



wwPDB EM Validation Summary Report ⓘ

Mar 27, 2026 – 10:19 PM UTC

PDB ID : 8SES / pdb_00008ses
EMDB ID : EMD-40427
Title : Cryo-EM Structure of RyR1 + Adenine
Authors : Cholak, S.; Saville, J.W.; Zhu, X.; Berezuk, A.M.; Tuttle, K.S.; Haji-Ghassemi, O.; Van Petegem, F.; Subramaniam, S.
Deposited on : 2023-04-10
Resolution : 3.98 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

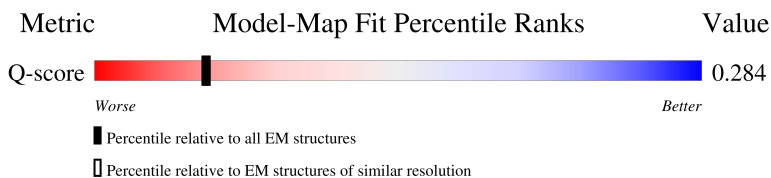
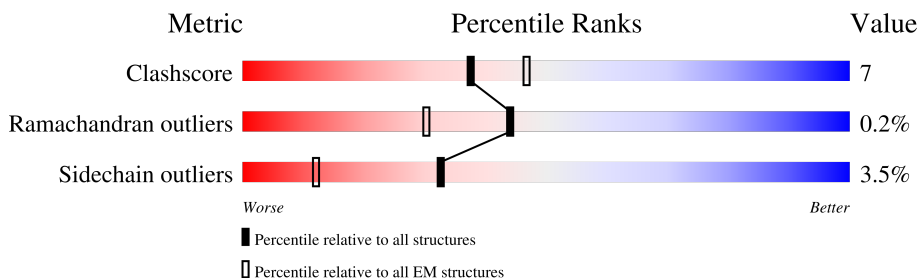
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.98 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7512 (3.48 - 4.48)

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	5037	
1	B	5037	
1	C	5037	
1	D	5037	

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Mol	Chain	Length	Quality of chain
2	E	350	 21%9%69%
2	F	350	 21%9%69%
2	G	350	 22%9%69%
2	H	350	 22%9%69%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 142940 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4377	Total	C	N	O	S	9	0
			34906	22208	6024	6438	236		
1	B	4377	Total	C	N	O	S	9	0
			34906	22208	6024	6438	236		
1	C	4377	Total	C	N	O	S	9	0
			34906	22208	6024	6438	236		
1	D	4377	Total	C	N	O	S	9	0
			34906	22208	6024	6438	236		

- Molecule 2 is a protein called Glutathione S-transferase class-mu 26 kDa isozyme,Peptidyl-prolyl cis-trans isomerase FKBP1B.

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

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-242	MET	-	expression tag	UNP P08515
E	-241	LYS	-	expression tag	UNP P08515
E	-240	SER	-	expression tag	UNP P08515
E	-239	SER	-	expression tag	UNP P08515
E	-238	HIS	-	expression tag	UNP P08515
E	-237	HIS	-	expression tag	UNP P08515
E	-236	HIS	-	expression tag	UNP P08515
E	-235	HIS	-	expression tag	UNP P08515

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-234	HIS	-	expression tag	UNP P08515
E	-233	HIS	-	expression tag	UNP P08515
E	-232	GLY	-	expression tag	UNP P08515
E	-231	SER	-	expression tag	UNP P08515
E	-230	SER	-	expression tag	UNP P08515
E	-11	GLY	-	linker	UNP P08515
E	-10	ILE	-	linker	UNP P08515
E	-9	GLU	-	linker	UNP P08515
E	-8	GLU	-	linker	UNP P08515
E	-7	ASN	-	linker	UNP P08515
E	-6	LEU	-	linker	UNP P08515
E	-5	TYR	-	linker	UNP P08515
E	-4	PHE	-	linker	UNP P08515
E	-3	GLN	-	linker	UNP P08515
E	-2	SER	-	linker	UNP P08515
E	-1	ASN	-	linker	UNP P08515
E	0	ALA	-	linker	UNP P08515
F	-242	MET	-	expression tag	UNP P08515
F	-241	LYS	-	expression tag	UNP P08515
F	-240	SER	-	expression tag	UNP P08515
F	-239	SER	-	expression tag	UNP P08515
F	-238	HIS	-	expression tag	UNP P08515
F	-237	HIS	-	expression tag	UNP P08515
F	-236	HIS	-	expression tag	UNP P08515
F	-235	HIS	-	expression tag	UNP P08515
F	-234	HIS	-	expression tag	UNP P08515
F	-233	HIS	-	expression tag	UNP P08515
F	-232	GLY	-	expression tag	UNP P08515
F	-231	SER	-	expression tag	UNP P08515
F	-230	SER	-	expression tag	UNP P08515
F	-11	GLY	-	linker	UNP P08515
F	-10	ILE	-	linker	UNP P08515
F	-9	GLU	-	linker	UNP P08515
F	-8	GLU	-	linker	UNP P08515
F	-7	ASN	-	linker	UNP P08515
F	-6	LEU	-	linker	UNP P08515
F	-5	TYR	-	linker	UNP P08515
F	-4	PHE	-	linker	UNP P08515
F	-3	GLN	-	linker	UNP P08515
F	-2	SER	-	linker	UNP P08515
F	-1	ASN	-	linker	UNP P08515
F	0	ALA	-	linker	UNP P08515

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-242	MET	-	expression tag	UNP P08515
G	-241	LYS	-	expression tag	UNP P08515
G	-240	SER	-	expression tag	UNP P08515
G	-239	SER	-	expression tag	UNP P08515
G	-238	HIS	-	expression tag	UNP P08515
G	-237	HIS	-	expression tag	UNP P08515
G	-236	HIS	-	expression tag	UNP P08515
G	-235	HIS	-	expression tag	UNP P08515
G	-234	HIS	-	expression tag	UNP P08515
G	-233	HIS	-	expression tag	UNP P08515
G	-232	GLY	-	expression tag	UNP P08515
G	-231	SER	-	expression tag	UNP P08515
G	-230	SER	-	expression tag	UNP P08515
G	-11	GLY	-	linker	UNP P08515
G	-10	ILE	-	linker	UNP P08515
G	-9	GLU	-	linker	UNP P08515
G	-8	GLU	-	linker	UNP P08515
G	-7	ASN	-	linker	UNP P08515
G	-6	LEU	-	linker	UNP P08515
G	-5	TYR	-	linker	UNP P08515
G	-4	PHE	-	linker	UNP P08515
G	-3	GLN	-	linker	UNP P08515
G	-2	SER	-	linker	UNP P08515
G	-1	ASN	-	linker	UNP P08515
G	0	ALA	-	linker	UNP P08515
H	-242	MET	-	expression tag	UNP P08515
H	-241	LYS	-	expression tag	UNP P08515
H	-240	SER	-	expression tag	UNP P08515
H	-239	SER	-	expression tag	UNP P08515
H	-238	HIS	-	expression tag	UNP P08515
H	-237	HIS	-	expression tag	UNP P08515
H	-236	HIS	-	expression tag	UNP P08515
H	-235	HIS	-	expression tag	UNP P08515
H	-234	HIS	-	expression tag	UNP P08515
H	-233	HIS	-	expression tag	UNP P08515
H	-232	GLY	-	expression tag	UNP P08515
H	-231	SER	-	expression tag	UNP P08515
H	-230	SER	-	expression tag	UNP P08515
H	-11	GLY	-	linker	UNP P08515
H	-10	ILE	-	linker	UNP P08515
H	-9	GLU	-	linker	UNP P08515
H	-8	GLU	-	linker	UNP P08515

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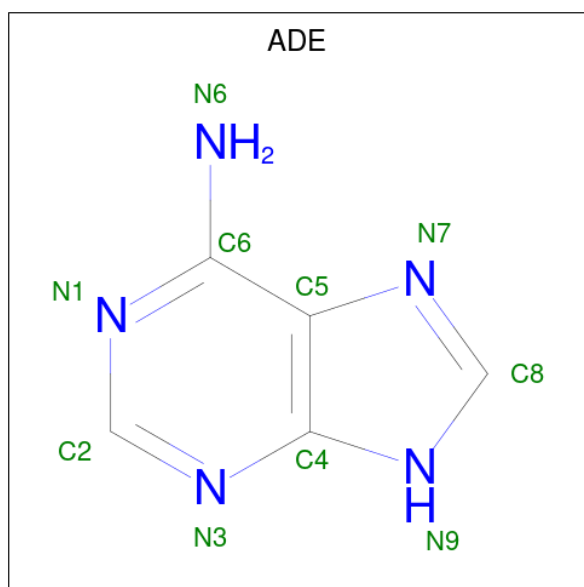
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Chain	Residue	Modelled	Actual	Comment	Reference
H	-7	ASN	-	linker	UNP P08515
H	-6	LEU	-	linker	UNP P08515
H	-5	TYR	-	linker	UNP P08515
H	-4	PHE	-	linker	UNP P08515
H	-3	GLN	-	linker	UNP P08515
H	-2	SER	-	linker	UNP P08515
H	-1	ASN	-	linker	UNP P08515
H	0	ALA	-	linker	UNP P08515

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is ADENINE (CCD ID: ADE) (formula: C₅H₅N₅) (labeled as "Ligand of Interest" by depositor).

