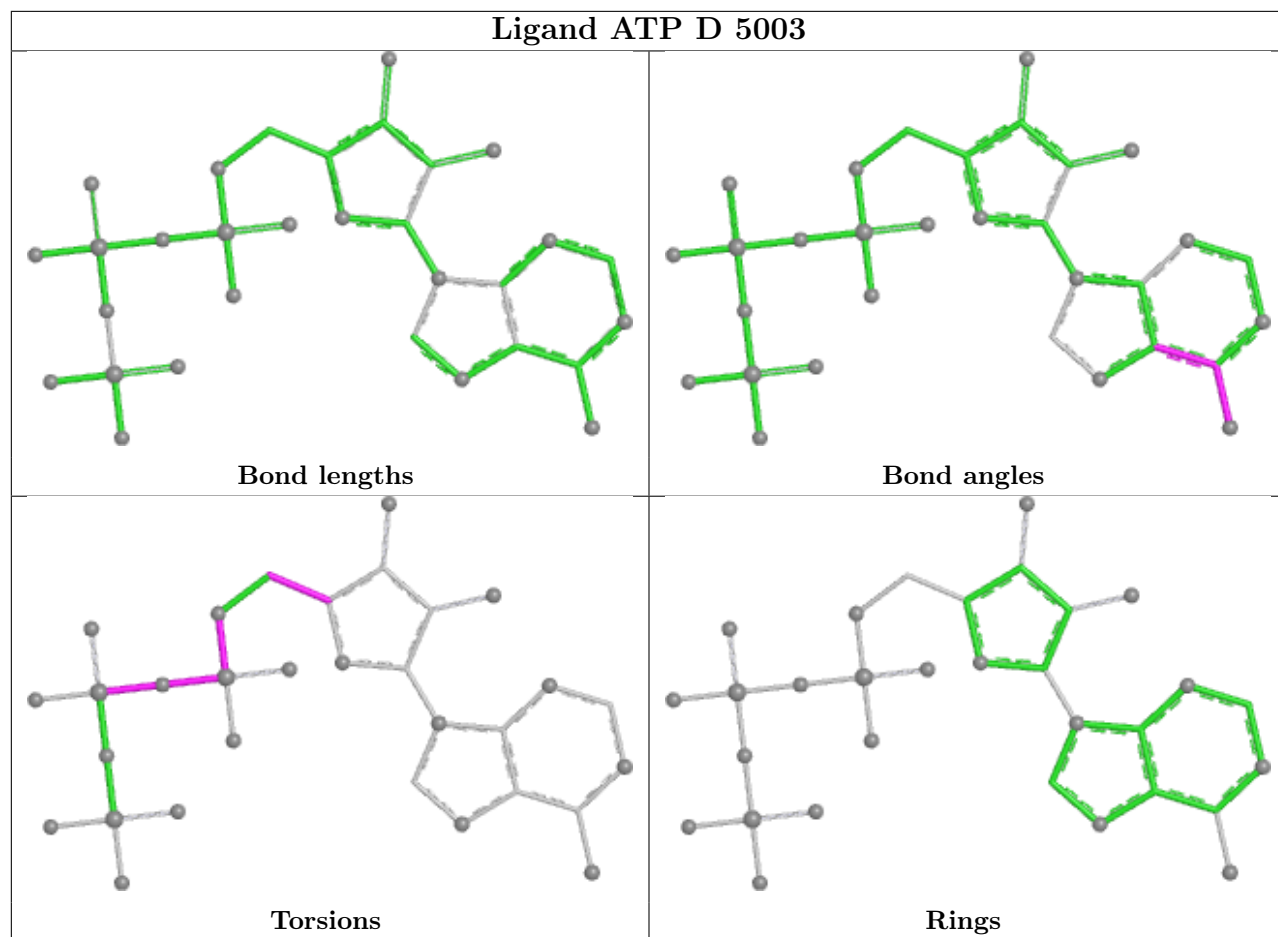


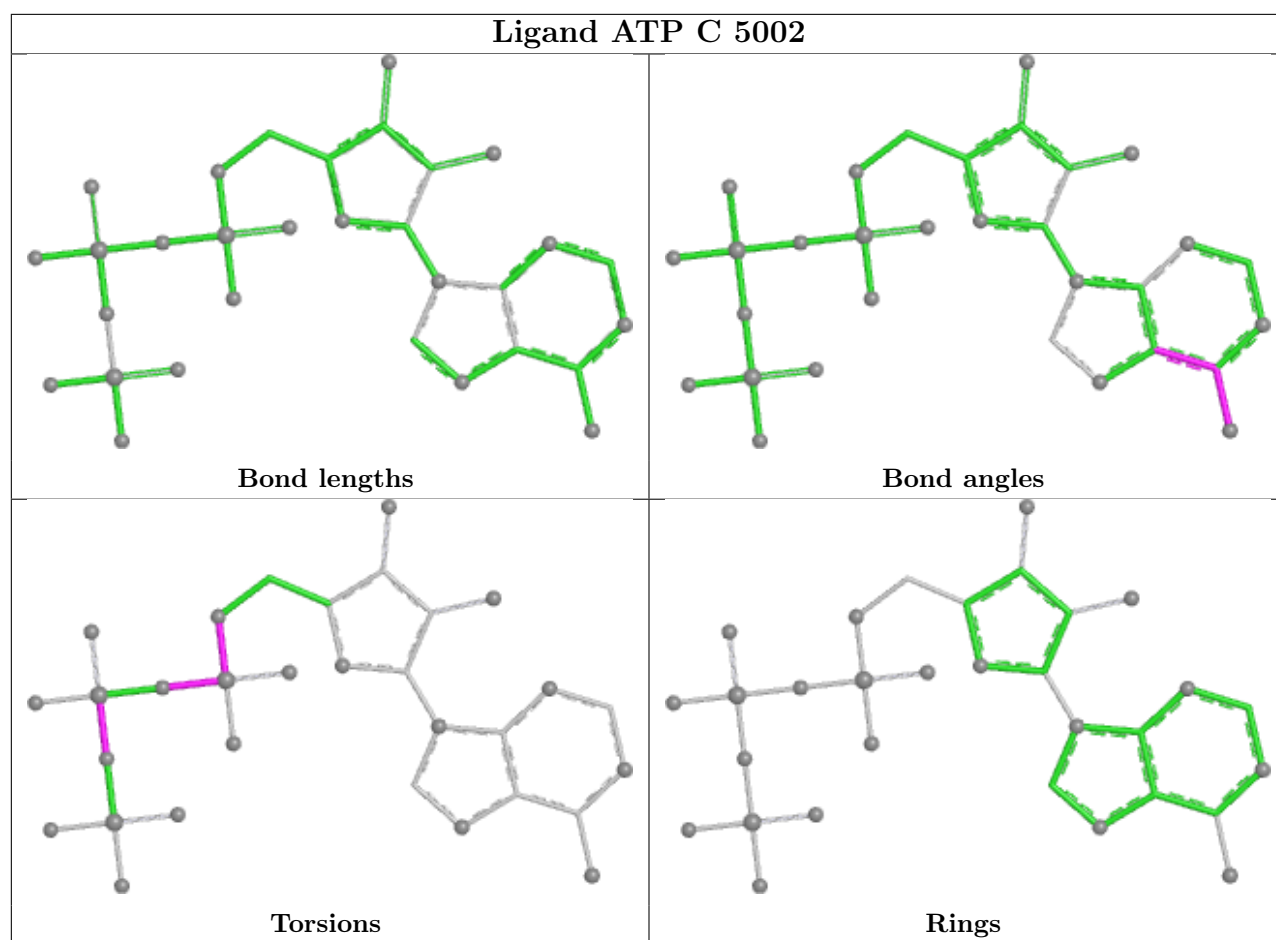












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42762. These allow visual inspection of the internal detail of the map and identification of artifacts.

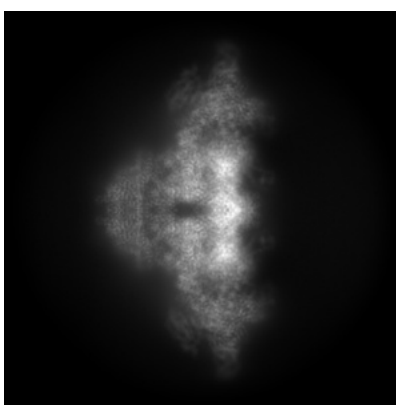
