



wwPDB EM Validation Summary Report ⓘ

Oct 21, 2024 – 07:24 AM EDT

PDB ID : 8UXG
EMDB ID : EMD-42763
Title : Structure of PKA phosphorylated human RyR2-R420W in the closed state in the presence of ARM210
Authors : Miotto, M.C.; Marks, A.R.
Deposited on : 2023-11-09
Resolution : 3.08 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

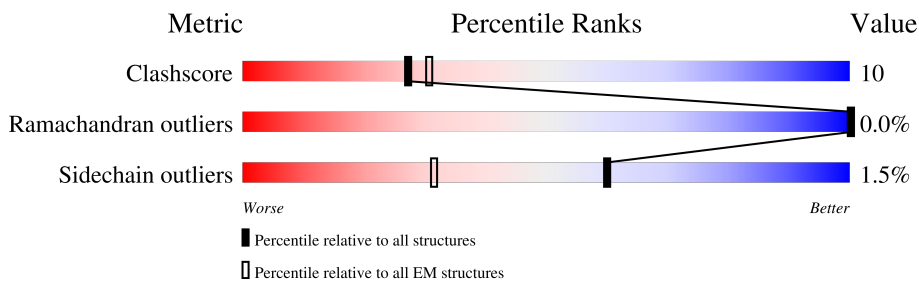
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.08 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	
1	B	4967	
1	C	4967	
1	D	4967	
2	E	108	
2	F	108	
2	G	108	
2	H	108	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 138712 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
			Total	C	N	O	S		
1	A	4224	33774	21521	5743	6280	230	2	0
1	B	4224	33774	21521	5743	6280	230	2	0
1	C	4224	33774	21521	5743	6280	230	2	0
1	D	4224	33774	21521	5743	6280	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

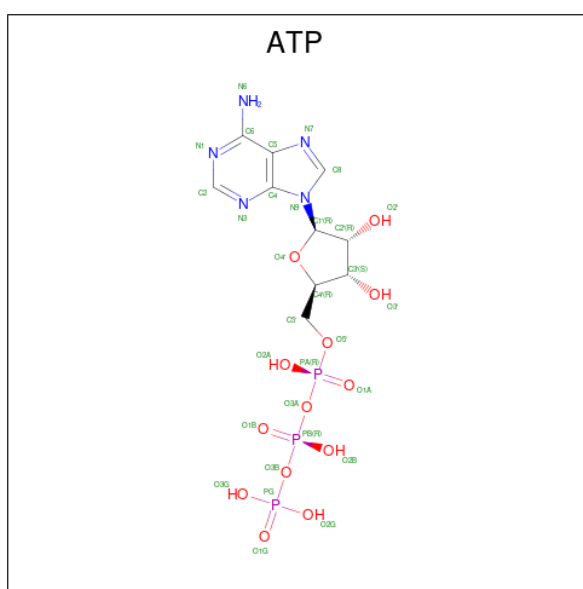
- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	E	107	818	516	144	154	4	0	0
2	F	107	818	516	144	154	4	0	0
2	G	107	818	516	144	154	4	0	0
2	H	107	818	516	144	154	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: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



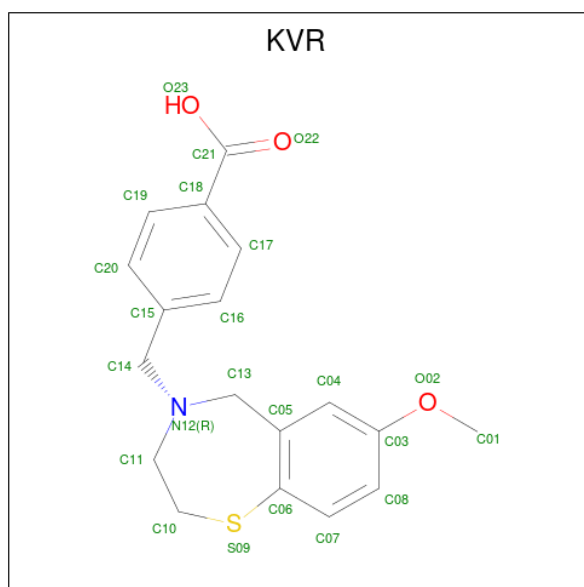
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	D	1	Total	C	N	O	P	0
			31	10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

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

- Molecule 5 is 4-[(7-methoxy-2,3-dihydro-1,4-benzothiazepin-4(5H)-yl)methyl]benzoic acid (three-letter code: KVR) (formula: C₁₈H₁₉NO₃S) (labeled as "Ligand of Interest" by depositor).

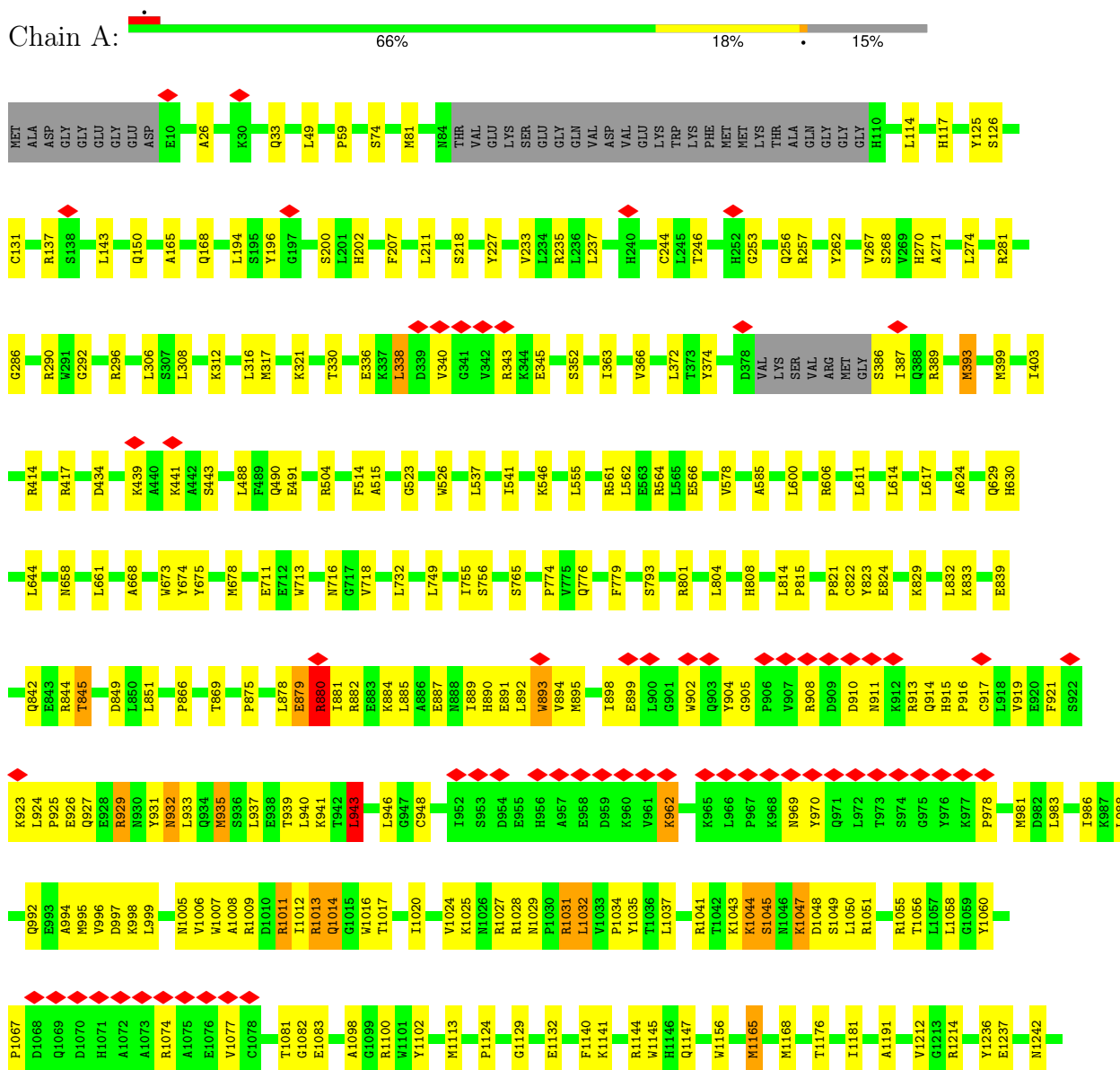


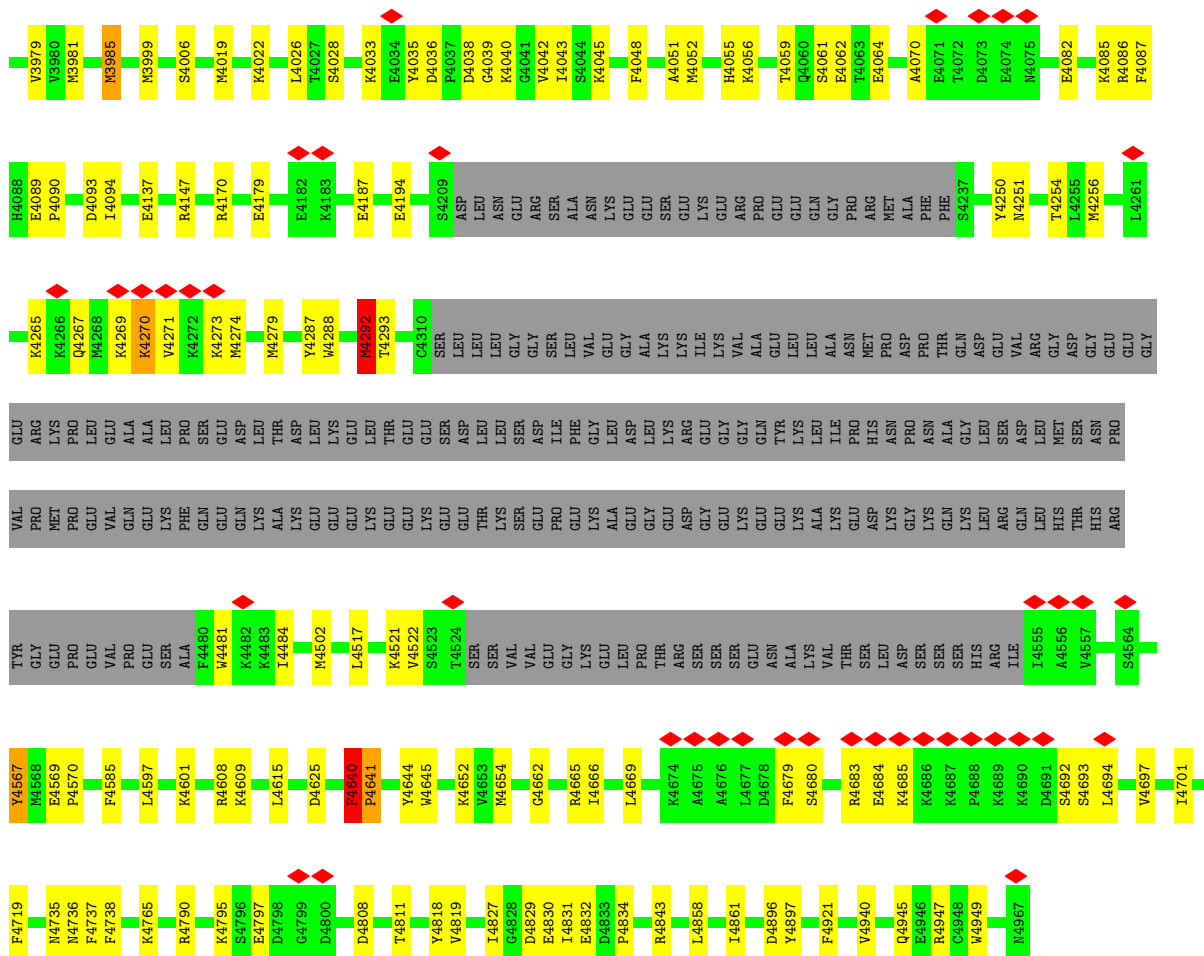
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
5	A	1	23	18	1	3	1	0
5	B	1	23	18	1	3	1	0
5	C	1	23	18	1	3	1	0
5	D	1	23	18	1	3	1	0

3 Residue-property plots

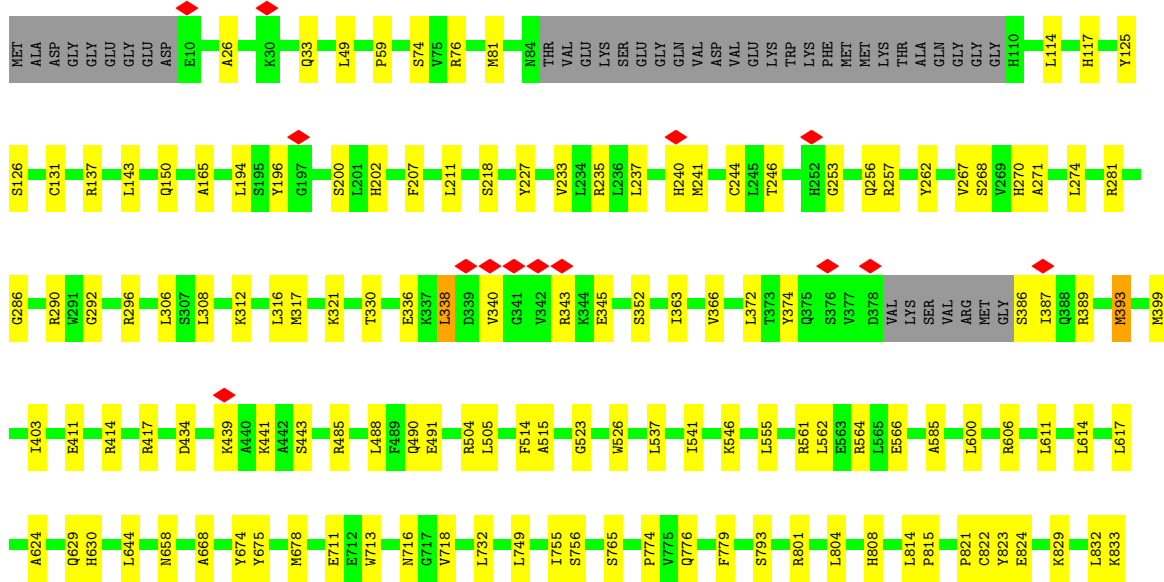
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Ryanodine receptor 2