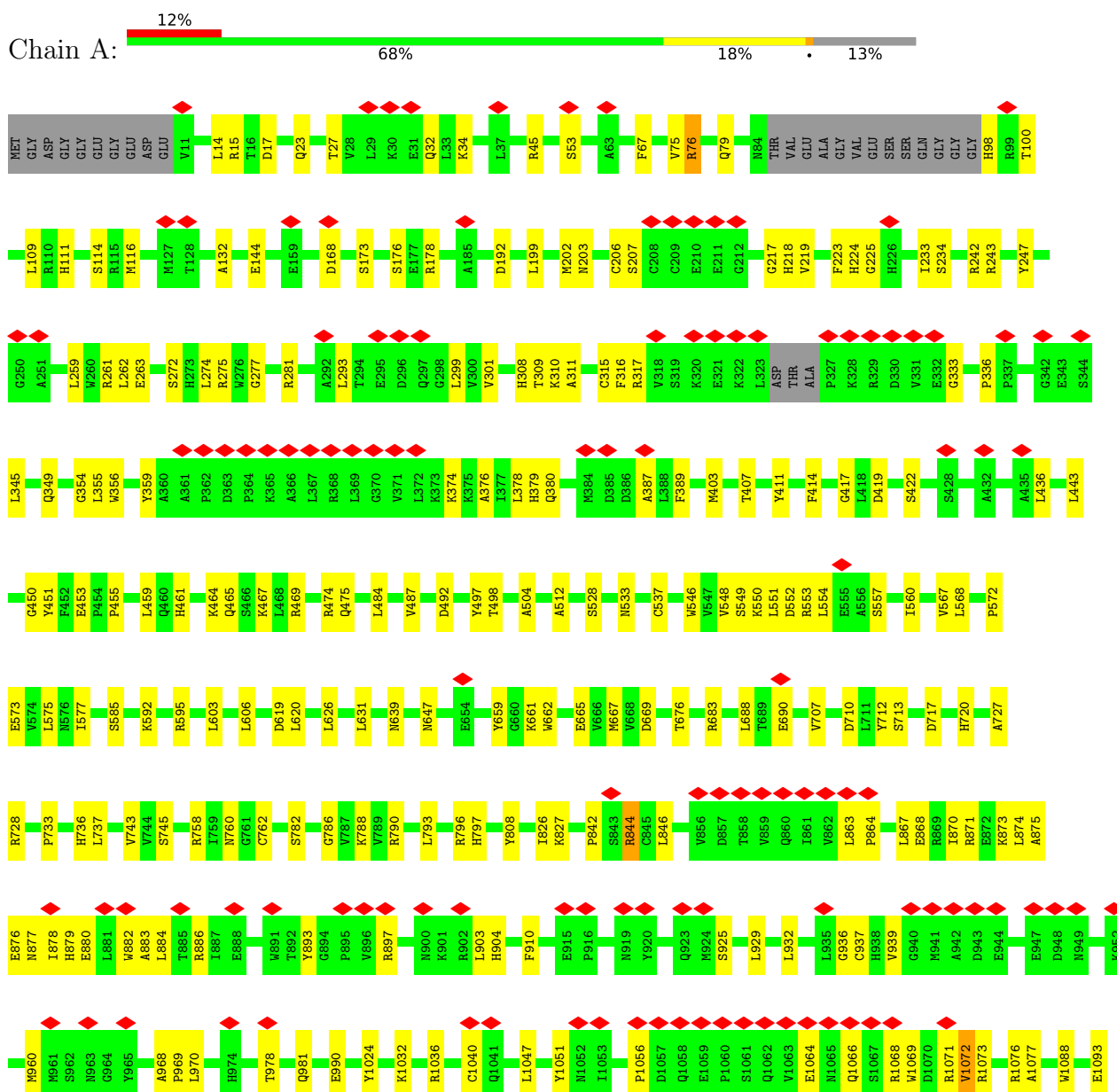


Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total 10	C 5	N 5	0
4	B	1	Total 10	C 5	N 5	0
4	C	1	Total 10	C 5	N 5	0
4	D	1	Total 10	C 5	N 5	0

3 Residue-property plots

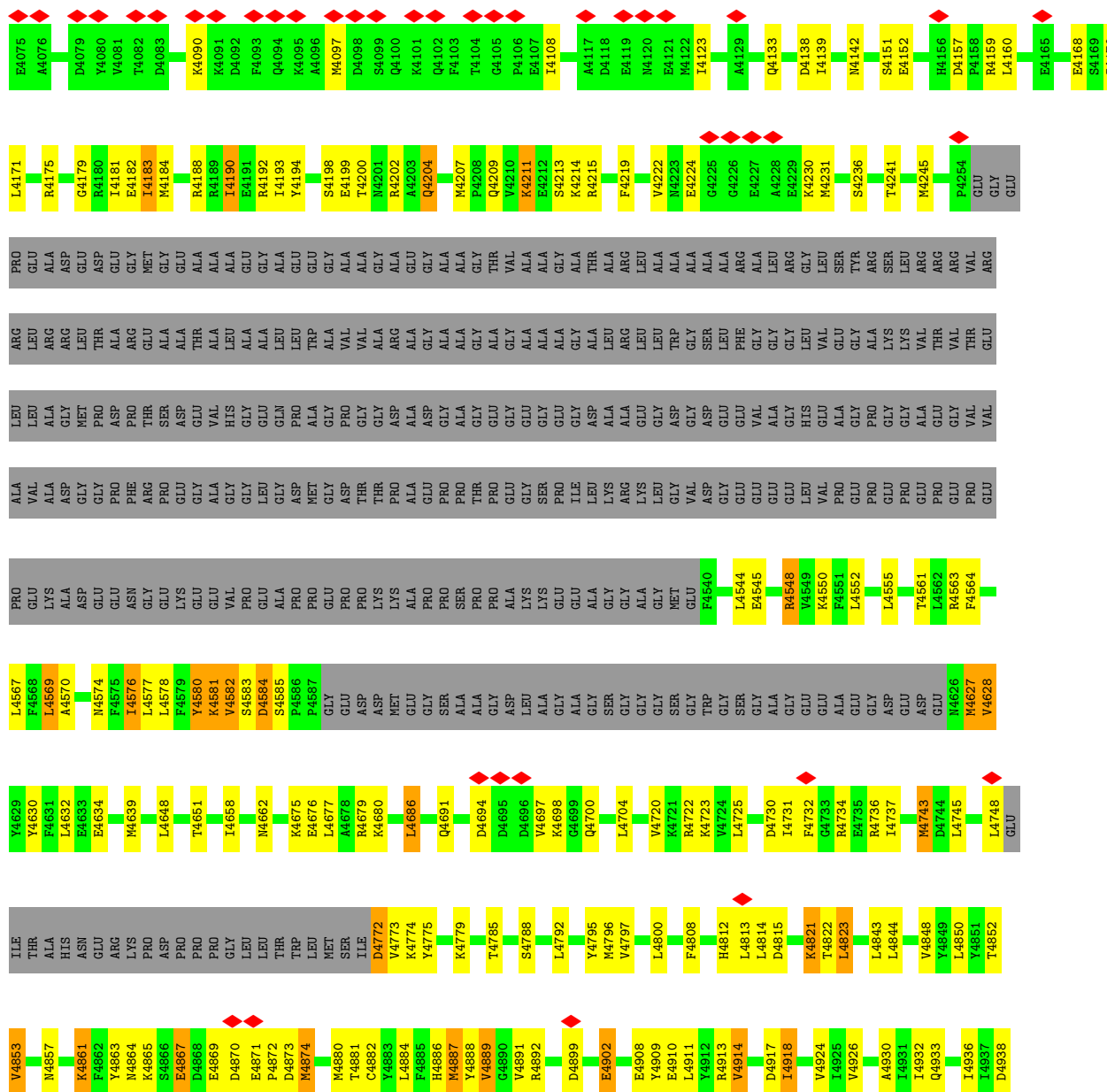
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Ryanodine receptor 1