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

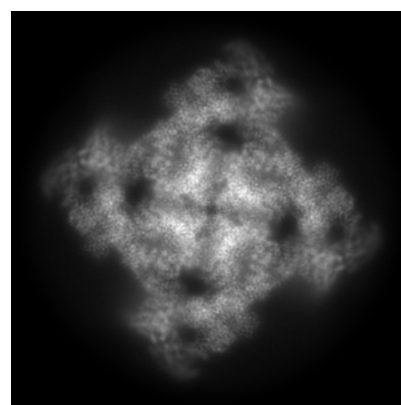
6.1.1 Primary map



X



Y

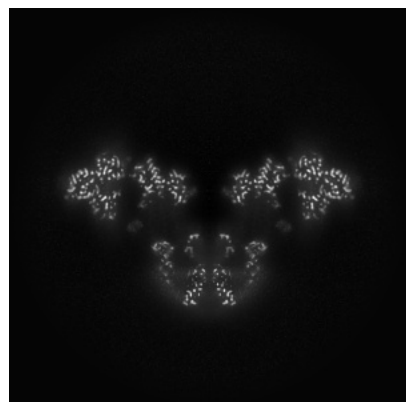


Z

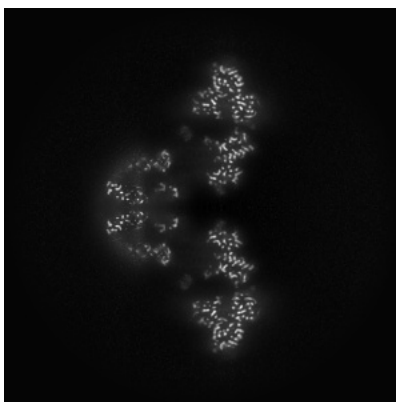
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