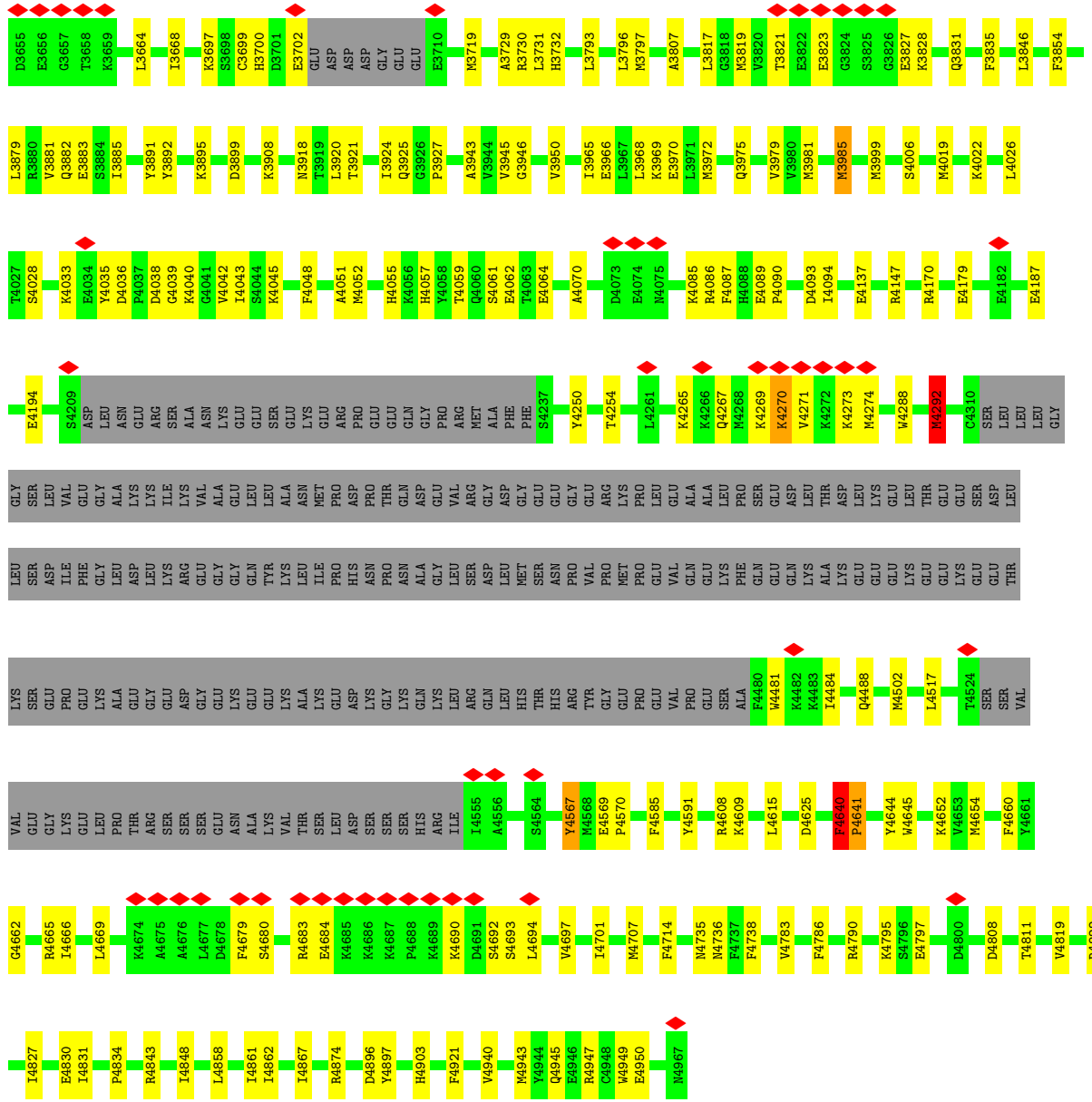




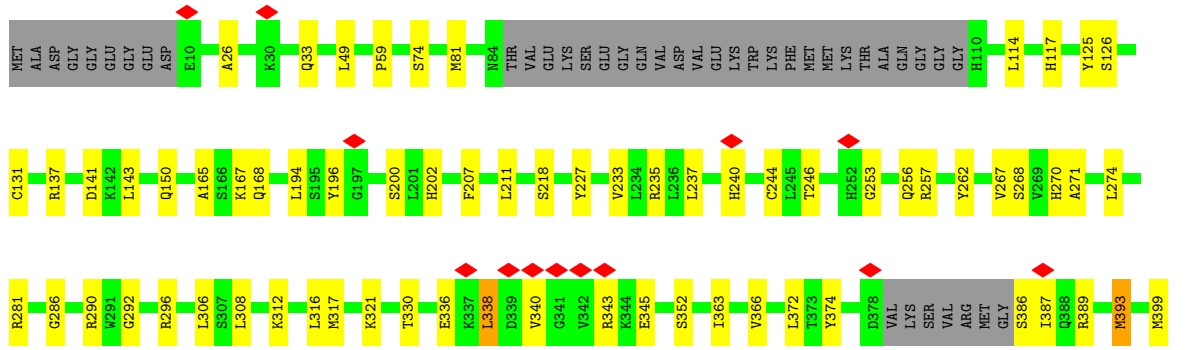
• Molecule 1: Ryanodine receptor 2

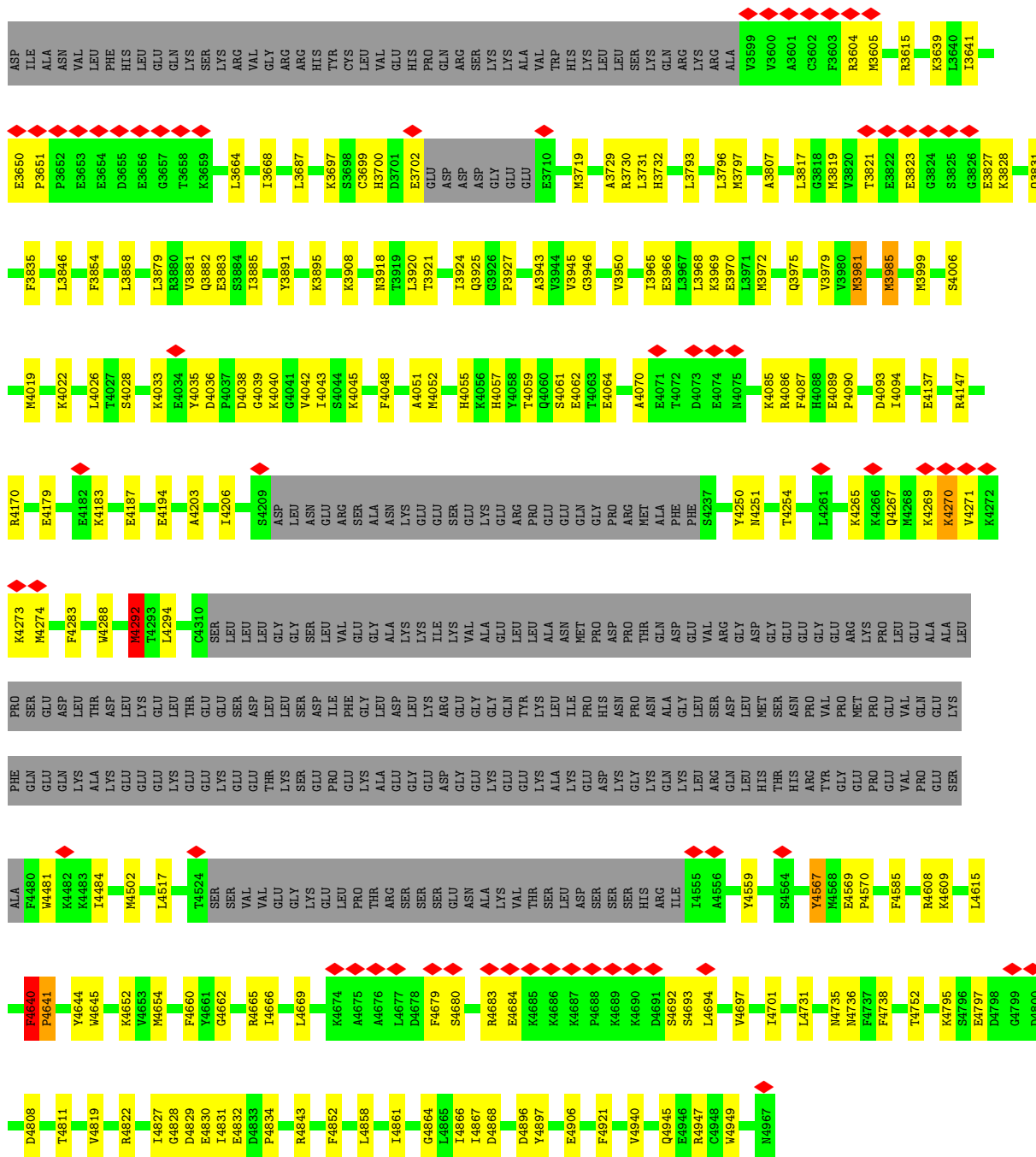


ASN	L2763	L2665	L2666	L2496	L2497	A2498	T2504	L2507	M2512	L2520	E2539	E2377	E2378	D2379	D2380	T2381	I2382	I2388	M2389	T2390	I2409	K2413	Q2414	E2415	R2420	I2427	D2431	G2434	V2435	I2436	S2437	I2438	I2439	F2440	Q2441	M2442	P2443	F2460	K2465	F2471	V2475	H2486	L2487	L2488	E2489	V2490																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
L2496	R2497	A2498	T2504	L2507	M2512	L2520	E2539	I2545	L2548	H2550	R2566	E2570	L2580	R2581	M2585	L2589	L2592	V2593	K2604	M2605	P2606	L2610	K2619	L2623	W2627	G2628	N2629	F2630	E2635	L2638	R2642	K2643	L2644	E2660	L2664	L2665	L2666	L2669	D2679	E2682	S2683	M2684	V2685	M2689	R2691	Q2692	S2693	S2694	M2695	G2696	S2697	E2698	N2702	F2703	Q2704	F2705	V2706	K2723	E2726	K2731	M2734	A2738	M2739	G2740	W2741	Y2743	G2744	E2745	I2746	Y2747	M2748	D2749	S2750	S2751	K2752	L2753	Q2754	M2757	K2758	P2759	L2762																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
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F2921	Q2927	R2931	D2934	Q2938	E2942	F2943	D2944	G2945	G2946	S2947	R2948	G2949	K2950	G2951	E2952	H2953	F2954	F2955	Y2956	E2957	Q2958	E2959	I2960	V2966	P2969	L2970	R2979	F2982	L2983	S2984	R2988	F2989	S2997	E3000	K3001	E3002	T3005	S3006	D3007	L3011	L3014	R3018	L3019	S3020	L3022	D3025	I3029	L3033	H3034	I3035	Q3038	L3039	L3040	D3041	A3042	V3045	M3046	L3050	E3051	S3052	V3053	K3054	A3059	N3063	K3070	L3071	M3072	E3073	L3075	K3076	F3080	T3081	HIS	THR	ARG	ASN	GLN	PRO	K3088	Y3096	L3102	L3108	F3109	I3112	M3115	E3216	F3117	G3118	E3119	L3122	L3123	E3124	D3125	Q3127	S3128	S3129	L3133	L3134	L3137	K3144	V3148	E3149	R3150	Q3151	R3152	L3155	L3159	F3162	L3166	F3167	V3168	L3171	H3174	L3175	I3183	Y3184	K3187	S3188	S3189	R3190	E3191	R3192	P3198	Y3204	L3211	E3212	K3213	L3214	M3215	E3216	F3117	G3118	E3119	L3218																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
L3021	F3022	D3025	I3029	L3033	H3034	I3035	Q3038	L3039	L3040	D3041	A3042	V3045	M3046	L3050	E3051	S3052	V3053	K3054	A3059	N3063	K3070	L3071	M3072	E3073	L3075	K3076	F3080	T3081	HIS	THR	ARG	ASN	GLN	PRO	K3088	Y3096	L3102	L3108	F3109	I3112	M3115	E3216	F3117	G3118	E3119	L3218																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
V3219	E3223	R3227	T3229	Q3230	H3233	V3234	M3235	I3238	L3239	Y3245	R3248	W3249	E3251	N3256	R3260	T3266	A3267	L3268	N3269	S3270	E3271	L3277	I3280	L3281	I3284	Y3285	L3288	G3289	I3290	D3291	E3292	G3293	M3296	L3299	Q3304	I3307	L3314	L3318	L3319	L3320	L3322	R3323	E3324	L3326	K3327	K3328	T3332	V3334	E3337	ASP	HIS	LEU	LEU	LYS	ALA	ALA	GLU	ALA	ALA	TRP	ARG	GLY	ASP	ARG	MET	TYR	VAL	ASP	ALA	GLU	ASP	MET	GLN	VAL	PHE	ALA	THR	SER	ILE	ALA	VAL	TRP	ILE	TRP	GLN	VAL	VAL	MET	ALA	ALA	ALA	LEU	TYR	LYS	ASP	ALA	ALA	GLU	ASP	PRO	ALA	ALA	THR	SER	ILE	ALA	VAL	TRP	ILE	TRP	GLN	VAL	VAL	MET	ALA	ALA	LEU	TYR	LYS	ASP	ALA	ALA	GLU	ASP	PRO	ALA	ALA	THR	SER	ILE	ALA	VAL	TRP	ILE	TRP	GLN	VAL	VAL	MET	ALA	ALA	LEU	TYR	LYS	ASP	ALA	ALA	GLU	ASP	PRO	ALA	ALA	THR	SER	ILE	ALA	VAL	TRP	ILE	TRP	GLN	VAL	VAL	MET	ALA	ALA	LEU	TYR	LYS	ASP	ALA	ALA	GLU	ASP	PRO	ALA	ALA	THR	SER	ILE	ALA	VAL	TRP	ILE	TRP	GLN	VAL	VAL	MET	ALA	ALA	LEU	TYR	LYS	ASP	ALA	ALA	GLU	ASP	PRO	ALA	ALA	THR	SER	ILE	ALA	VAL	TRP	ILE	TRP	GLN	VAL	VAL	MET	ALA	ALA	LEU	TYR	LYS	ASP	ALA	ALA	GLU	ASP	PRO	ALA	ALA	THR	SER	ILE	ALA	VAL	TRP	ILE	TRP	GLN	VAL	VAL	MET	ALA	ALA	LEU	TYR	LYS	ASP	ALA	ALA	GLU	ASP	PRO	ALA	ALA	THR	SER	ILE	ALA	VAL	TRP	ILE	TRP	GLN	VAL	VAL	MET	ALA	ALA	LEU	TYR	LYS	ASP	ALA	ALA	GLU	ASP	PRO	ALA	ALA	THR	SER	ILE	ALA	VAL	TRP	ILE	TRP	GLN	VAL	VAL	MET	ALA	ALA	LEU	TYR	LYS	ASP	ALA	ALA	GLU	ASP	PRO	ALA	ALA	THR	SER	ILE	ALA	VAL	TRP	ILE	TRP	GLN	VAL	VAL	MET	ALA	ALA	LEU	TYR	LYS	ASP	ALA	ALA	GLU	ASP	PRO	ALA	ALA	THR	SER	ILE	ALA	VAL	TRP	ILE	TRP	GLN	VAL	VAL	MET	ALA	ALA	LEU	TYR	LYS	ASP	ALA	ALA	GLU	ASP	PRO	ALA	ALA	THR	SER	ILE	ALA	VAL	TRP	ILE	TRP	GLN	VAL	VAL	MET	ALA	ALA	LEU	TYR	LYS	ASP	ALA	ALA	GLU	ASP	PRO	ALA	ALA	THR	SER	ILE	ALA	VAL	TRP	ILE	TRP	GLN	VAL	VAL	MET	ALA	ALA	LEU	TYR	LYS	ASP	ALA	ALA	GLU	ASP	PRO	ALA	ALA	THR	SER	ILE	ALA	VAL	TRP	ILE	TRP	GLN	VAL	VAL	MET	ALA	ALA	LEU	TYR	LYS	ASP	ALA	ALA	GLU	ASP	PRO	ALA	ALA	THR	SER	ILE	ALA	VAL	TRP	ILE	TRP	GLN	VAL	VAL	MET	ALA	ALA	LEU	TYR	LYS	ASP	ALA	ALA	GLU	ASP	PRO	ALA	ALA	THR	SER	ILE	ALA	VAL	TRP	ILE	TRP	GLN	VAL	VAL	MET	ALA	ALA	LEU	TYR	LYS	ASP	ALA	ALA	GLU	ASP	PRO	ALA	ALA	THR	SER	ILE	ALA	VAL	TRP	ILE	TRP	GLN	VAL	VAL	MET	ALA	ALA	LEU	TYR	LYS	ASP	ALA	ALA	GLU	ASP	PRO	ALA	ALA	THR	SER	ILE	ALA	VAL	TRP	ILE	TRP	GLN	VAL	VAL	MET	ALA	ALA	LEU	TYR	LYS	ASP	ALA	ALA	GLU	ASP	