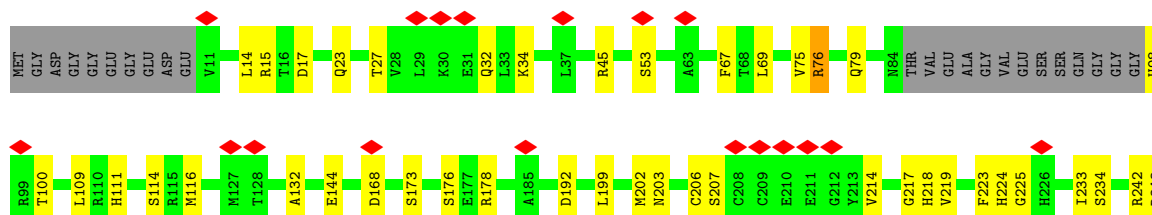




Q3927	G3786	Y3576	S3474	R3366	R2682	T3157	R3051	L2963	A2896	LYS	S2776
Q3928	K3787	L3579	K3475	E3377	E3265	L3158	H3052	M2967	K2897	LYS	Y2777
S3929	G3788	P3580	S3476	M3266	M3266	D3159	R3053	M2967	G2898	THR	G2778
D3932	T3797	G3581	K3477	R3380	E3271	D3160	L3056	Q2970	G2899	ARG	E2779
W3935	L3800	R3582	M3478	L3381	E3271	D3162	V3064	S2970	G2900	LYS	N2780
G3939	L3805	E3583	A3479	E3382	P3275	S3171	L3075	F2973	T2901	ILE	N2781
E3944	N3809	E3584	LYS	A3383	M3276	S3174	M3081	E2978	D2902	GLN	D2782
E3945	E3810	D3585	ALA	K3384	E3290	S3174	G3084	A2979	P2903	THR	E2783
Q3946	E3811	A3586	GLY	A3385	A3291	R3187	E3086	L2904	L2904	ALA	E2784
G3947	V3812	A3587	ALA	E3386	P3292	P3188	P3085	L2905	L2905	GLN	L2785
L3948	V3690	E3387	GLN	E3387	P3293	G3191	E3086	V2906	V2906	THR	K2786
E3965	E3691	E3388	GLY	E3388	P3294	G3191	E3086	P2907	P2907	ASP	T2787
T3966	E3692	E3389	GLY	E3389	A3295	S3174	E3086	Y2908	Y2908	ARG	H2788
E3967	K3693	A3588	ASP	A3295	A3295	R3187	E3086	D2909	D2909	THR	L2789
Y3968	K3694	E3589	GLN	A3296	L3194	P3188	E3086	T2910	T2910	THR	L2790
L3985	P3695	R3392	GLN	P3297	R3194	P3188	E3086	L2911	L2911	THR	L2791
V3989	E3718	R3393	ARG	A3298	K3201	P3202	E3086	T2912	T2912	ASP	R2792
K3842	D3719	R3403	LYS	G3299	P3202	A3204	E3086	K2914	K2914	PRO	P2793
R3849	Y3725	Y3406	LYS	P3301	P3208	P3208	E3086	E2915	E2915	GLU	K2794
Q3850	T3728	R3414	R3498	P3303	N3211	N3211	E3086	K2916	K2916	GLY	K2795
G3857	K3729	Y3415	R3499	C3304	N3211	N3211	E3086	A2917	A2917		F2796
M3858	L3735	V3416	G3500	S3309	N3211	N3211	E3086	R2918	R2918		F2797
V3859	E3736	R3419	D3501	N3318	N3211	N3211	E3086	S2863	S2863		S2798
N3860	E3736	R3420	Q3506	N3318	A3215	A3215	E3086	G2864	G2864		E2799
E3861	E3736	A3421	K3516	L3320	S3217	S3217	E3086	V2865	V2865		K2800
D3862	E3736	V3423	K3516	R3321	S3217	S3217	E3086	T2866	T2866		D2801
G3863	E3736	L3424	K3517	I3322	V3218	V3218	E3086	K2802	K2802		K2802
T3864	E3736	T3425	M3518	R3322	T3221	T3221	E3086	E2803	E2803		E2803
V3865	E3736	E3426	P3519	N3326	K3224	K3224	E3086	L2804	L2804		L2804
N3866	E3736	P3427	N3524	N3326	P3224	P3224	E3086	K2805	K2805		K2805
L3866	E3736	L3434	N3524	N3326	R3225	R3225	E3086	R2806	R2806		R2806
N3867	E3736	N3437	A3541	L3329	T3229	T3229	E3086	L2871	L2871		L2871
Q3868	E3736	N3437	L3542	D3330	L3230	L3230	E3086	Q2872	Q2872		Q2872
N3870	E3736	T3441	K3543	A3332	L3230	L3230	E3086	F2808	F2808		F2808
E3872	E3736	N3450	N3555	K3336	G3231	G3231	E3086	T2809	T2809		T2809
M3875	E3736	R3453	N3556	R3337	E3238	E3238	E3086	K2810	K2810		K2810
D3876	E3736	E3454	L3557	L3338	P3241	P3241	E3086	E2811	E2811		E2811
R3886	E3736	N3457	H3558	V3340	D3242	D3242	E3086	L2813	L2813		L2813
F3887	E3736	N3465	L3559	Q3343	T3243	T3243	E3086	K2814	K2814		K2814
L3888	E3736	N3466	Q3560	P3344	P3244	P3244	E3086	E2815	E2815		E2815
Q3889	E3736	N3467	G3561	I3345	V3245	V3245	E3086	L2816	L2816		L2816
L3890	E3736	N3468	K3562	R3350	D3247	D3247	E3086	L2817	L2817		L2817
L3891	E3736	N3469	V3563	R3350	R3248	R3248	E3086	A2818	A2818		A2818
Q3900	E3736	N3470	E3564	L3354	K3249	K3249	E3086	W2819	W2819		W2819
	E3736	N3471	G3565	F3356	N3250	N3250	E3086	E2820	E2820		E2820
	E3736	N3472	S3566	F3356	K3254	K3254	E3086	W2821	W2821		W2821
	E3736	N3473	L3569	T3361	G3254	G3254	E3086	T2822	T2822		T2822
	E3736	N3474	L3573	T3361	G3254	G3254	E3086	L2823	L2823		L2823
	E3736	N3475	M3573	T3361	G3254	G3254	E3086	E2824	E2824		E2824
	E3736	N3476	M3573	T3361	G3254	G3254	E3086	K2825	K2825		K2825
	E3736	N3477	M3573	T3361	G3254	G3254	E3086	L2826	L2826		L2826
	E3736	N3478	M3573	T3361	G3254	G3254	E3086	R2827	R2827		R2827
	E3736	N3479	M3573	T3361	G3254	G3254	E3086	E2828	E2828		E2828
	E3736	N3480	M3573	T3361	G3254	G3254	E3086	G2829	G2829		G2829
	E3736	N3481	M3573	T3361	G3254	G3254	E3086	L2894	L2894		L2894
	E3736	N3482	M3573	T3361	G3254	G3254	E3086	E2895	E2895		E2895
	E3736	N3483	M3573	T3361	G3254	G3254	E3086	L2960	L2960		L2960
	E3736	N3484	M3573	T3361	G3254	G3254	E3086				
	E3736	N3485	M3573	T3361	G3254	G3254	E3086				
	E3736	N3486	M3573	T3361	G3254	G3254	E3086				
	E3736	N3487	M3573	T3361	G3254	G3254	E3086				
	E3736	N3488	M3573	T3361	G3254	G3254	E3086				
	E3736	N3489	M3573	T3361	G3254	G3254	E3086				
	E3736	N3490	M3573	T3361	G3254	G3254	E3086				
	E3736	N3491	M3573	T3361	G3254	G3254	E3086				
	E3736	N3492	M3573	T3361	G3254	G3254	E3086				
	E3736	N3493	M3573	T3361	G3254	G3254	E3086				
	E3736	N3494	M3573	T3361	G3254	G3254	E3086				
	E3736	N3495	M3573	T3361	G3254	G3254	E3086				
	E3736	N3496	M3573	T3361	G3254	G3254	E3086				
	E3736	N3497	M3573	T3361	G3254	G3254	E3086				
	E3736	N3498	M3573	T3361	G3254	G3254	E3086				
	E3736	N3499	M3573	T3361	G3254	G3254	E3086				
	E3736	N3500	M3573	T3361	G3254	G3254	E3086				
	E3736	N3501	M3573	T3361	G3254	G3254	E3086				
	E3736	N3502	M3573	T3361	G3254	G3254	E3086				
	E3736	N3503	M3573	T3361	G3254	G3254	E3086				
	E3736	N3504	M3573	T3361	G3254	G3254	E3086				
	E3736	N3505	M3573	T3361	G3254	G3254	E3086				
	E3736	N3506	M3573	T3361	G3254	G3254	E3086				
	E3736	N3507	M3573	T3361	G3254	G3254	E3086				
	E3736	N3508	M3573	T3361	G3254	G3254	E3086				
	E3736	N3509	M3573	T3361	G3254	G3254	E3086				
	E3736	N3510	M3573	T3361	G3254	G3254	E3086				
	E3736	N3511	M3573	T3361	G3254	G3254	E3086				
	E3736	N3512	M3573	T3361	G3254	G3254	E3086				
	E3736	N3513	M3573	T3361	G3254	G3254	E3086				
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	E3736	N3515	M3573	T3361	G3254	G3254	E3086				
	E3736	N3516	M3573	T3361	G3254	G3254	E3086				
	E3736	N3517	M3573	T3361	G3254	G3254	E3086				
	E3736	N3518	M3573	T3361	G3254	G3254	E3086				
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	E3736	N3522	M3573	T3361	G3254	G3254	E3086				
	E3736	N3523	M3573	T3361	G3254	G3254	E3086				
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	E3736	N3525	M3573	T3361	G3254	G3254	E3086				
	E3736	N3526	M3573	T3361	G3254	G3254	E3086				
	E3736	N3527	M3573	T3361	G3254	G3254	E3086				
	E3736	N3528	M3573	T3361	G3254	G3254	E3086				
	E3736	N3529	M3573	T3361	G3254	G3254	E3086				
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• Molecule 1: Ryanodine receptor 1