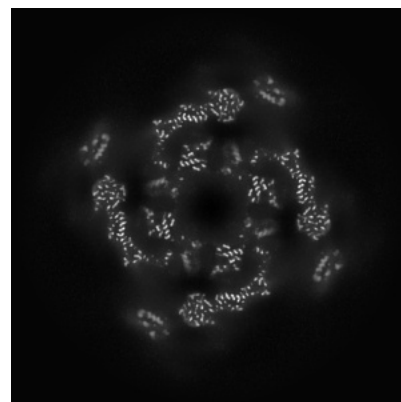
6.2.1 Primary map



X Index: 256



Y Index: 256

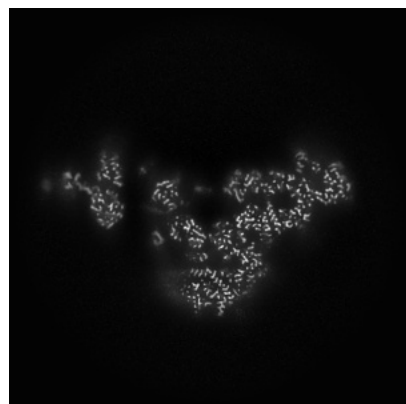


Z Index: 256

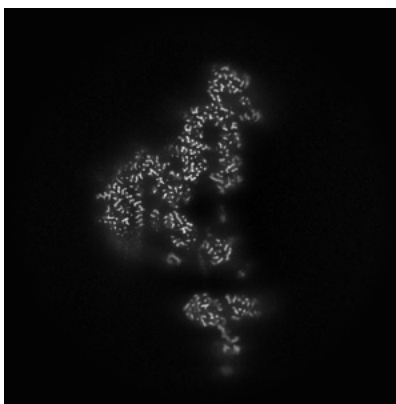
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

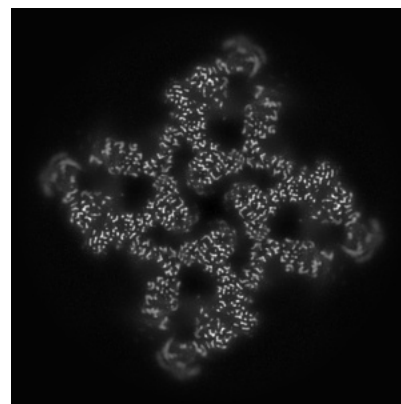
6.3.1 Primary map



X Index: 238



Y Index: 274

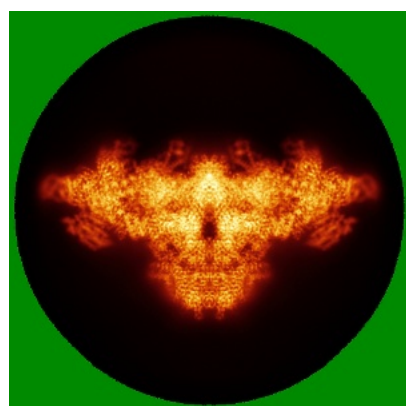


Z Index: 282

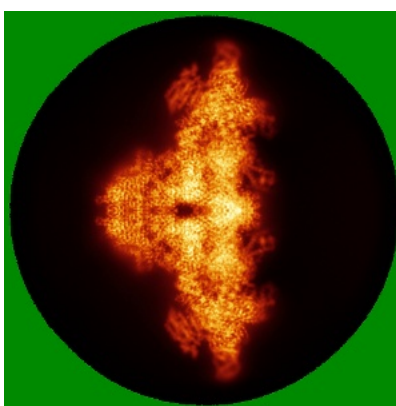
The images above show the largest variance slices of the map in three orthogonal directions.