PRO	ALA	ALA	THR	SER	ILE	ALA	VAL	TRP	ILE	TRP	GLN	VAL	VAL	MET	ALA	ALA	LEU	TYR	LYS	ASP	ALA	ALA	GLU	ASP	PRO	ALA	ALA	THR	SER	ILE	ALA	VAL	TRP	ILE	TRP	GLN	VAL	VAL	MET	ALA	ALA	LEU	TYR	LYS	ASP	ALA	ALA	GLU	ASP	PRO	ALA	ALA	THR	SER	ILE	ALA	VAL	TRP	ILE	TRP	GLN	VAL	VAL	MET	ALA	ALA	LEU	TYR	LYS	ASP	ALA	ALA	GLU	ASP	PRO	ALA	ALA	THR	SER	ILE	ALA	VAL	TRP	ILE	TRP	GLN	VAL	VAL	MET	ALA	ALA	LEU	TYR	LYS	ASP	ALA	ALA	GLU	ASP	PRO	ALA	ALA	THR	SER	ILE	ALA	VAL	TRP	ILE	TRP	GLN	VAL	VAL	MET	ALA	ALA	LEU	TYR	LYS	ASP	ALA	ALA	GLU	ASP	PRO	ALA	ALA	THR	SER	ILE	ALA	VAL	TRP	ILE	TRP	GLN	VAL	VAL	MET	ALA	ALA	LEU	TYR	LYS	ASP	ALA	ALA	GLU	ASP	PRO	ALA	ALA	THR	SER	ILE	ALA	VAL	TRP	ILE	TRP	GLN	VAL	VAL	MET	ALA	ALA	LEU	TYR	LYS	ASP	ALA	ALA	GLU	ASP	PRO	ALA	ALA	THR	SER	ILE	ALA	VAL	TRP	ILE	TRP	GLN	VAL	VAL	MET	ALA	ALA	LEU	TYR	LYS	ASP	ALA	ALA	GLU	ASP	PRO	ALA	ALA	THR	SER	ILE	ALA	VAL	TRP	ILE	TRP	GLN	VAL	VAL	MET	ALA	ALA	LEU	TYR	LYS	ASP	ALA	ALA	GLU	ASP	PRO	ALA	ALA	THR	SER	ILE	ALA	VAL	TRP	ILE	TRP	GLN	VAL	VAL	MET	ALA	ALA	LEU	TYR	LYS	ASP	ALA	ALA	GLU	ASP	PRO	ALA	ALA	THR	SER	ILE	ALA	VAL	TRP	ILE	TRP	GLN	VAL	VAL	MET	ALA	ALA	LEU	TYR	LYS	ASP	ALA	ALA	GLU	ASP	PRO	ALA	ALA	THR	SER	ILE	ALA	VAL	TRP	ILE	TRP	GLN	VAL	VAL	MET	ALA	ALA	LEU	TYR	LYS	ASP	ALA	ALA	GLU	ASP	PRO	ALA	ALA	THR	SER	ILE	ALA	VAL	TRP	ILE	TRP	GLN	VAL	VAL	MET	ALA	ALA	LEU	TYR	LYS	ASP	ALA	ALA	GLU	ASP	PRO	ALA	ALA	THR	SER	ILE	ALA	VAL	TRP	ILE	TRP	GLN	VAL	VAL	MET	ALA	ALA	LEU	TYR	LYS	ASP	ALA	ALA	GLU	ASP	PRO	ALA	ALA	THR	SER	ILE	ALA	VAL	TRP	ILE	TRP	GLN	VAL	VAL	MET	ALA	ALA	LEU	TYR	LYS	ASP	ALA	ALA	GLU	ASP	PRO	ALA	ALA	THR	SER	ILE	ALA	VAL	TRP	ILE	TRP	GLN	VAL	VAL	MET	ALA	ALA	LEU	TYR	LYS	ASP	ALA	ALA	GLU	ASP	PRO	ALA	ALA	THR	SER	ILE	ALA	VAL	TRP	ILE	TRP	GLN	VAL	VAL	MET	ALA	ALA	LEU	TYR	LYS	ASP	ALA	ALA	GLU	ASP	PRO	ALA	ALA	THR	SER	ILE	ALA	VAL	TRP	ILE	TRP	GLN	VAL	VAL	MET	ALA	ALA	LEU	TYR	LYS	ASP	ALA	ALA	GLU	ASP	PRO	ALA	ALA	THR	SER	ILE	ALA	VAL	TRP	ILE	TRP	GLN	VAL	VAL	MET	ALA	ALA	LEU	TYR	LYS	ASP	ALA	ALA	GLU	ASP	PRO	ALA	ALA	THR	SER	ILE	ALA	VAL	TRP	ILE	TRP	GLN	VAL	VAL	MET	ALA	ALA	LEU	TYR	LYS	ASP	ALA	ALA	GLU	ASP	PRO	ALA	ALA	THR	SER	ILE	ALA	VAL	TRP	ILE	TRP	GLN	VAL	VAL	MET	ALA	ALA	LEU	TYR	LYS	ASP	ALA	ALA	GLU	ASP	PRO	ALA	ALA	THR	SER	ILE	ALA	VAL	TRP	ILE	TRP	GLN	VAL	VAL	MET	ALA	ALA	LEU	TYR	LYS	ASP	ALA	ALA	GLU	ASP	PRO	ALA	ALA	THR	SER	ILE	ALA	VAL	TRP	ILE	TRP	GLN	VAL	VAL	MET	ALA	ALA	LEU	TYR	LYS	ASP	ALA	ALA	GLU	ASP	PRO	ALA	ALA	THR	SER	ILE	ALA	VAL	TRP	ILE	TRP	GLN	VAL	VAL	MET	ALA	ALA	LEU	TYR	LYS	ASP	ALA	ALA	GLU	ASP	PRO	ALA	ALA	THR	SER	ILE	ALA	VAL	TRP	ILE	TRP	GLN	VAL	VAL	MET	ALA	ALA	LEU	TYR	LYS	ASP	ALA	ALA	GLU	ASP	PRO	ALA	ALA	THR	SER	ILE	ALA	VAL	TRP	ILE	TRP	GLN	VAL	VAL	MET	ALA	ALA	LEU	TYR	LYS	ASP	ALA	ALA	GLU	ASP	PRO	ALA	ALA	THR	SER	ILE	ALA	VAL	TRP	ILE	TRP	GLN	VAL	VAL	MET	ALA	ALA	LEU	TYR	LYS	ASP	ALA	ALA	GLU	ASP	PRO	ALA	ALA	THR	SER	ILE	ALA	VAL	TRP	ILE	TRP	GLN	VAL	VAL	MET	ALA	ALA	LEU	TYR	LYS	ASP	ALA	ALA	GLU	ASP	PRO	ALA	ALA	THR	SER	ILE	ALA	VAL	TRP	ILE	TRP	GLN	VAL	VAL	MET	ALA	ALA	LEU	TYR	LYS	ASP	ALA	ALA	GLU	ASP	PRO	ALA	ALA	THR	SER	ILE	ALA	VAL	TRP	ILE	TRP	GLN	VAL	VAL	MET	ALA	ALA	LEU	TYR	LYS	ASP	ALA	ALA	GLU	ASP	PRO	ALA	ALA	THR	SER	ILE	ALA	VAL	TRP	ILE	TRP	GLN	VAL	VAL	MET	ALA	ALA	LEU	TYR	LYS	ASP	ALA	ALA	GLU	ASP	PRO	ALA	ALA	THR	SER	ILE	ALA	VAL	TRP	ILE	TRP	GLN	VAL	VAL	MET	ALA	ALA	LEU	TYR	LYS	ASP	ALA	ALA	GLU	ASP	PRO	ALA	ALA	THR	SER	ILE	ALA	VAL



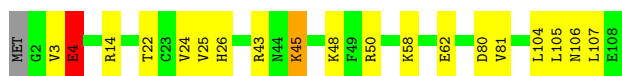
• Molecule 1: Ryanodine receptor 2





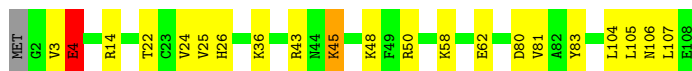
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E: 81% 16%

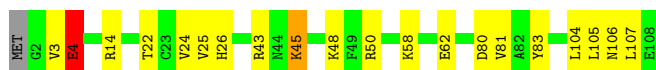
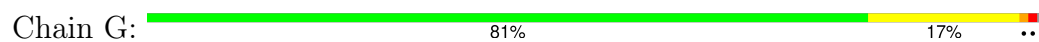


• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

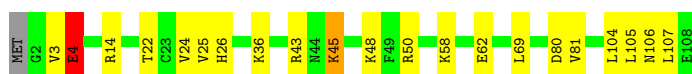
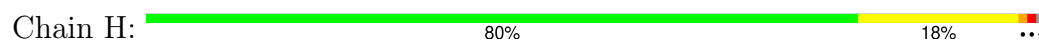
Chain F: 80% 18%



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	181724	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	0.623	Depositor
Minimum map value	-0.012	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	430.592, 430.592, 430.592	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.841, 0.841, 0.841	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: KVR, ATP, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.26	0/34516	0.50	9/46623 (0.0%)
1	B	0.26	0/34516	0.50	9/46623 (0.0%)
1	C	0.26	0/34516	0.50	9/46623 (0.0%)
1	D	0.26	0/34516	0.50	9/46623 (0.0%)
2	E	0.29	0/834	0.56	1/1123 (0.1%)
2	F	0.29	0/834	0.56	1/1123 (0.1%)
2	G	0.29	0/834	0.56	1/1123 (0.1%)
2	H	0.29	0/834	0.56	1/1123 (0.1%)
All	All	0.26	0/141400	0.51	40/190984 (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	5
1	B	0	5
1	C	0	5
1	D	0	5
All	All	0	20

There are no bond length outliers.