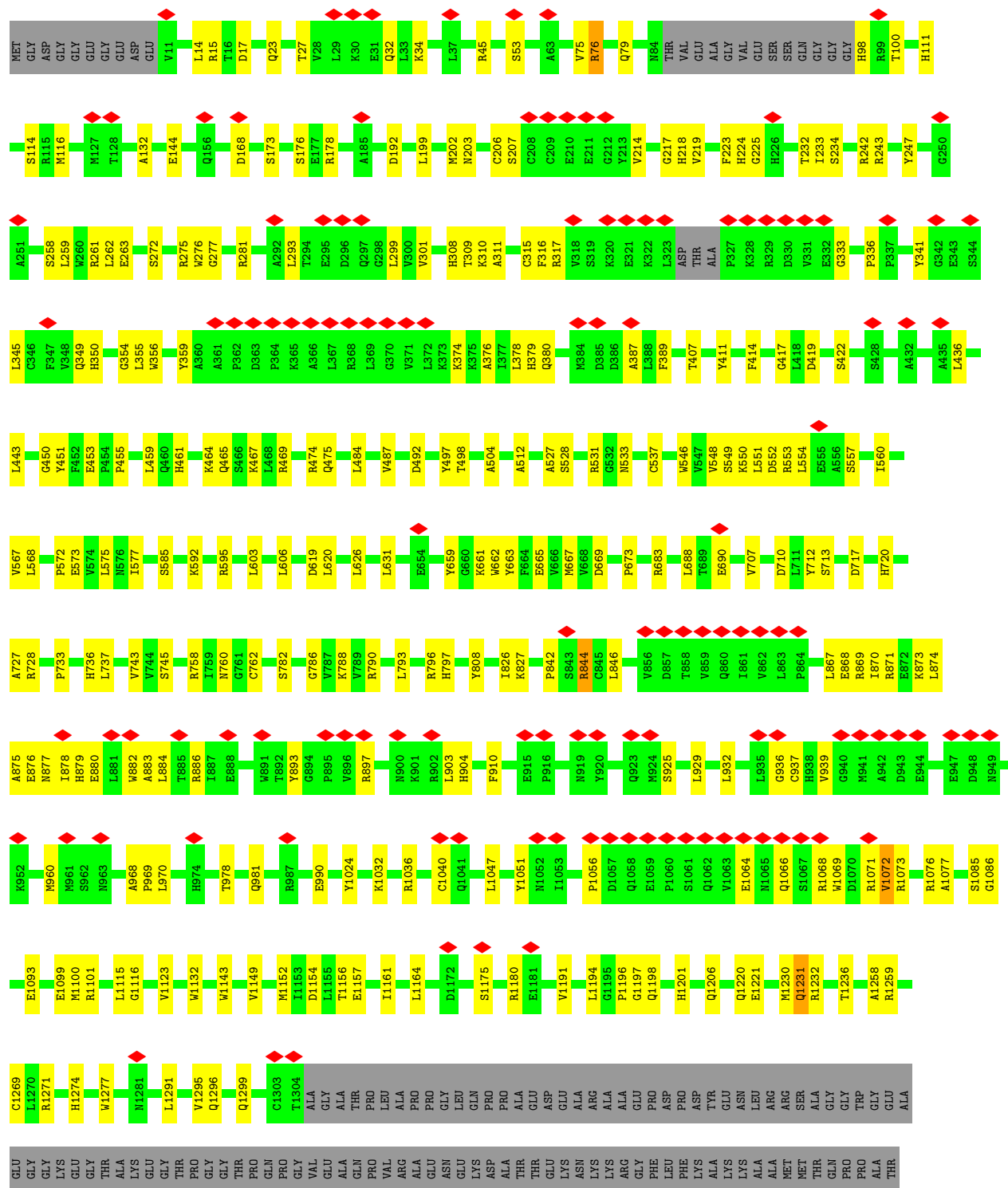
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G3231	L3136	R2939	R2939	E2880	E2820	F2758	W2680	K2564	HIS	E2219	VAL	T1985
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P3293	G3191	S2983	S2983	L2904	ALA	E2783	ALA	P2640	G2480	R2126	GLY	GLY
P3294	L3194	G2984	G2984	L2905	GLN	E2784	THR	L2643	K2481	P2146	GLU	GLU
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N3318	C3216	F2997	F2997	K2916	L2862	T2797	L2743		N2514	G2396	LEU	LEU
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I3322	K3123	L3002	L3002	K2922	T2866	D2801	I2747					
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		Y3009	Y3009	E2925	V2865	L2804	K2750					
		F3010	F3010	L2926	T2866	Y2805	L2761					
				L2927	L2867	R2806						
				K2928	L2867	W2807						
				F2929	L2867	P2808						
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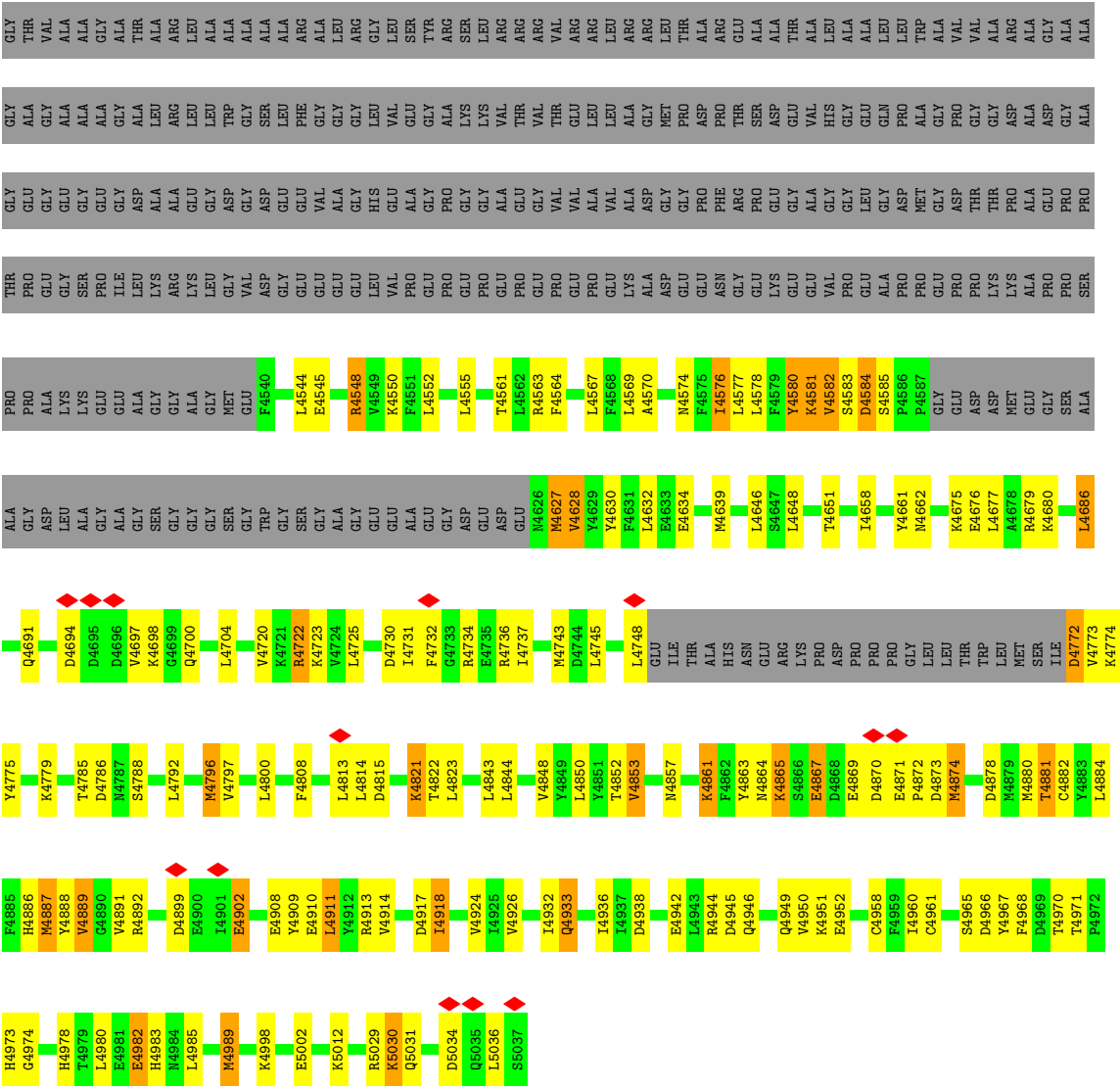
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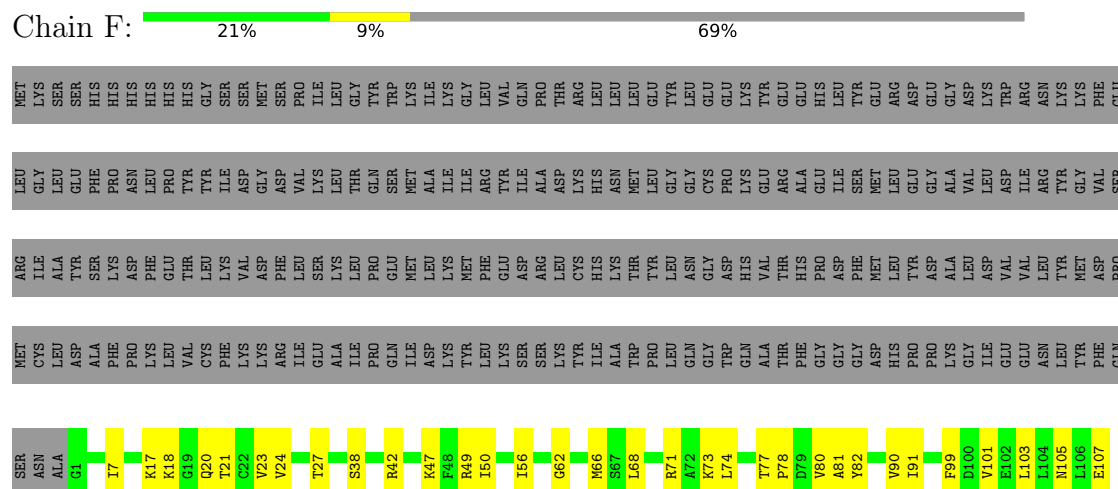