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

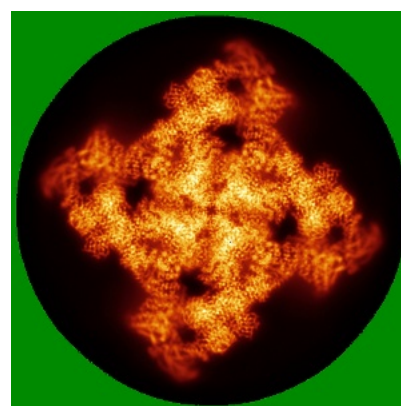
6.4.1 Primary map



X



Y

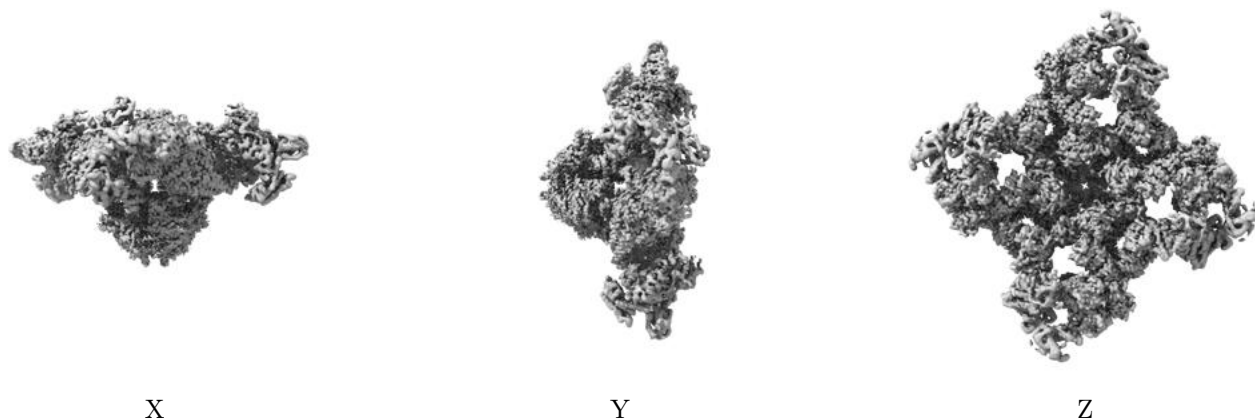


Z

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 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

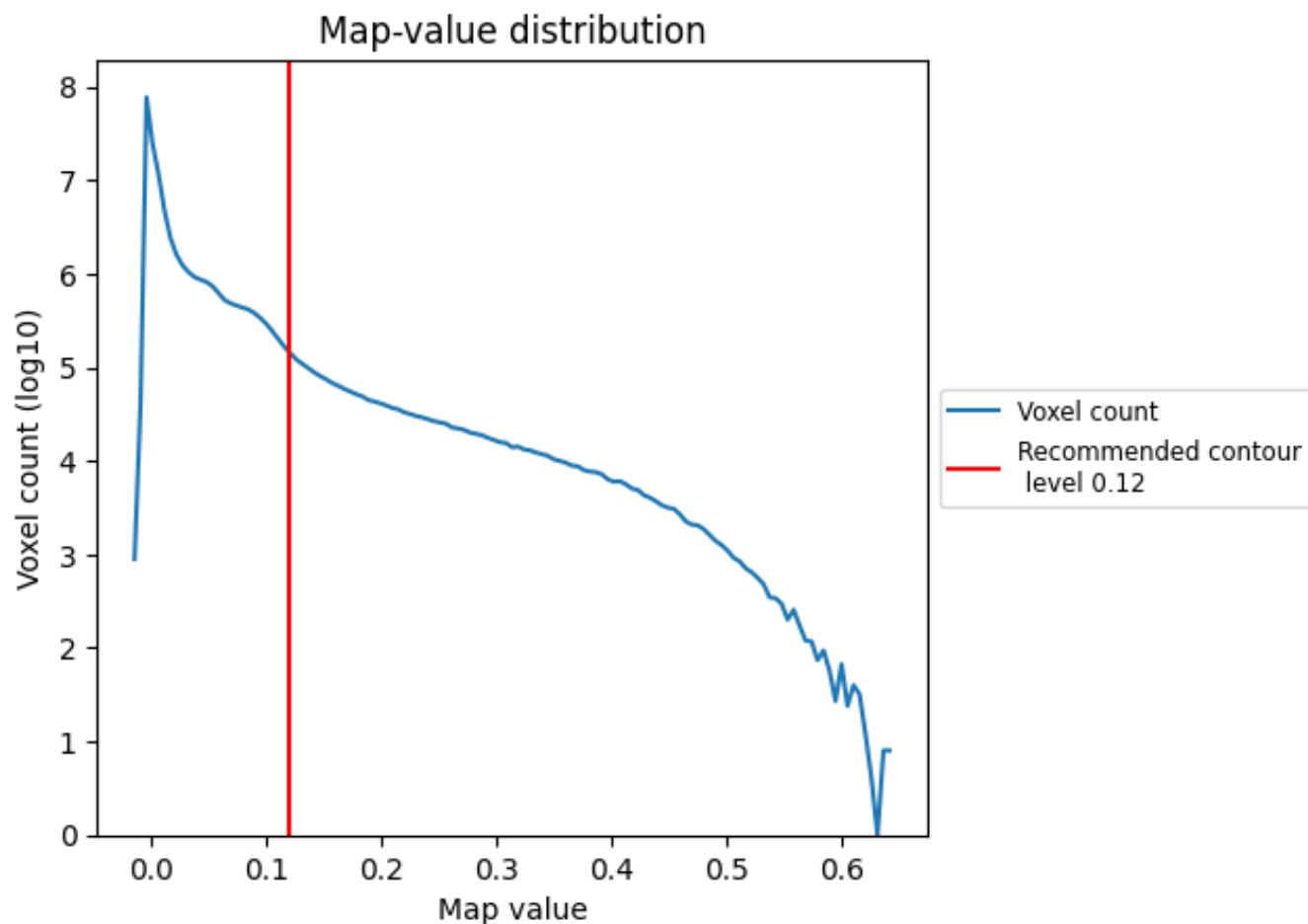
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