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	943	LEU	CA-CB-CG	12.40	143.83	115.30
1	C	943	LEU	CA-CB-CG	12.39	143.81	115.30
1	D	943	LEU	CA-CB-CG	12.39	143.81	115.30
1	B	943	LEU	CA-CB-CG	12.38	143.78	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2734	MET	CA-CB-CG	9.25	129.03	113.30

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2766	LYS	Peptide
1	A	439	LYS	Peptide
1	A	4640	PHE	Peptide
1	A	879	GLU	Peptide
1	A	880	ARG	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	33774	0	33452	652	0
1	B	33774	0	33452	665	0
1	C	33774	0	33452	664	0
1	D	33774	0	33452	671	0
2	E	818	0	821	12	0
2	F	818	0	821	14	0
2	G	818	0	821	13	0
2	H	818	0	821	14	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	2	0
4	B	62	0	24	2	0
4	C	62	0	24	2	0
4	D	62	0	24	2	0
5	A	23	0	0	1	0
5	B	23	0	0	1	0
5	C	23	0	0	1	0
5	D	23	0	0	1	0
All	All	138712	0	137188	2637	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 2637 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2779:LEU:HA	1:A:2782:MET:HG3	1.56	0.88
1:B:2779:LEU:HA	1:B:2782:MET:HG3	1.56	0.87
1:D:2779:LEU:HA	1:D:2782:MET:HG3	1.56	0.86
1:C:2779:LEU:HA	1:C:2782:MET:HG3	1.56	0.85
1:B:4279:MET:HE1	1:C:4488:GLN:HG2	1.57	0.85

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%)	4098 (98%)	98 (2%)	2 (0%)	100	100
1	B	4198/4967 (84%)	4099 (98%)	97 (2%)	2 (0%)	100	100
1	C	4198/4967 (84%)	4100 (98%)	96 (2%)	2 (0%)	100	100
1	D	4198/4967 (84%)	4099 (98%)	97 (2%)	2 (0%)	100	100
2	E	105/108 (97%)	105 (100%)	0	0	100	100
2	F	105/108 (97%)	105 (100%)	0	0	100	100
2	G	105/108 (97%)	105 (100%)	0	0	100	100
2	H	105/108 (97%)	105 (100%)	0	0	100	100
All	All	17212/20300 (85%)	16816 (98%)	388 (2%)	8 (0%)	100	100

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3927	PRO

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Mol	Chain	Res	Type
1	A	4641	PRO
1	B	3927	PRO
1	B	4641	PRO
1	C	3927	PRO

5.3.2 Protein sidechains [i](#)

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%)	3653 (98%)	55 (2%)	60	78
1	B	3708/4358 (85%)	3653 (98%)	55 (2%)	60	78
1	C	3708/4358 (85%)	3653 (98%)	55 (2%)	60	78
1	D	3708/4358 (85%)	3653 (98%)	55 (2%)	60	78
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%)	14956 (98%)	228 (2%)	60	78

5 of 228 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	4292	MET
1	D	3227	ARG
1	C	1045	SER
1	D	3033	LEU
1	D	1047	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	658	ASN

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Mol	Chain	Res	Type
1	D	3831	GLN
1	D	896	ASN
1	D	1014	GLN
1	B	1014	GLN

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 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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	C	5002	-	28,33,33	0.62	0	34,52,52	0.61	1 (2%)
4	ATP	D	5003	-	28,33,33	0.75	0	34,52,52	0.75	1 (2%)
5	KVR	D	5004	-	24,25,25	0.52	0	31,34,34	1.00	2 (6%)
4	ATP	D	5002	-	28,33,33	0.62	0	34,52,52	0.61	1 (2%)
5	KVR	C	5004	-	24,25,25	0.51	0	31,34,34	0.99	2 (6%)
4	ATP	A	5002	-	28,33,33	0.62	0	34,52,52	0.61	1 (2%)
4	ATP	C	5003	-	28,33,33	0.76	0	34,52,52	0.75	1 (2%)
4	ATP	B	5003	-	28,33,33	0.76	0	34,52,52	0.75	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	KVR	B	5004	-	24,25,25	0.51	0	31,34,34	0.99	2 (6%)
5	KVR	A	5004	-	24,25,25	0.51	0	31,34,34	0.99	2 (6%)
4	ATP	B	5002	-	28,33,33	0.63	0	34,52,52	0.61	1 (2%)
4	ATP	A	5003	-	28,33,33	0.75	0	34,52,52	0.75	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	C	5002	-	-	8/18/38/38	0/3/3/3
4	ATP	D	5003	-	-	5/18/38/38	0/3/3/3
5	KVR	D	5004	-	-	6/10/20/20	0/2/3/3
4	ATP	D	5002	-	-	8/18/38/38	0/3/3/3
5	KVR	C	5004	-	-	6/10/20/20	0/2/3/3
4	ATP	A	5002	-	-	8/18/38/38	0/3/3/3
4	ATP	C	5003	-	-	5/18/38/38	0/3/3/3
4	ATP	B	5003	-	-	5/18/38/38	0/3/3/3
5	KVR	B	5004	-	-	6/10/20/20	0/2/3/3
5	KVR	A	5004	-	-	6/10/20/20	0/2/3/3
4	ATP	B	5002	-	-	8/18/38/38	0/3/3/3
4	ATP	A	5003	-	-	5/18/38/38	0/3/3/3

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	5004	KVR	C10-S09-C06	3.36	107.46	102.71
5	C	5004	KVR	C10-S09-C06	3.34	107.44	102.71
5	A	5004	KVR	C10-S09-C06	3.34	107.44	102.71
5	B	5004	KVR	C10-S09-C06	3.33	107.42	102.71
5	D	5004	KVR	C14-N12-C11	2.99	115.95	111.09

There are no chirality outliers.

5 of 76 torsion outliers are listed below:

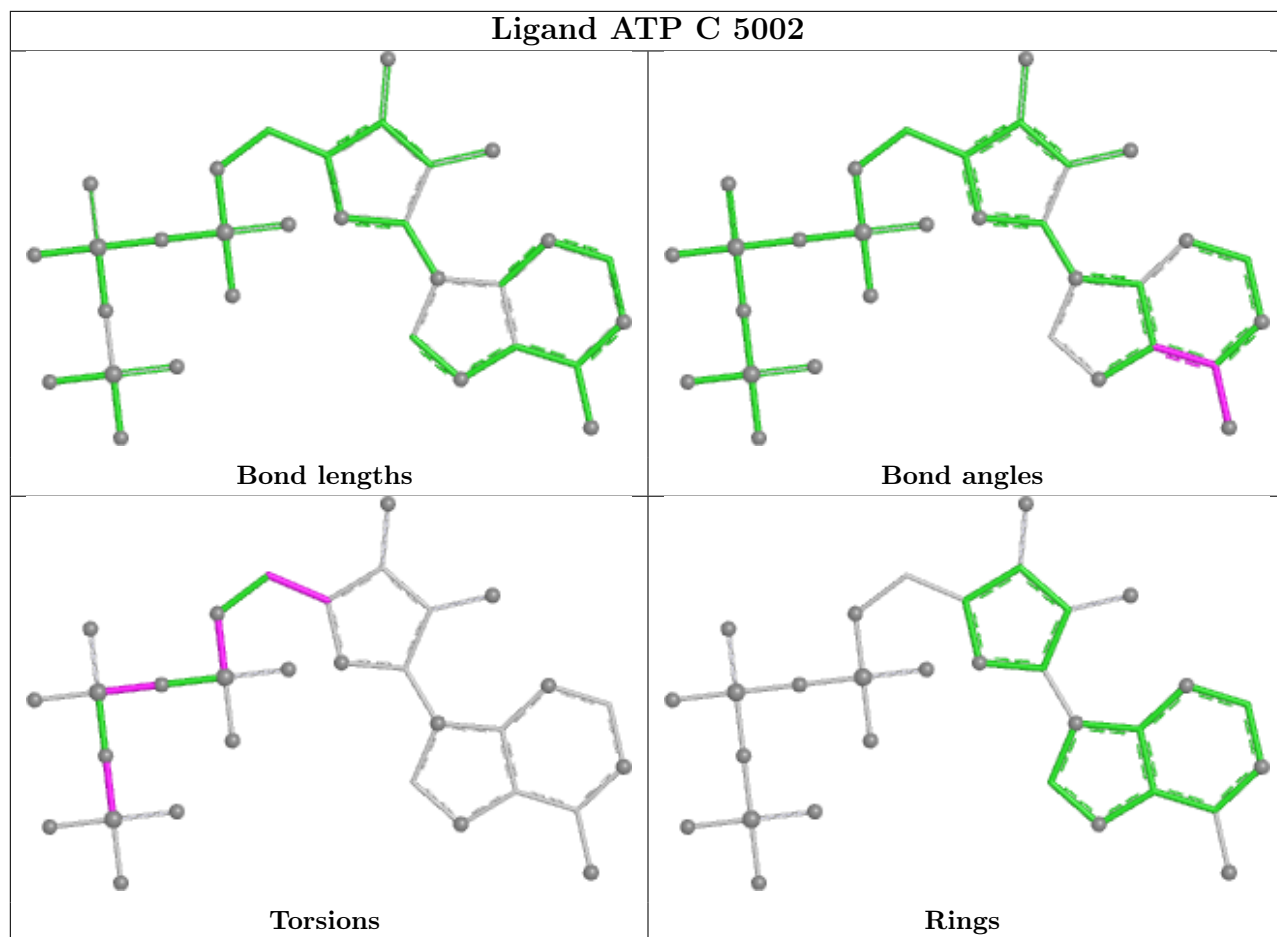
Mol	Chain	Res	Type	Atoms
4	A	5002	ATP	PB-O3B-PG-O3G
4	A	5002	ATP	C5'-O5'-PA-O1A
4	A	5002	ATP	C5'-O5'-PA-O3A
4	A	5003	ATP	C5'-O5'-PA-O3A
4	A	5003	ATP	C4'-C5'-O5'-PA

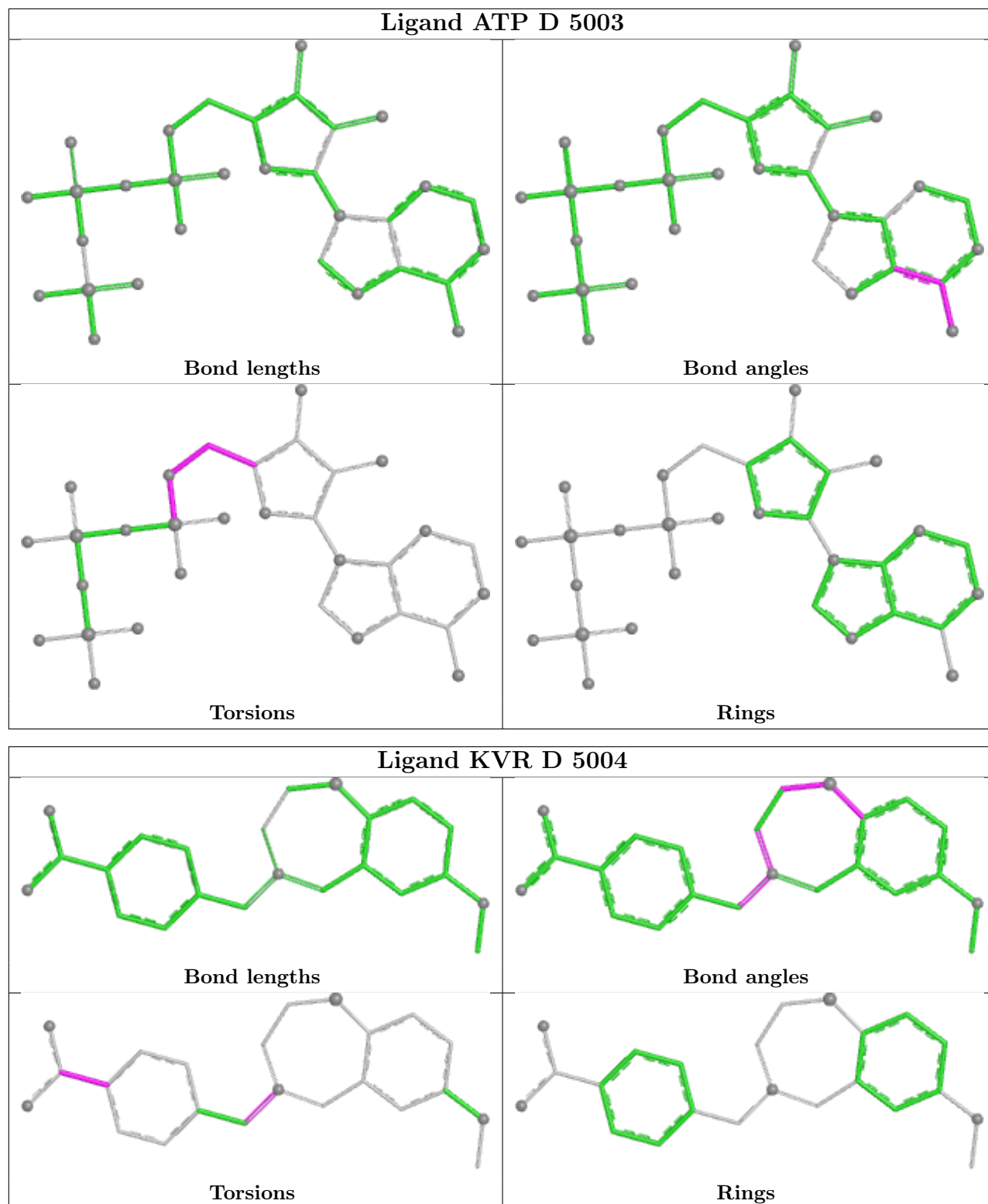
There are no ring outliers.