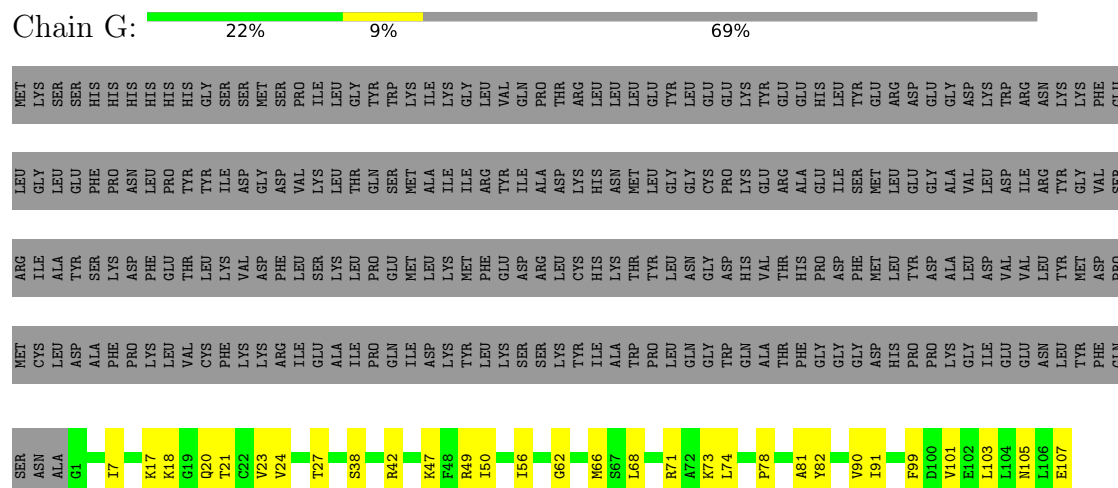
● Molecule 2: Glutathione S-transferase class-mu 26 kDa isozyme,Peptidyl-prolyl cis-trans isomerase FKBP1B



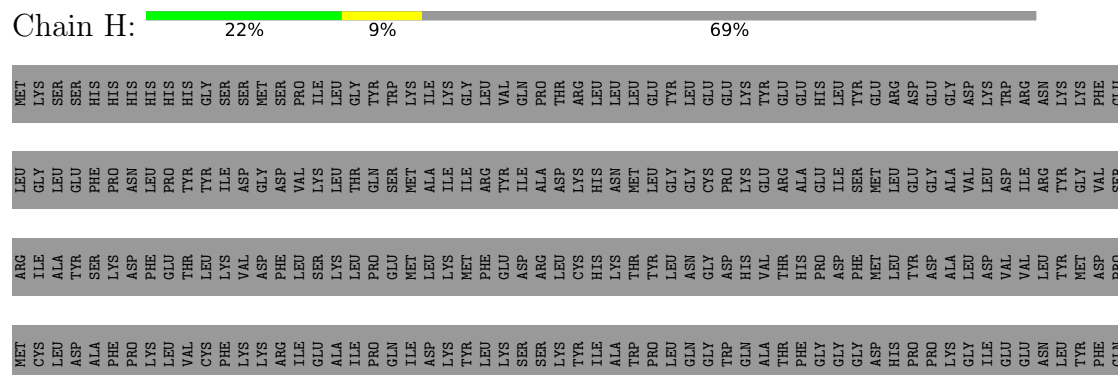
- Molecule 2: Glutathione S-transferase class-mu 26 kDa isozyme,Peptidyl-prolyl cis-trans isomerase FKBP1B



- Molecule 2: Glutathione S-transferase class-mu 26 kDa isozyme,Peptidyl-prolyl cis-trans isomerase FKBP1B



- Molecule 2: Glutathione S-transferase class-mu 26 kDa isozyme,Peptidyl-prolyl cis-trans isomerase FKBP1B



SER	ASN	ALA	G1	I7	K17	K18	G19	Q20	T21	C22	V23	V24	T27	S38	S39	R42	K47	F48	R49	I50	I56	G62	M66	S67	L68	R71	A72	K73	L74	P78	A81	Y82	V90	I91	F99	D100	V101	E102	L103	L104	N105	L106	E107
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21706	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.200	Depositor
Minimum map value	-0.744	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.065	Depositor
Recommended contour level	0.305	Depositor
Map size (Å)	515.2, 515.2, 515.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.288, 1.288, 1.288	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ADE, 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	0.30	0/35720	0.67	8/48374 (0.0%)
1	B	0.30	0/35720	0.67	8/48374 (0.0%)
1	C	0.30	0/35720	0.67	8/48374 (0.0%)
1	D	0.30	0/35720	0.67	6/48374 (0.0%)
2	E	0.26	0/834	0.64	0/1123
2	F	0.26	0/834	0.64	0/1123
2	G	0.26	0/834	0.64	0/1123
2	H	0.26	0/834	0.64	0/1123
All	All	0.30	0/146216	0.67	30/197988 (0.0%)

There are no bond length outliers.