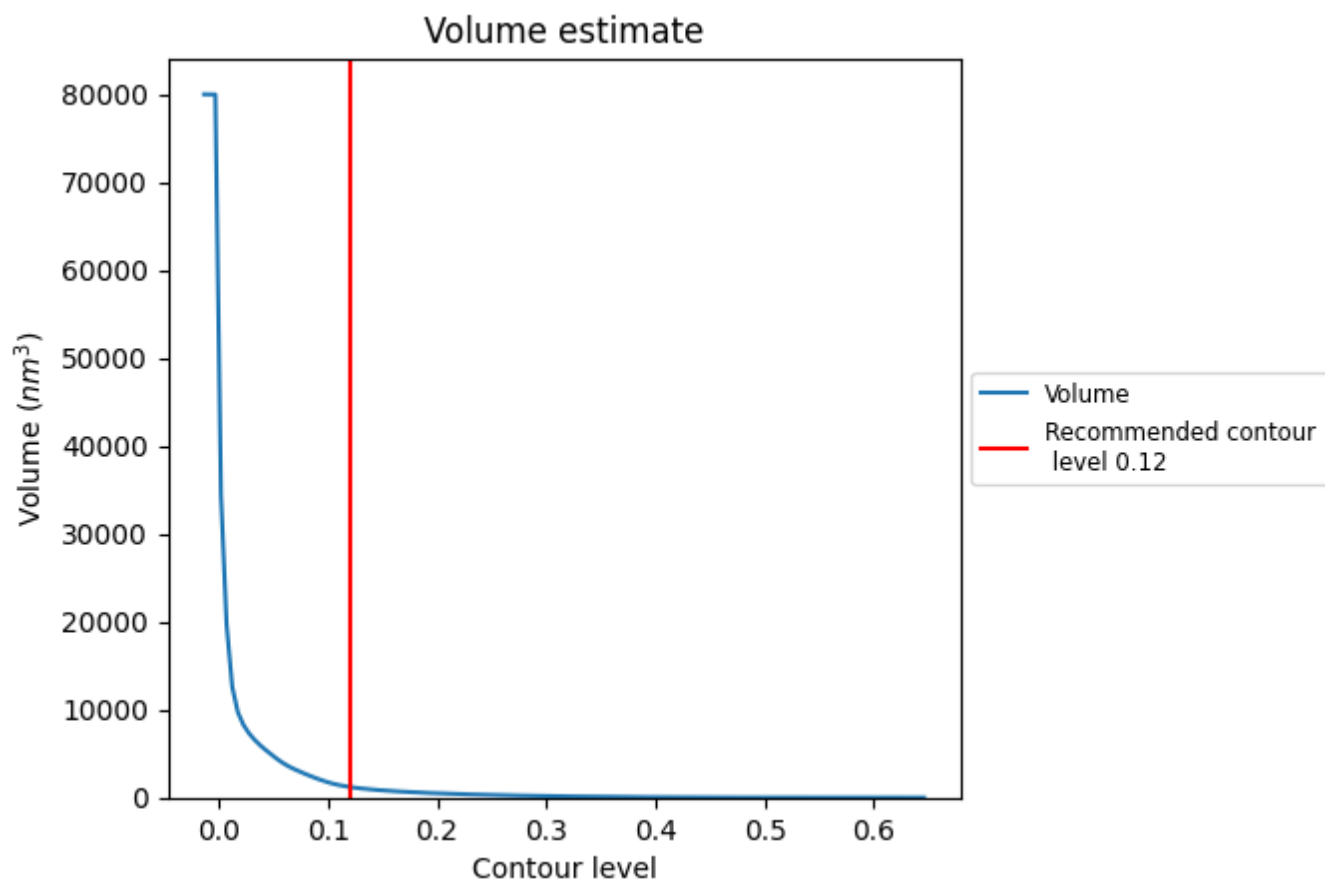
This section contains the results of statistical analysis of the map.