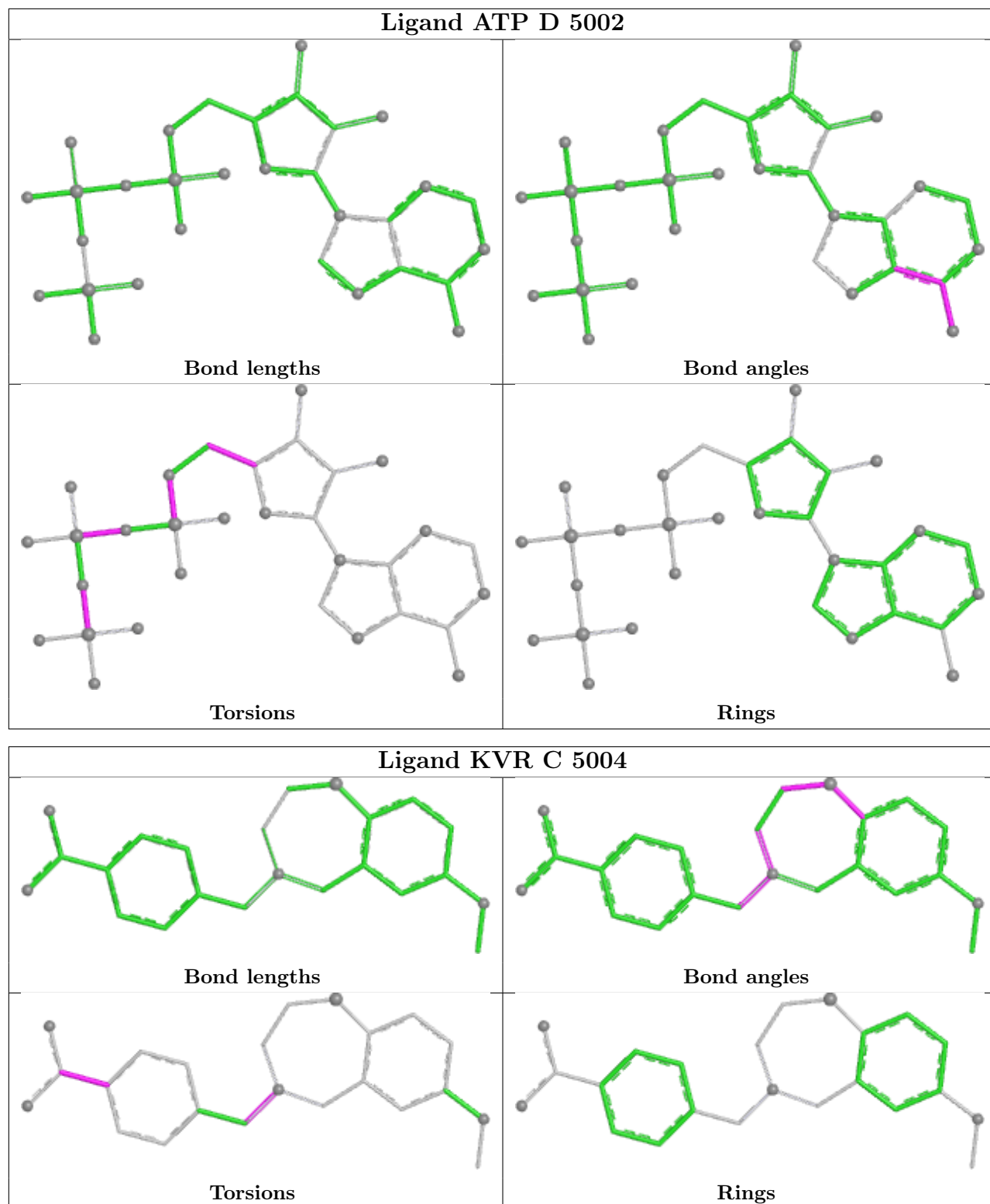
12 monomers are involved in 12 short contacts:

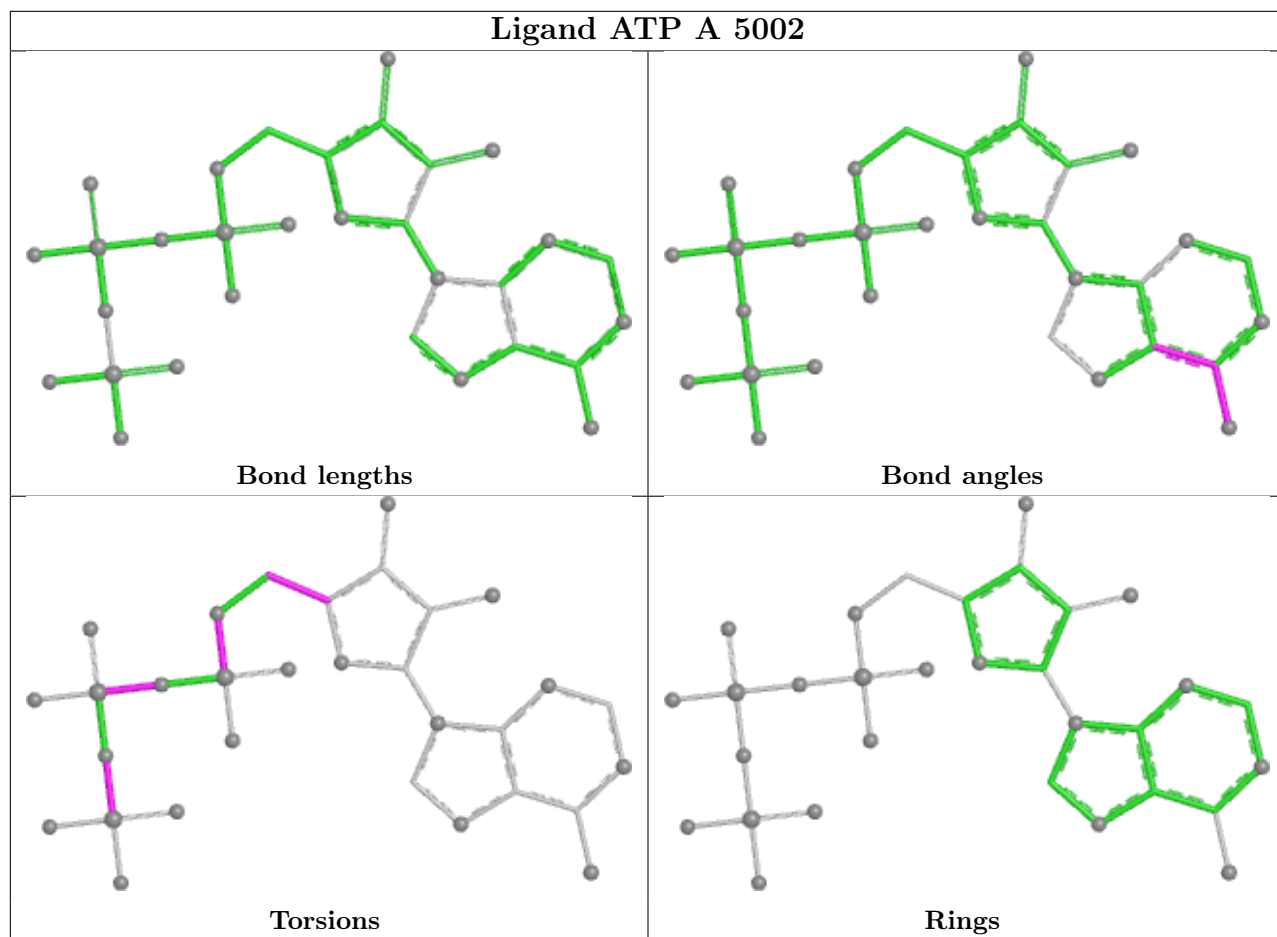
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	5002	ATP	1	0
4	D	5003	ATP	1	0
5	D	5004	KVR	1	0
4	D	5002	ATP	1	0
5	C	5004	KVR	1	0
4	A	5002	ATP	1	0
4	C	5003	ATP	1	0
4	B	5003	ATP	1	0
5	B	5004	KVR	1	0
5	A	5004	KVR	1	0
4	B	5002	ATP	1	0
4	A	5003	ATP	1	0

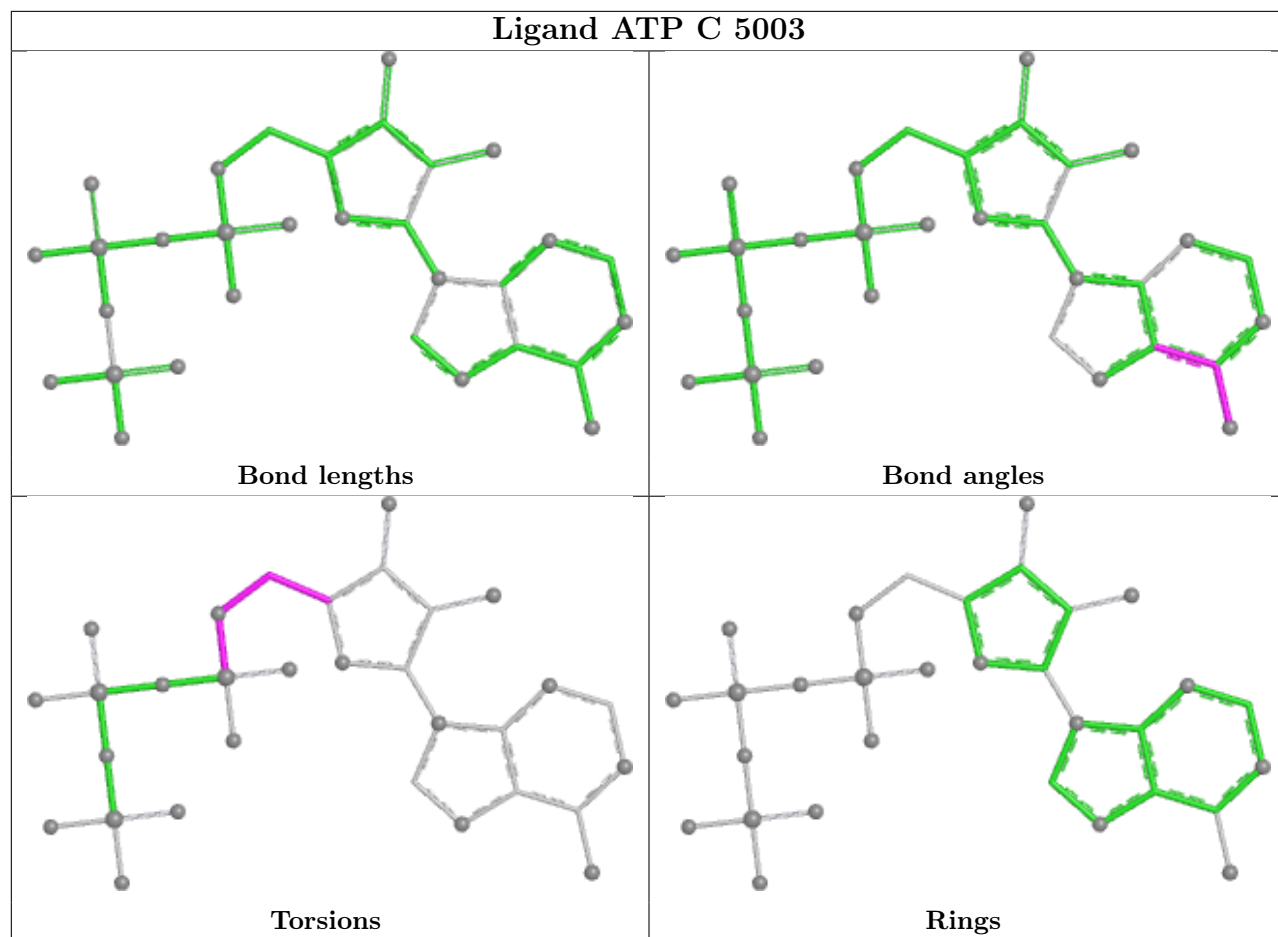
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