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	844	ARG	CA-CB-CG	7.34	128.78	114.10
1	D	844	ARG	CA-CB-CG	7.34	128.78	114.10
1	A	844	ARG	CA-CB-CG	7.33	128.77	114.10
1	B	844	ARG	CA-CB-CG	7.32	128.75	114.10
1	A	76	ARG	CG-CD-NE	6.59	126.51	112.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	34906	0	34529	508	0
1	B	34906	0	34529	520	0
1	C	34906	0	34529	524	0
1	D	34906	0	34529	523	0
2	E	818	0	824	20	0
2	F	818	0	824	20	0
2	G	818	0	824	19	0
2	H	818	0	824	20	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	10	0	4	1	0
4	B	10	0	4	1	0
4	C	10	0	4	1	0
4	D	10	0	4	1	0
All	All	142940	0	141428	2122	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 2122 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:844:ARG:HH12	1:C:1197:GLY:HA3	1.45	0.80
1:B:844:ARG:HH12	1:B:1197:GLY:HA3	1.45	0.80
1:A:844:ARG:HH12	1:A:1197:GLY:HA3	1.45	0.79
1:D:844:ARG:HH12	1:D:1197:GLY:HA3	1.45	0.79
1:B:34:LYS:H	1:B:53:SER:HB3	1.49	0.78

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	4353/5037 (86%)	4129 (95%)	217 (5%)	7 (0%)	43	75
1	B	4353/5037 (86%)	4128 (95%)	218 (5%)	7 (0%)	43	75
1	C	4353/5037 (86%)	4131 (95%)	215 (5%)	7 (0%)	43	75
1	D	4353/5037 (86%)	4129 (95%)	217 (5%)	7 (0%)	43	75
2	E	105/350 (30%)	95 (90%)	10 (10%)	0	100	100
2	F	105/350 (30%)	96 (91%)	9 (9%)	0	100	100
2	G	105/350 (30%)	95 (90%)	10 (10%)	0	100	100
2	H	105/350 (30%)	95 (90%)	10 (10%)	0	100	100
All	All	17832/21548 (83%)	16898 (95%)	906 (5%)	28 (0%)	44	75

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1069	TRP
1	A	3615	SER
1	A	4910	GLU
1	B	1069	TRP
1	B	3615	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	3805/4276 (89%)	3667 (96%)	138 (4%)	31	53
1	B	3805/4276 (89%)	3666 (96%)	139 (4%)	30	52
1	C	3805/4276 (89%)	3667 (96%)	138 (4%)	31	53
1	D	3805/4276 (89%)	3666 (96%)	139 (4%)	30	52
2	E	88/304 (29%)	88 (100%)	0	100	100
2	F	88/304 (29%)	88 (100%)	0	100	100
2	G	88/304 (29%)	88 (100%)	0	100	100
2	H	88/304 (29%)	88 (100%)	0	100	100

Continued on next page...

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	15572/18320 (85%)	15018 (96%)	554 (4%)	32 53

5 of 554 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	4632	LEU
1	D	4723	LYS
1	D	4628	VAL
1	D	4908	GLU
1	B	4697	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 190 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	2247	GLN
1	D	284	HIS
1	C	2991	HIS
1	C	4728	HIS
1	D	1229	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	ADE	A	5102	-	11,11,11	0.39	0	15,15,15	0.41	0
4	ADE	B	5102	-	11,11,11	0.39	0	15,15,15	0.41	0
4	ADE	C	5102	-	11,11,11	0.39	0	15,15,15	0.41	0
4	ADE	D	5102	-	11,11,11	0.39	0	15,15,15	0.41	0

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	ADE	A	5102	-	-	-	0/2/2/2
4	ADE	B	5102	-	-	-	0/2/2/2
4	ADE	C	5102	-	-	-	0/2/2/2
4	ADE	D	5102	-	-	-	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

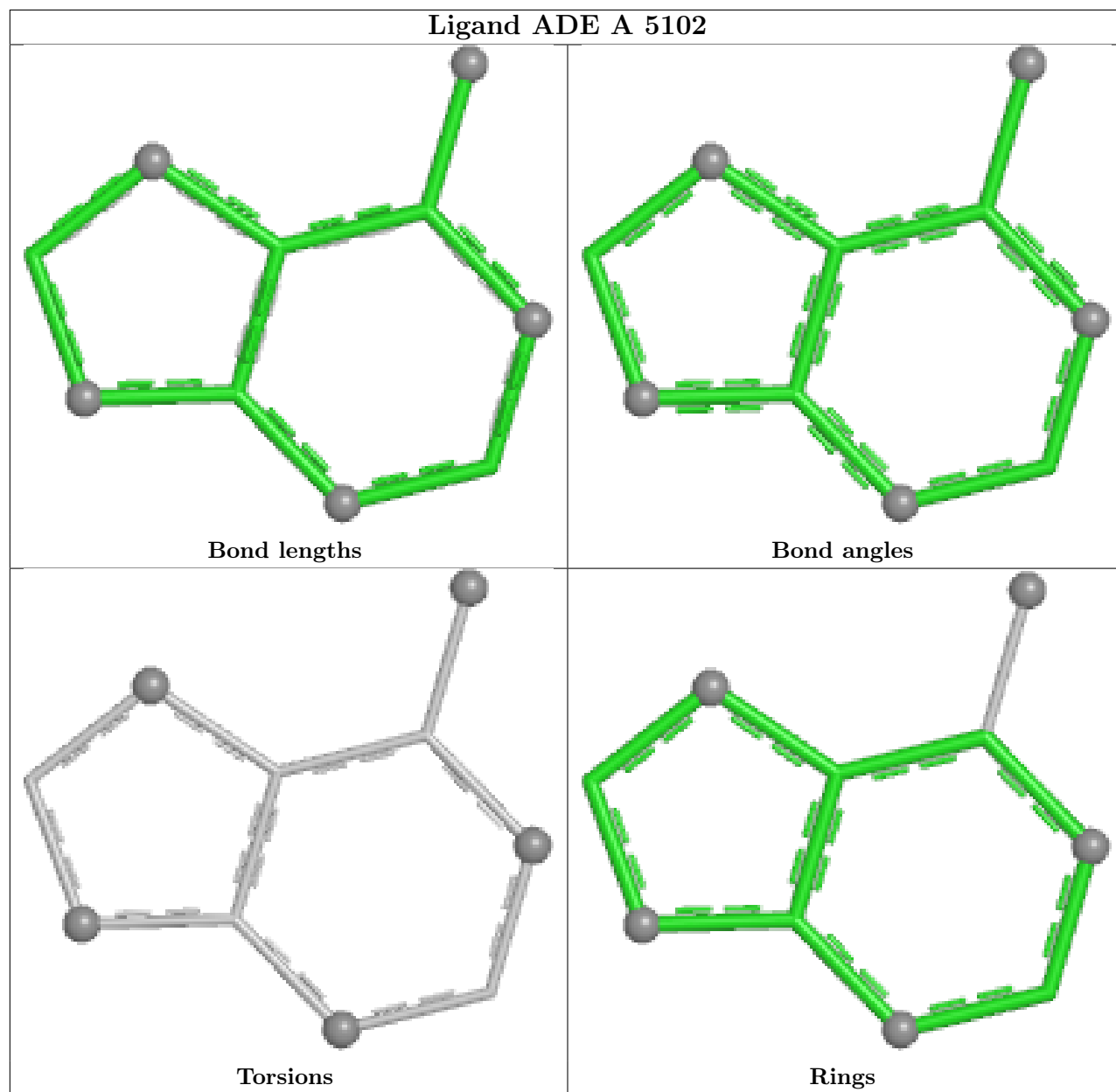
There are no ring outliers.