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.

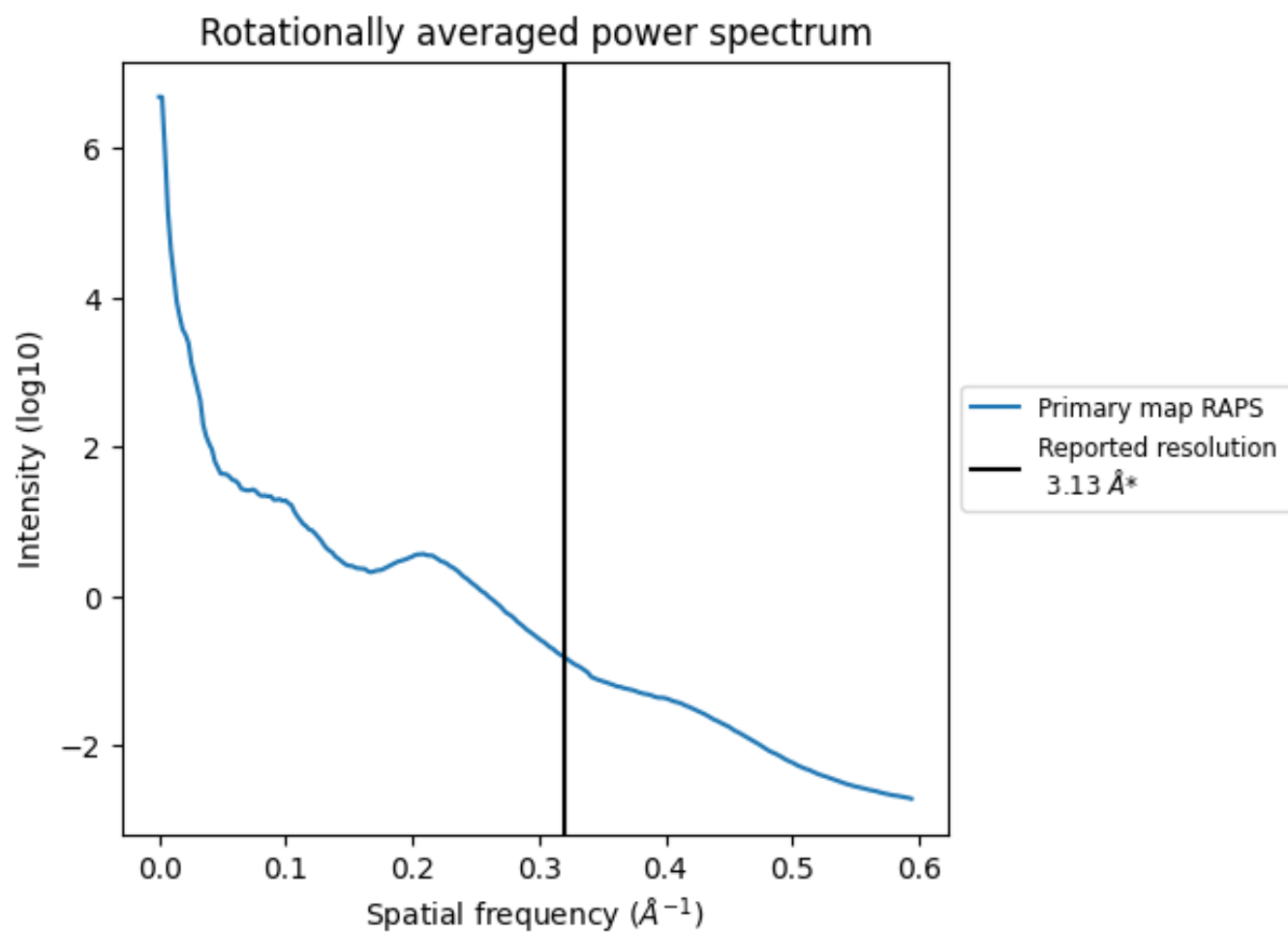
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1200 nm³; this corresponds to an approximate mass of 1084 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 0.319 Å⁻¹

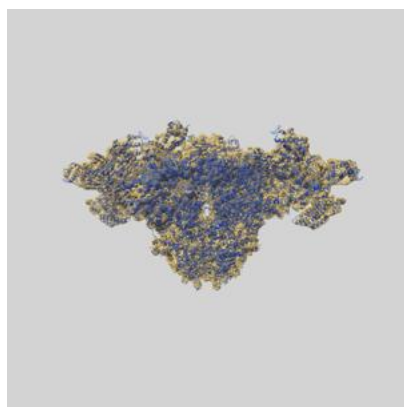
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

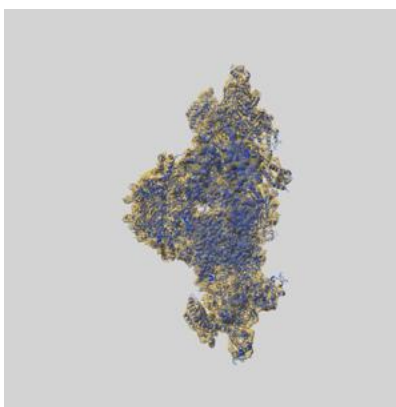
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-42762 and PDB model 8UXF. Per-residue inclusion information can be found in section [3](#) on page [6](#).