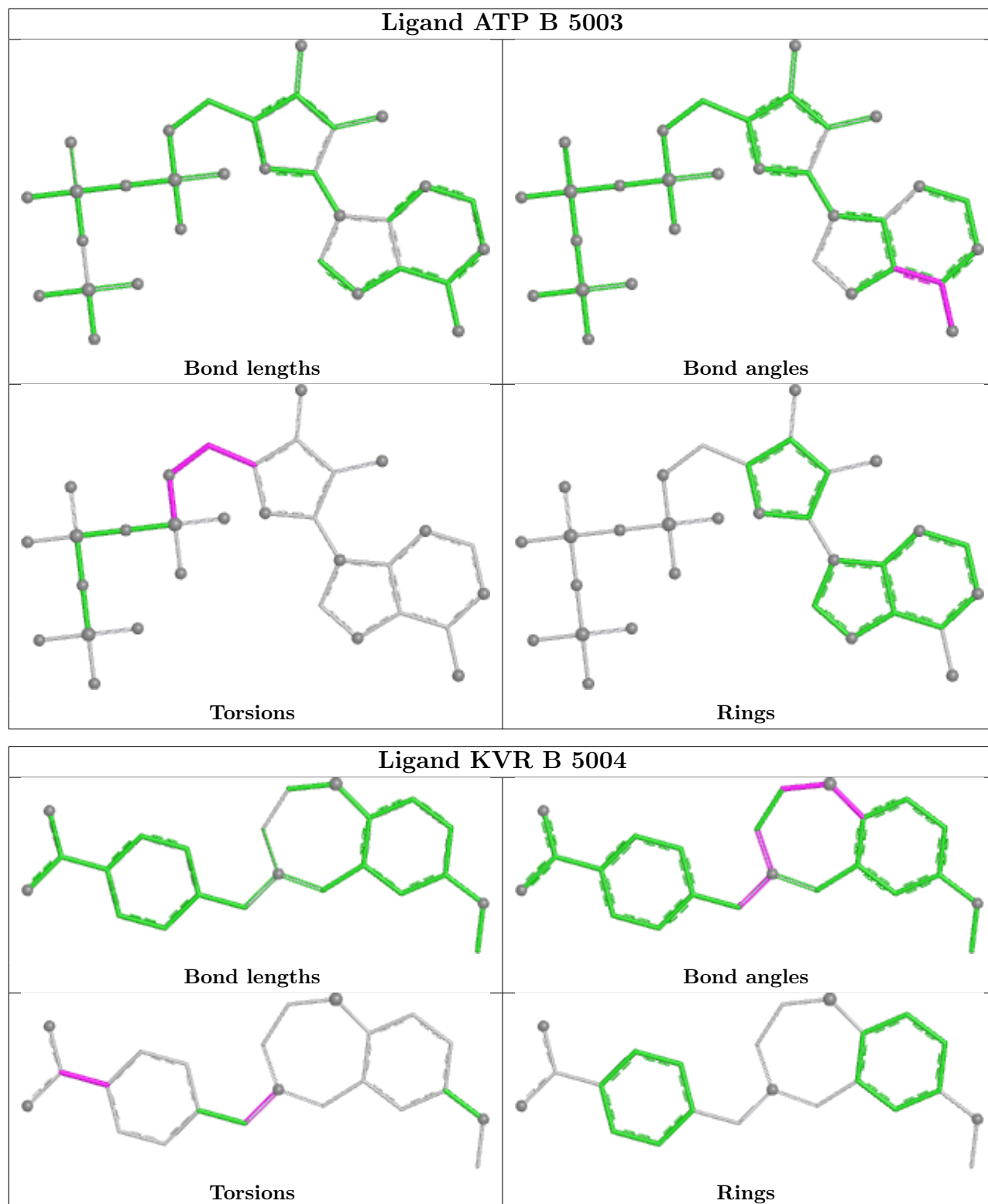


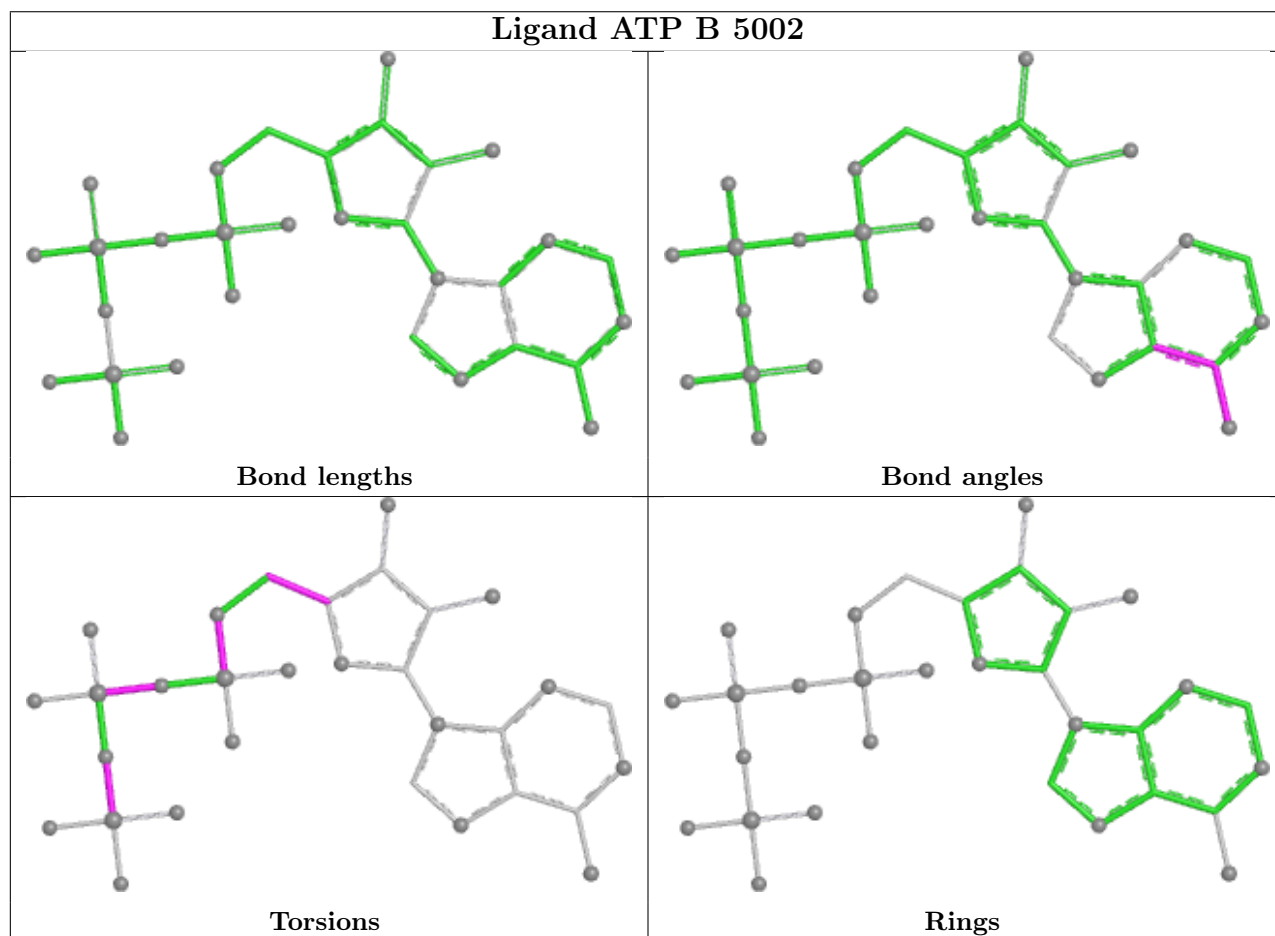
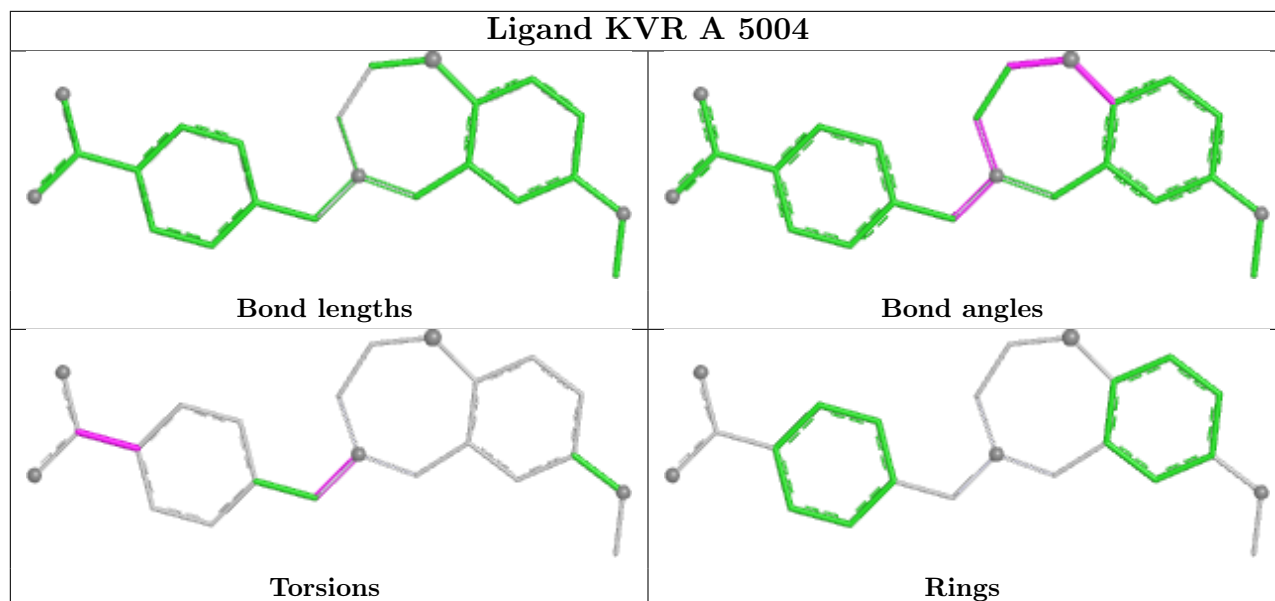


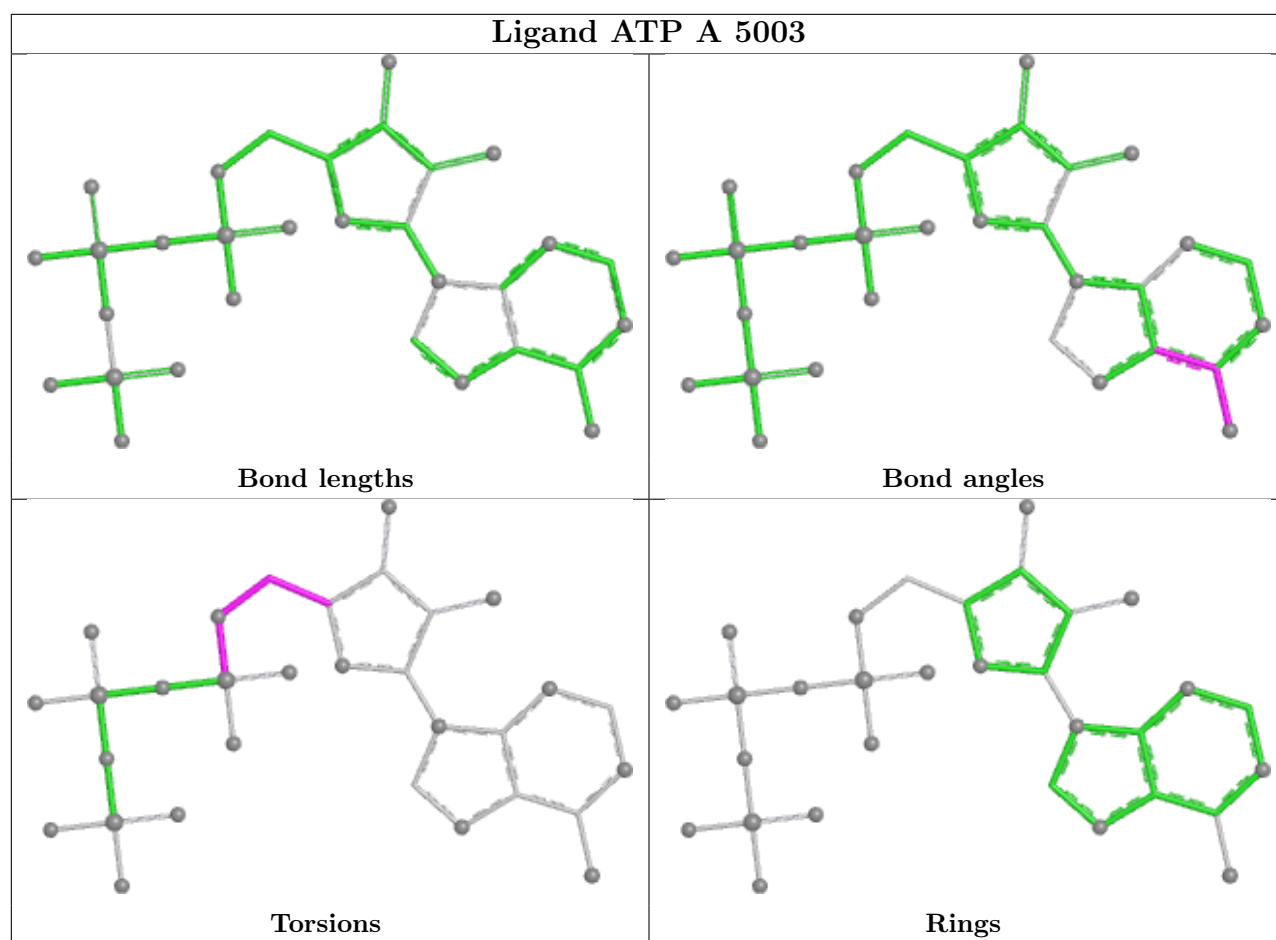












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

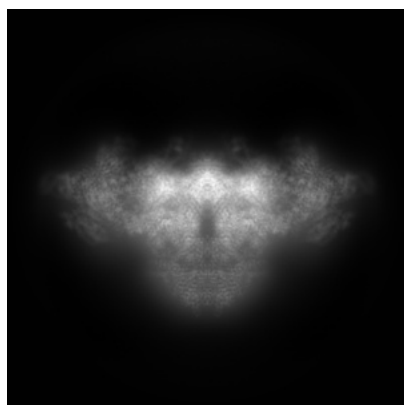
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42763. These allow visual inspection of the internal detail of the map and identification of artifacts.