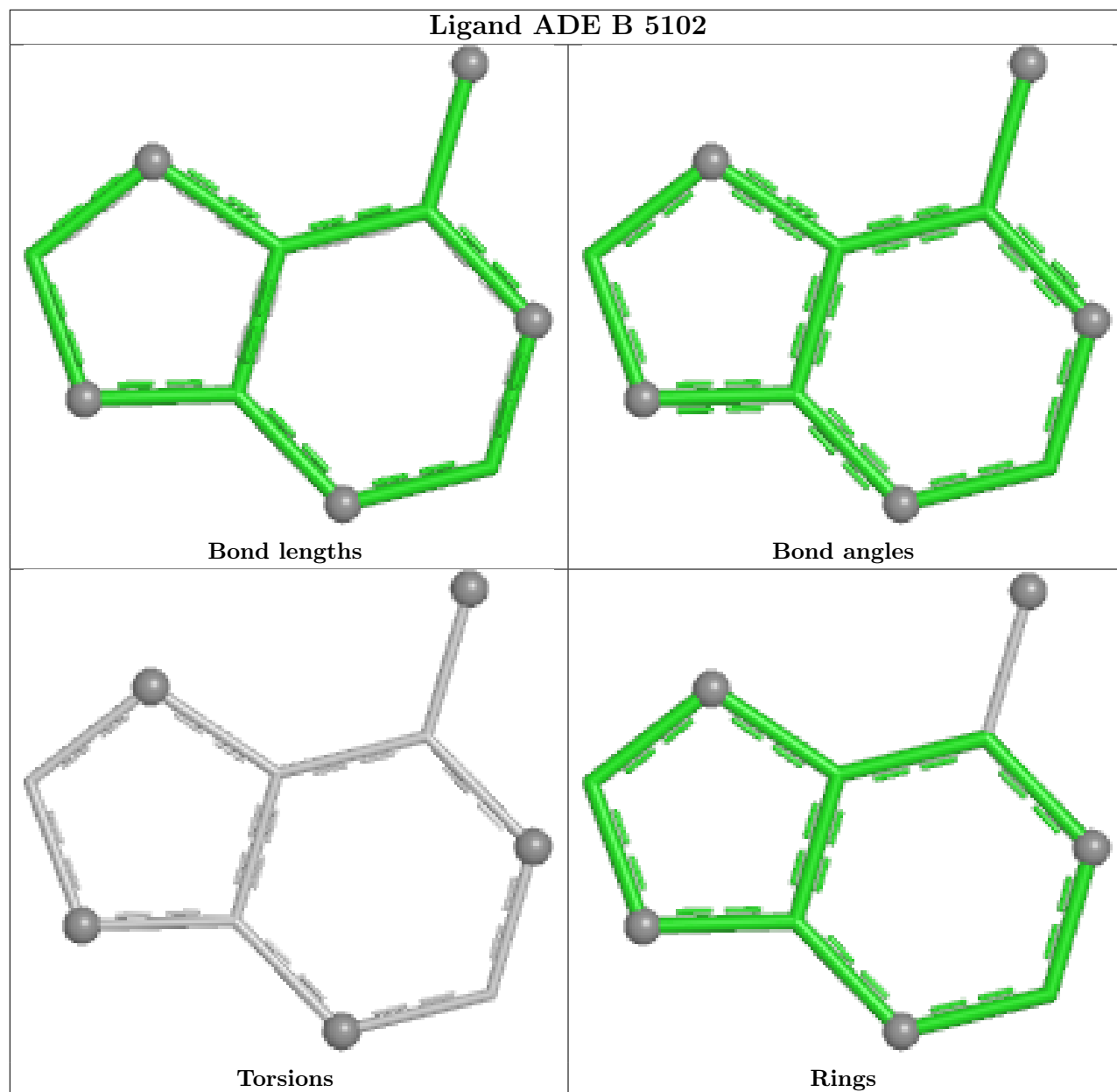
4 monomers are involved in 4 short contacts:

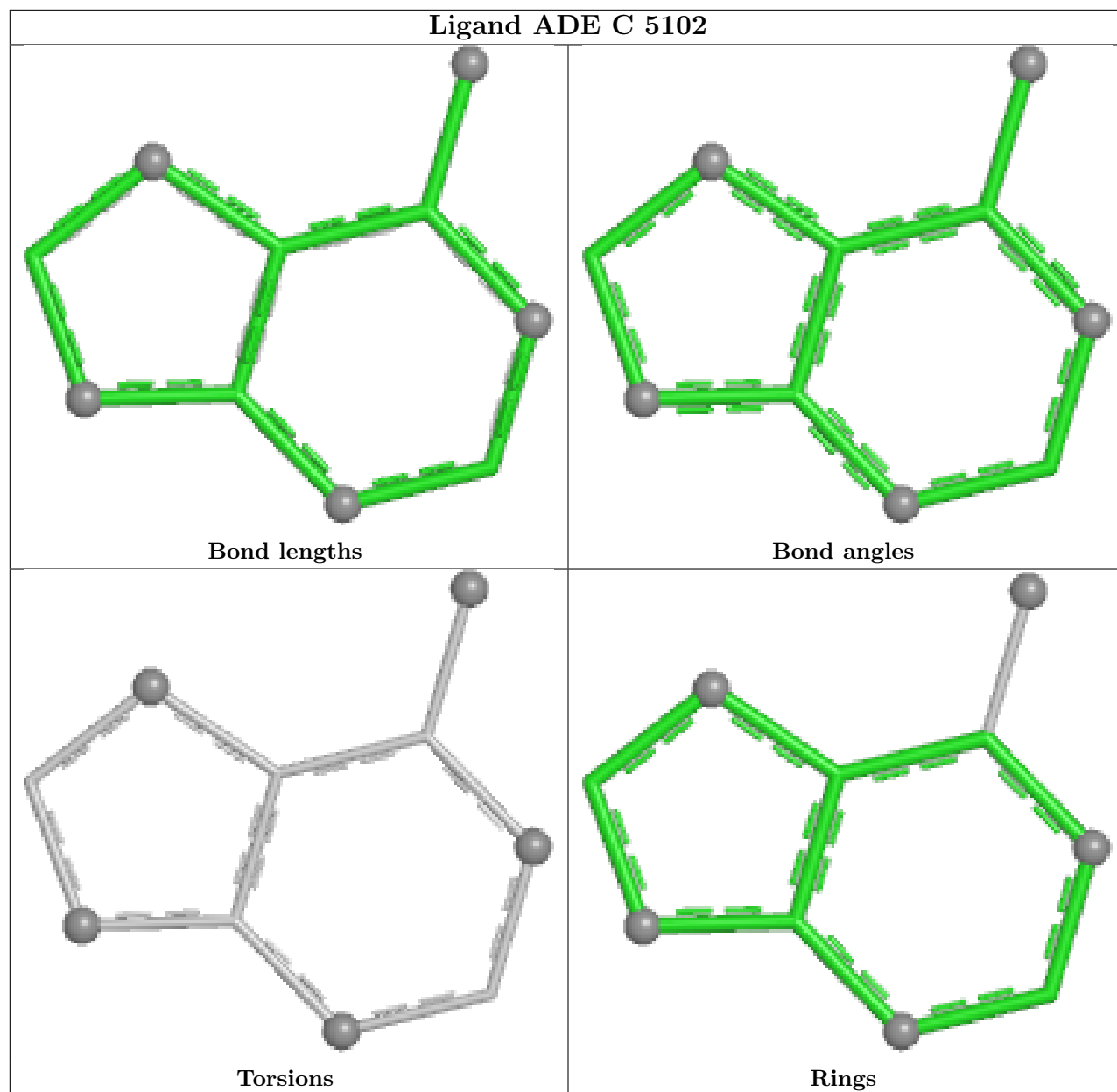
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	5102	ADE	1	0
4	B	5102	ADE	1	0
4	C	5102	ADE	1	0
4	D	5102	ADE	1	0