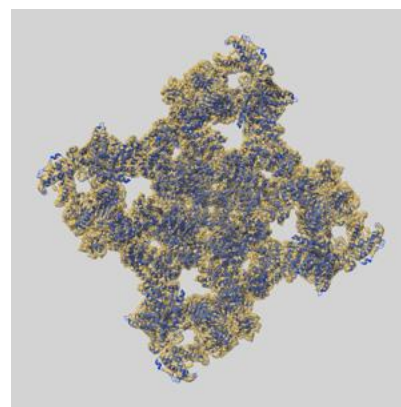
9.1 Map-model overlay [i](#)



X



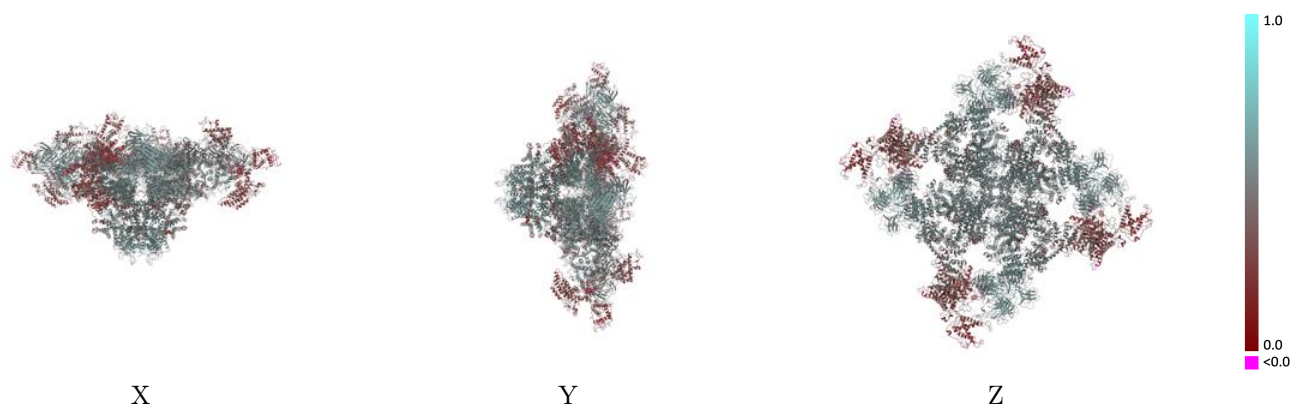
Y



Z

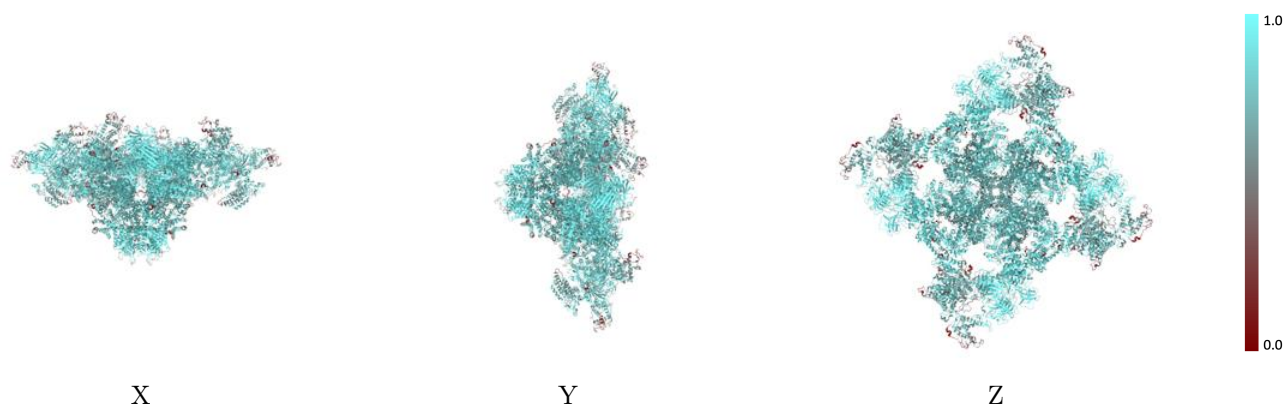
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