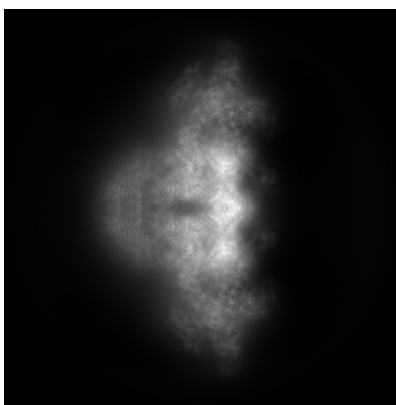
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

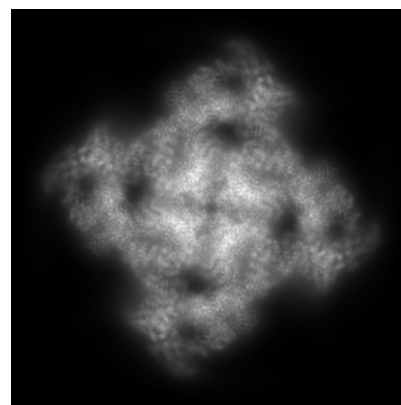
6.1.1 Primary map



X



Y



Z

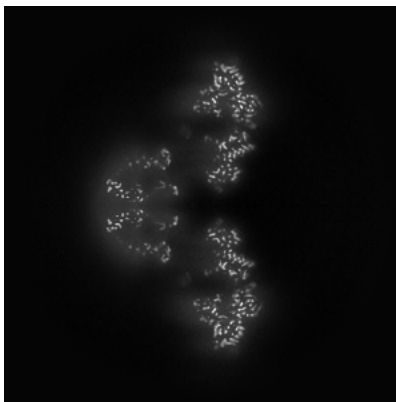
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

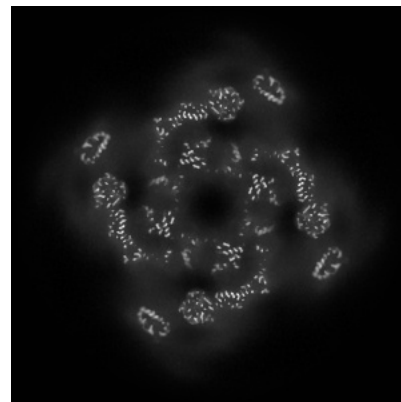
6.2.1 Primary map



X Index: 256



Y Index: 256

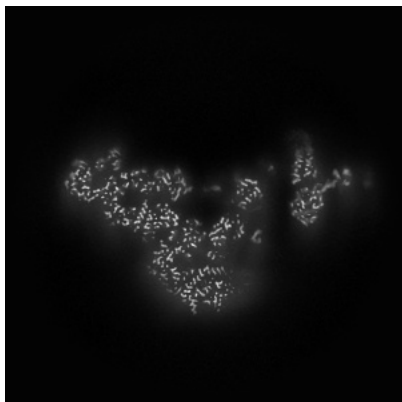


Z Index: 256

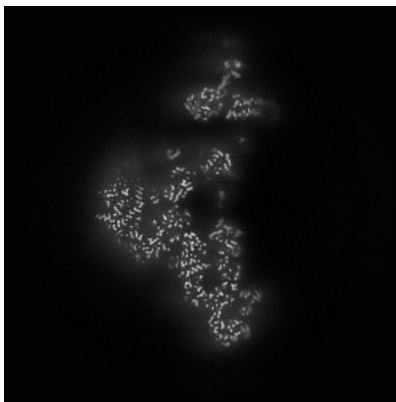
The images above show central slices of the map in three orthogonal directions.

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

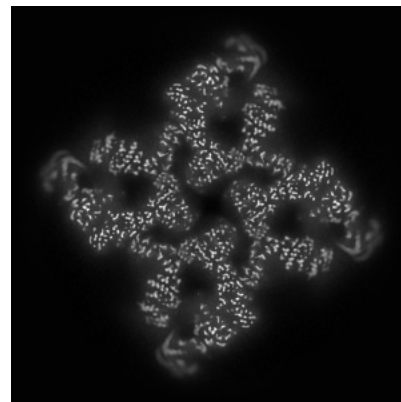
6.3.1 Primary map



X Index: 274



Y Index: 238

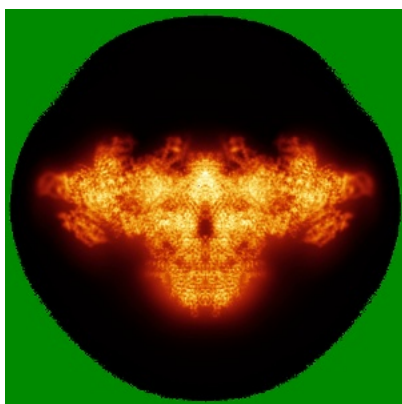


Z Index: 282

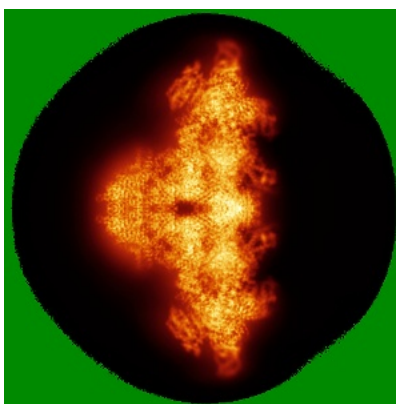
The images above show the largest variance slices of the map in three orthogonal directions.

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

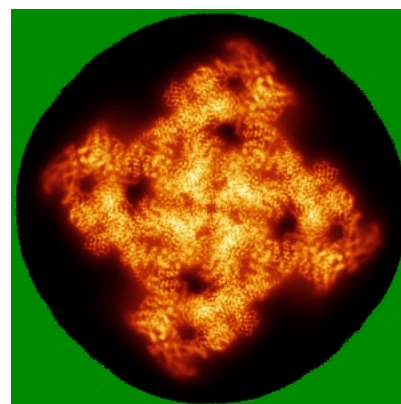
6.4.1 Primary map



X



Y

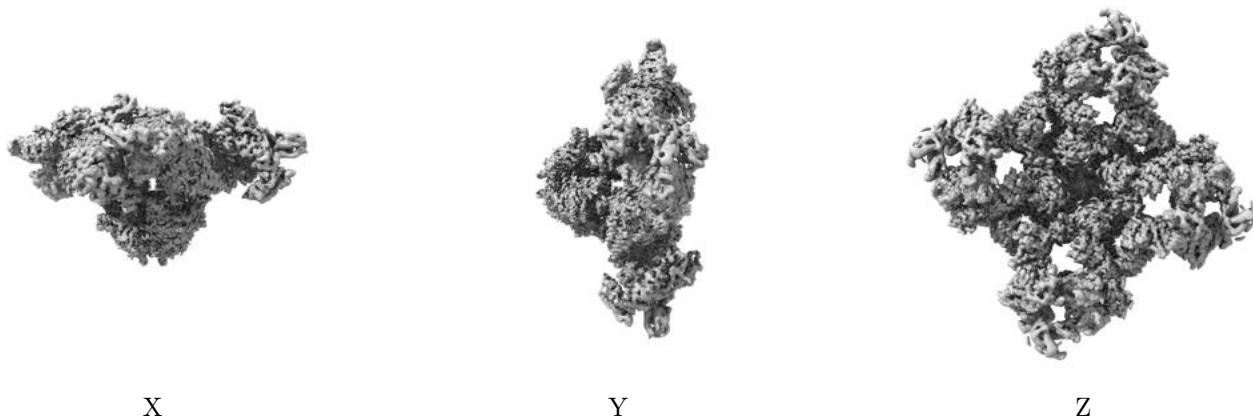


Z

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.

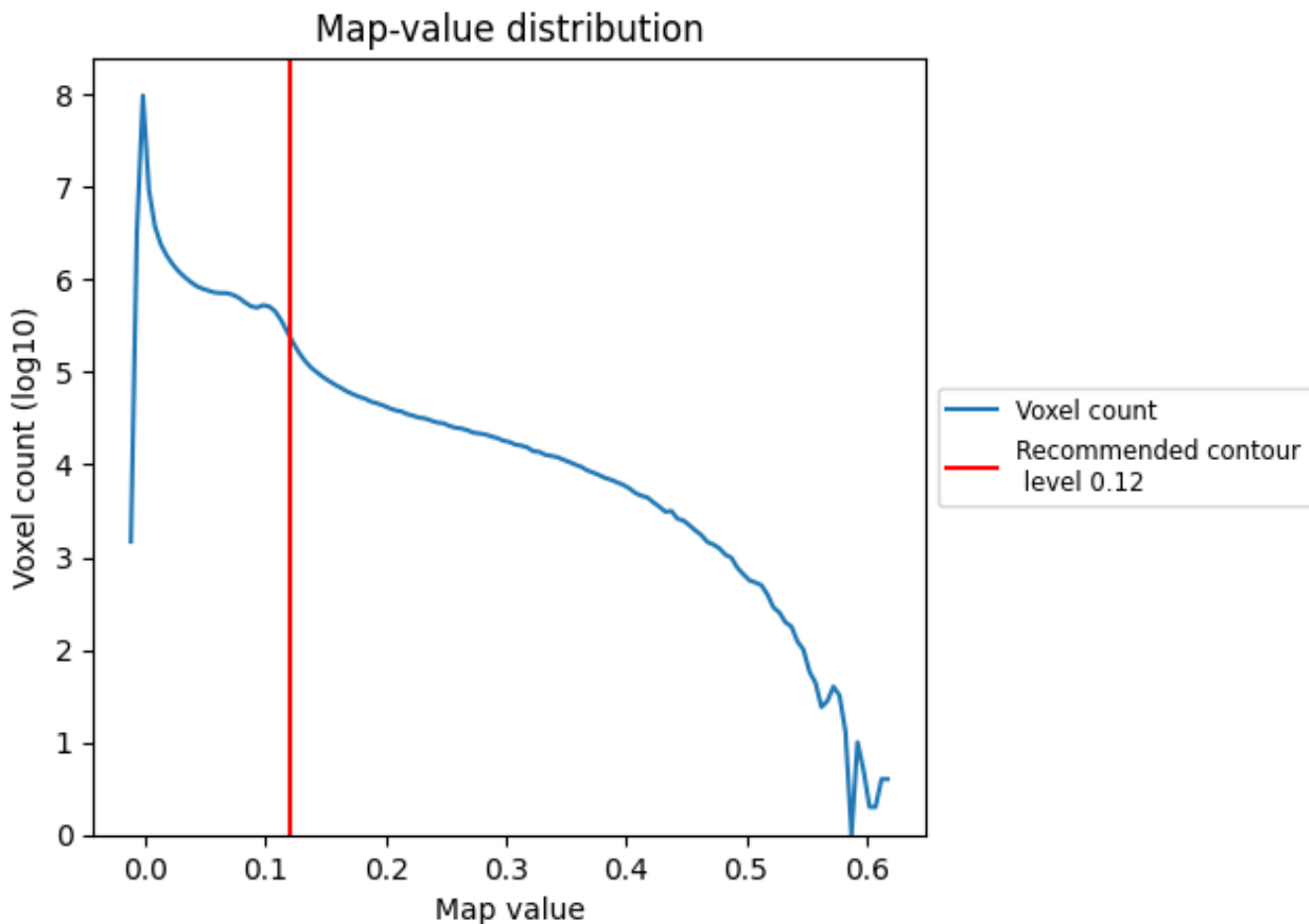
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

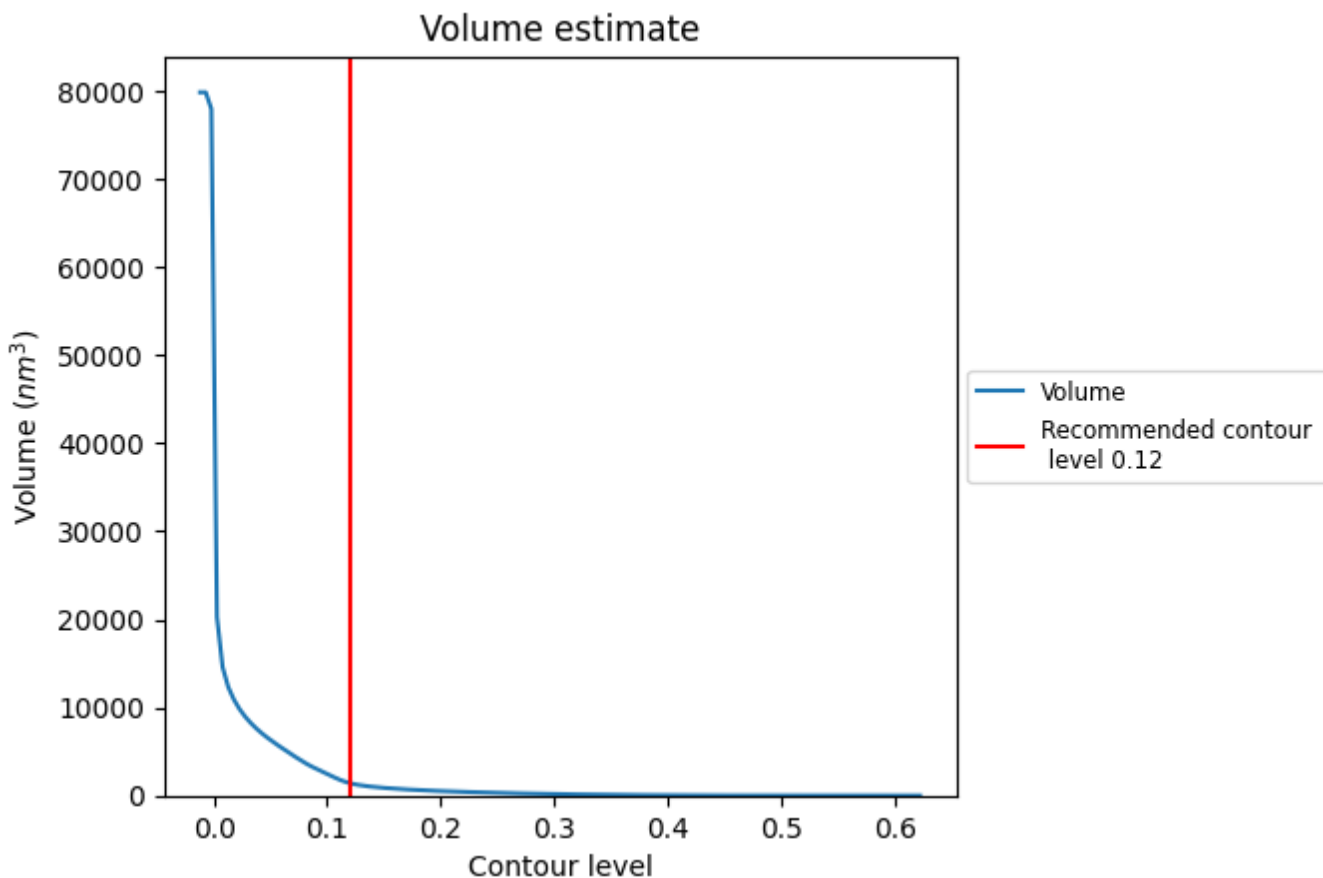
This section contains the results of statistical analysis of the map.