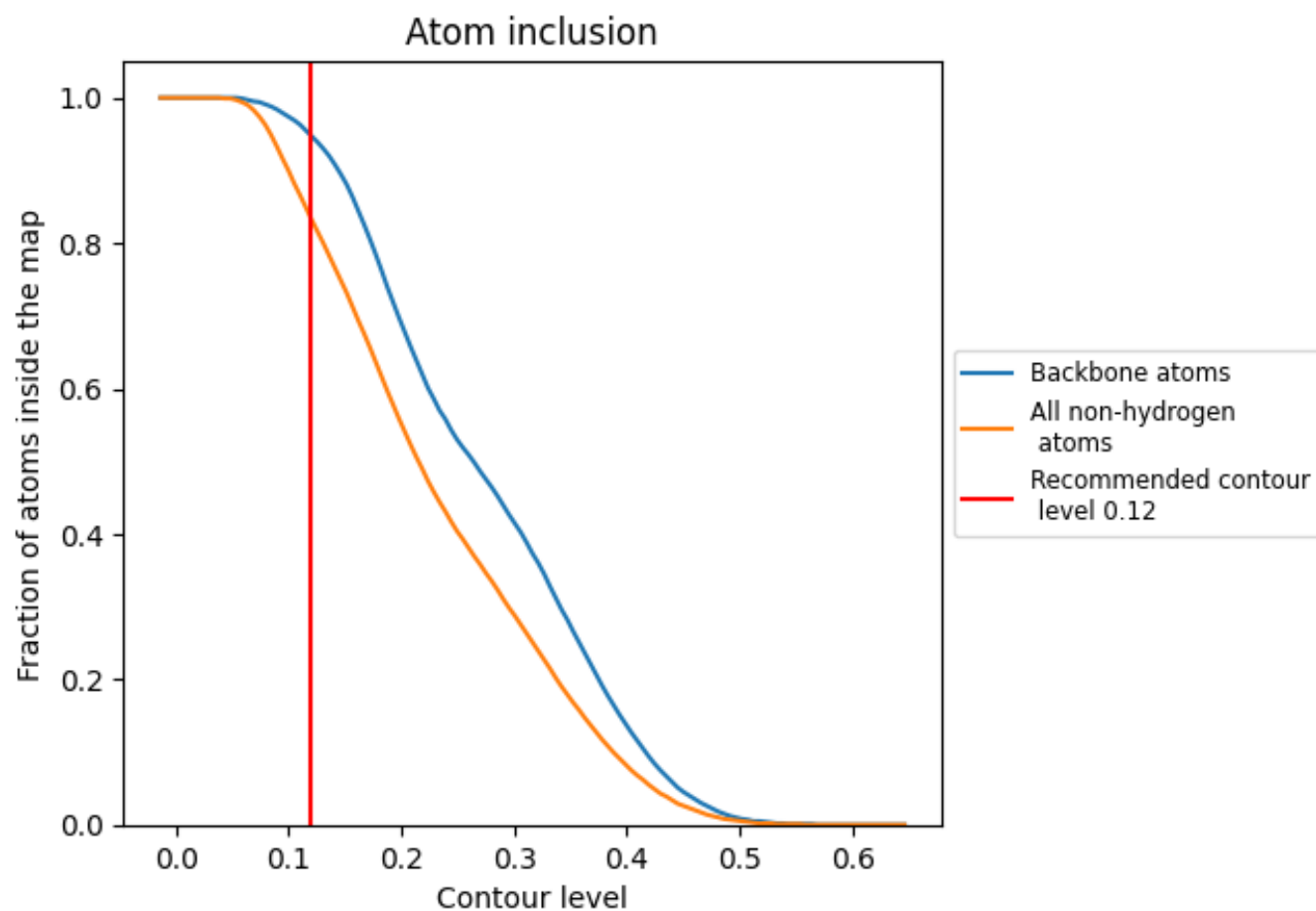
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).

9.4 Atom inclusion ⓘ



At the recommended contour level, 95% of all backbone atoms, 83% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8330	<div><div></div></div> 0.4540
A	<div><div></div></div> 0.8300	<div><div></div></div> 0.4510
B	<div><div></div></div> 0.8300	<div><div></div></div> 0.4510
C	<div><div></div></div> 0.8310	<div><div></div></div> 0.4530
D	<div><div></div></div> 0.8310	<div><div></div></div> 0.4520
E	<div><div></div></div> 0.9430	<div><div></div></div> 0.5530
F	<div><div></div></div> 0.9420	<div><div></div></div> 0.5530
G	<div><div></div></div> 0.9430	<div><div></div></div> 0.5540
H	<div><div></div></div> 0.9440	<div><div></div></div> 0.5540

1.0

0.0

<0.0