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.

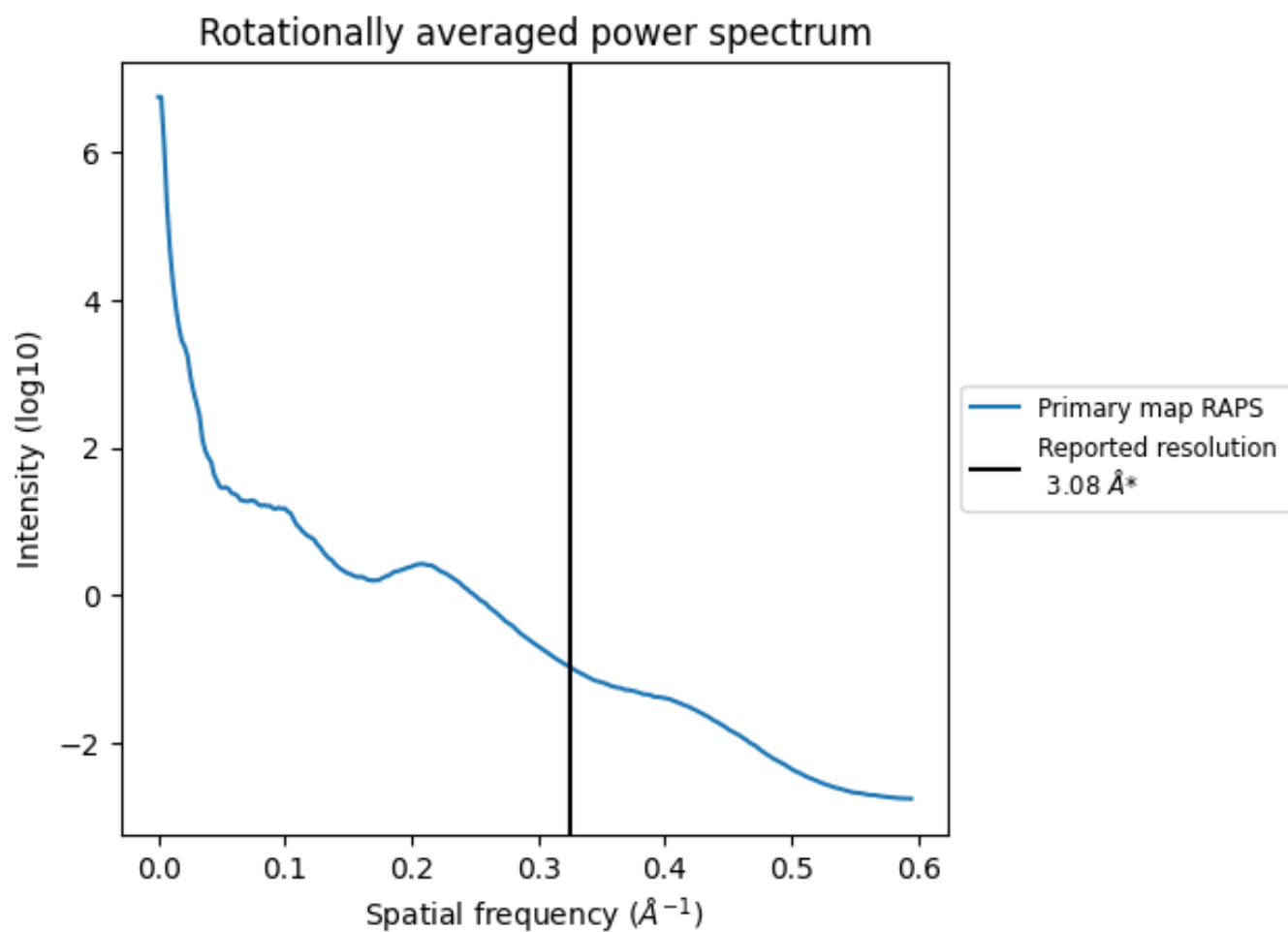
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1416 nm^3 ; this corresponds to an approximate mass of 1279 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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.325 Å⁻¹

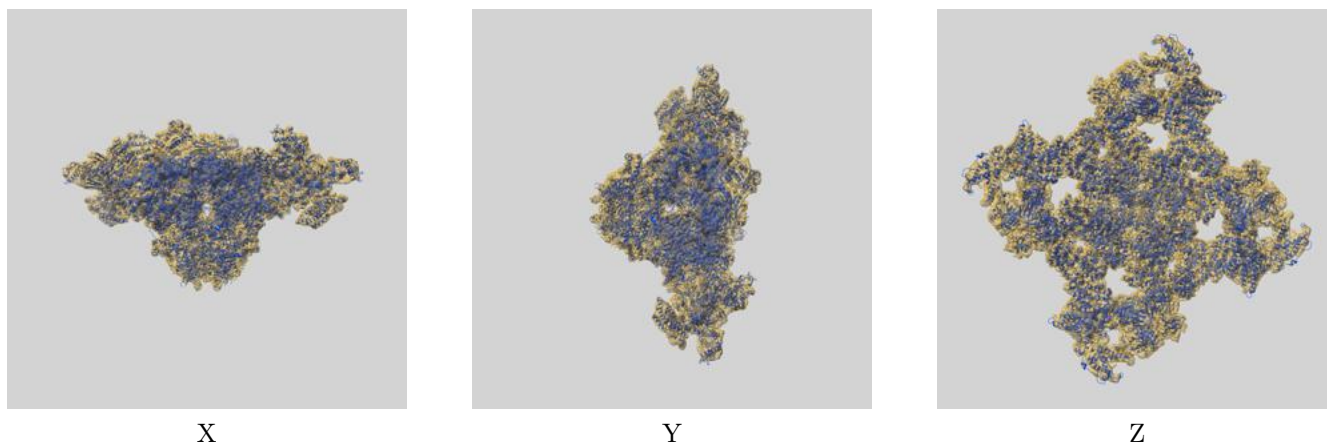
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

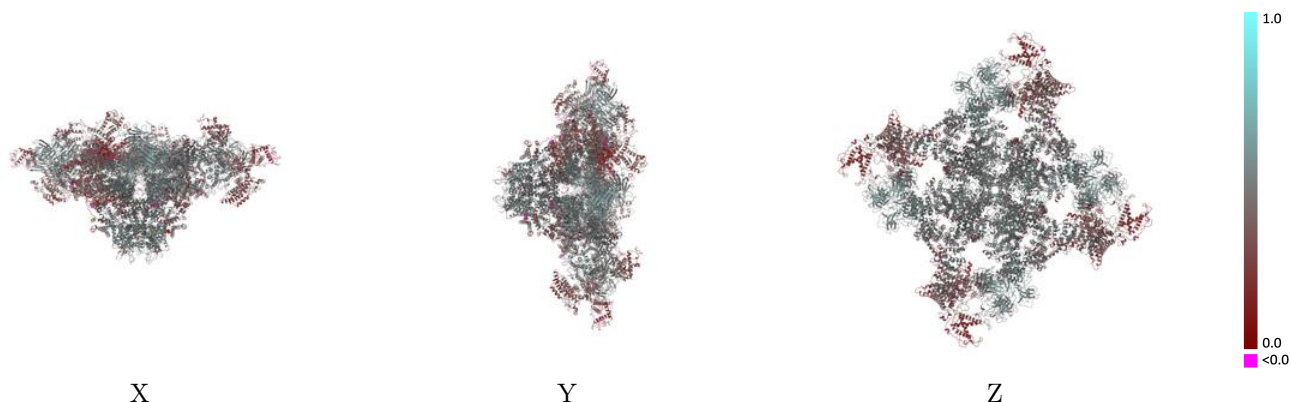
This section contains information regarding the fit between EMDB map EMD-42763 and PDB model 8UXG. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



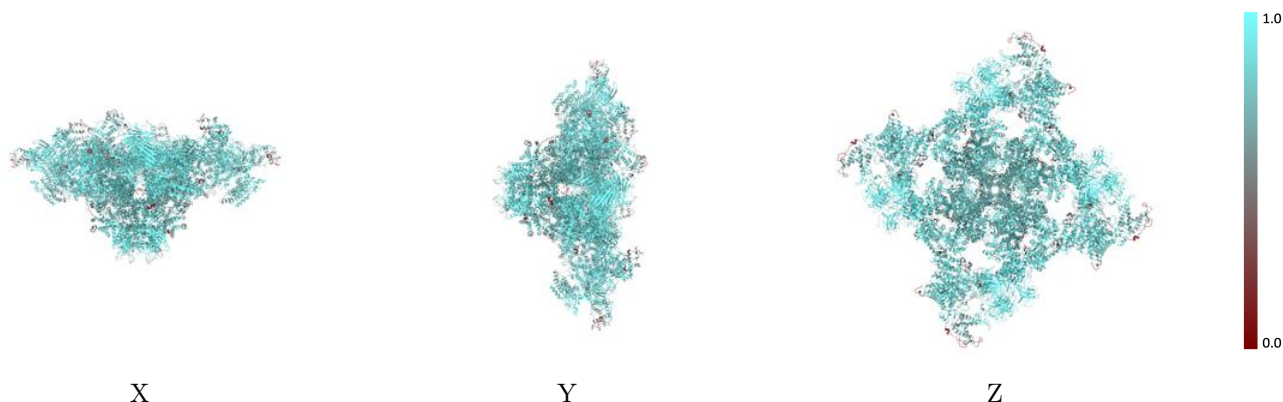
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



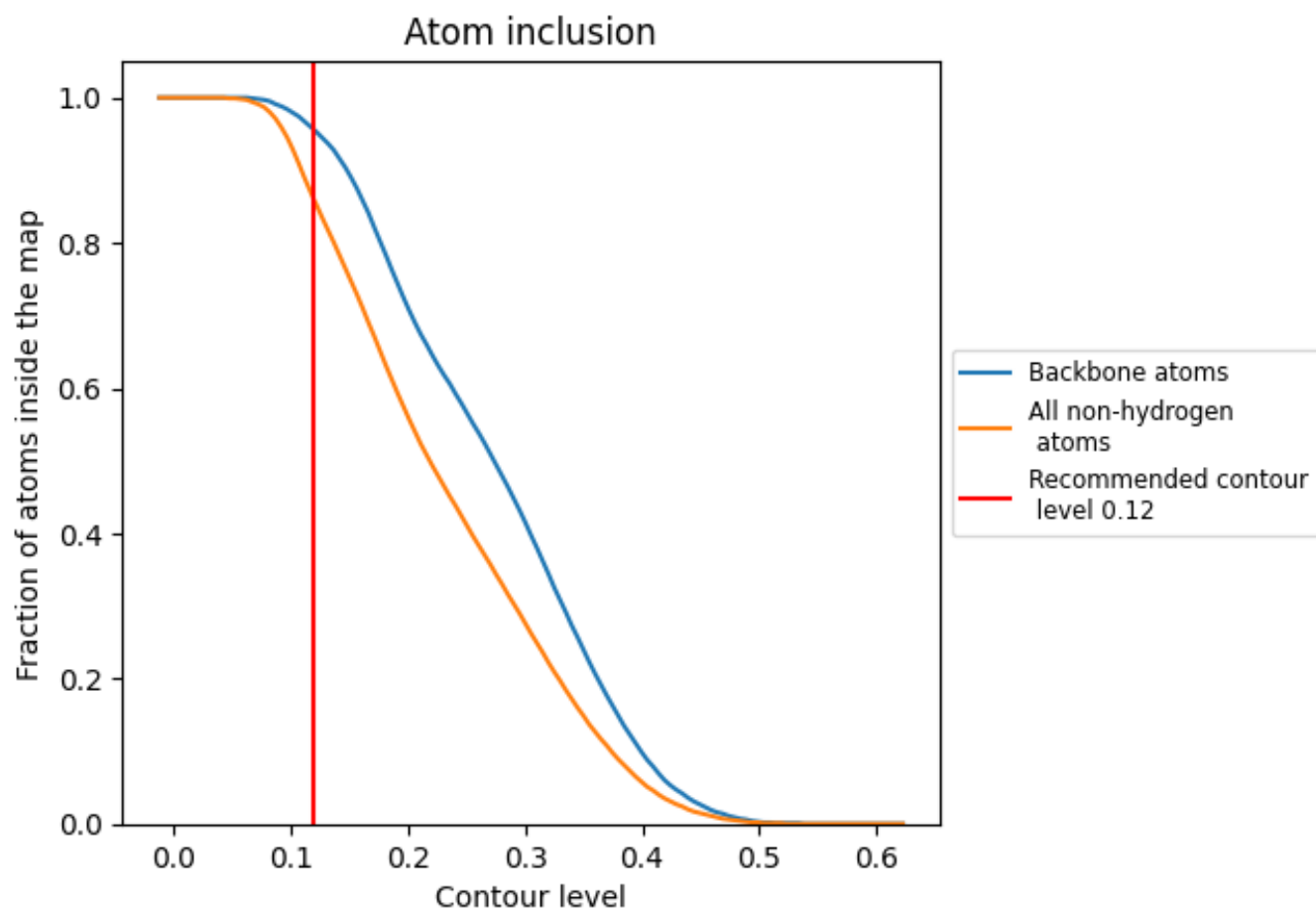
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



At the recommended contour level, 96% of all backbone atoms, 86% 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	 0.8590	 0.4340
A	 0.8580	 0.4310
B	 0.8580	 0.4300
C	 0.8590	 0.4340
D	 0.8560	 0.4300
E	 0.9330	 0.5340
F	 0.9290	 0.5330
G	 0.9340	 0.5350
H	 0.9340	 0.5360