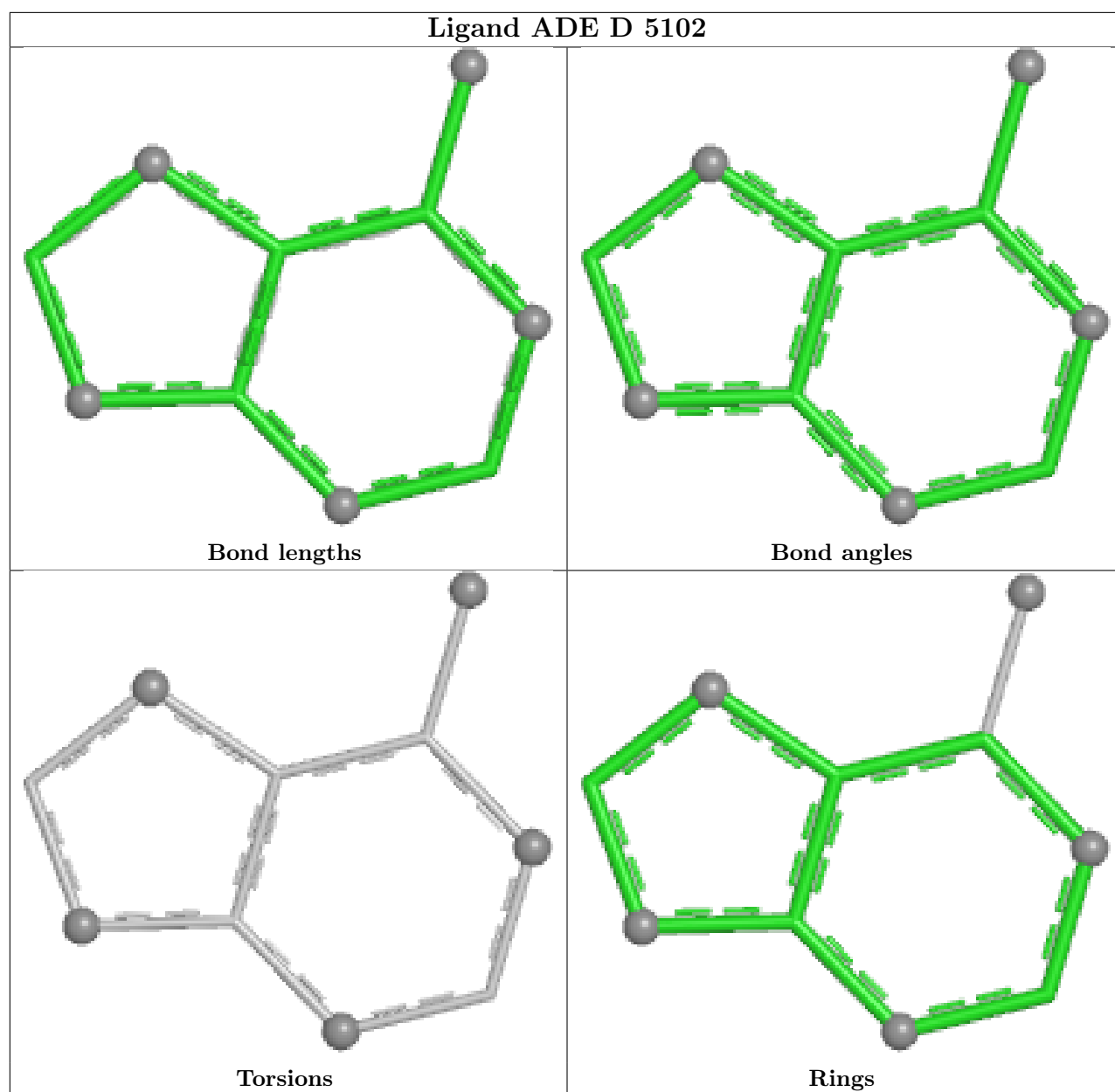
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

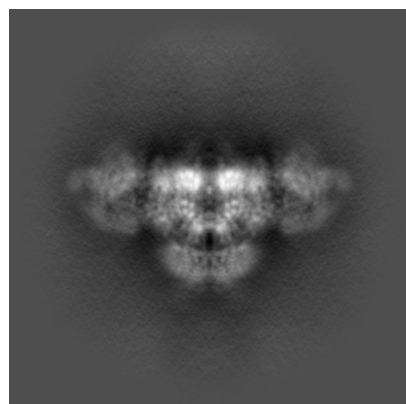
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40427. These allow visual inspection of the internal detail of the map and identification of artifacts.

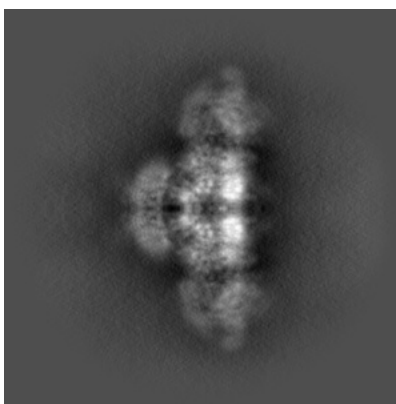
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

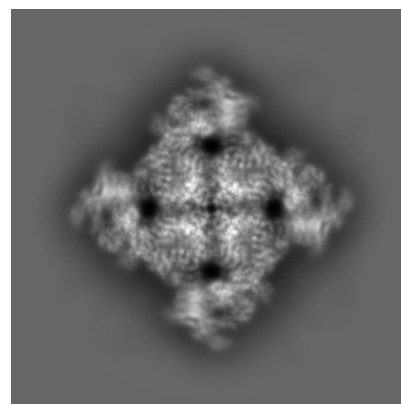
6.1.1 Primary map



X

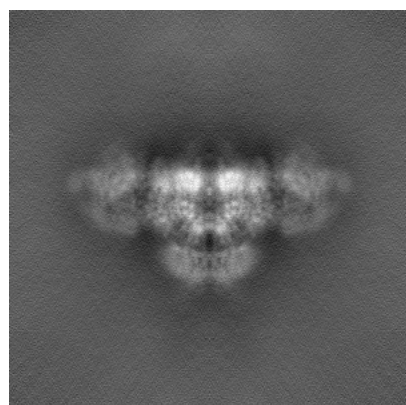


Y

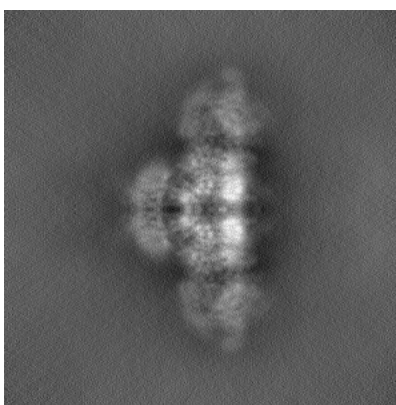


Z

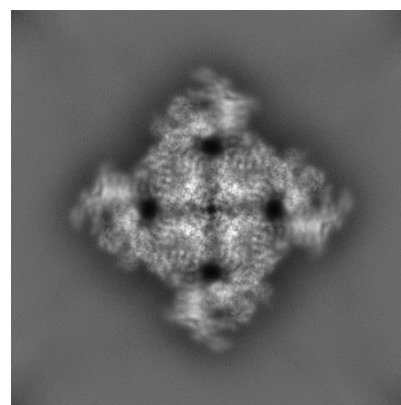
6.1.2 Raw map



X



Y

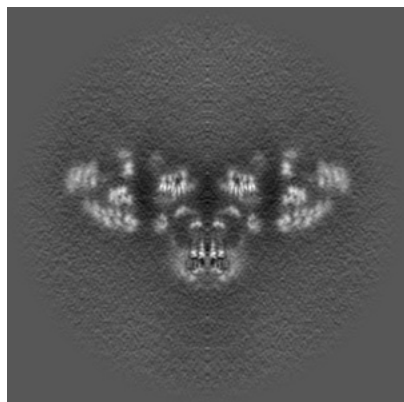


Z

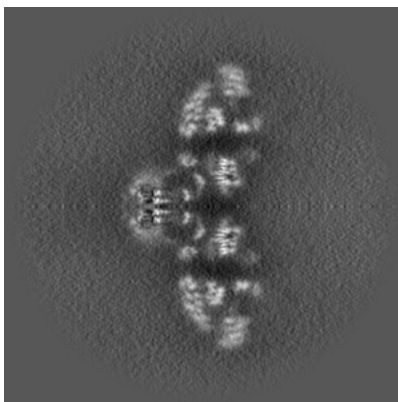
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

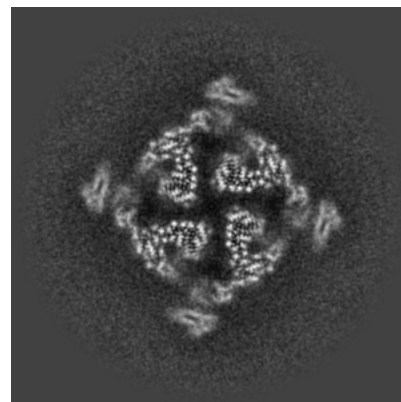
6.2.1 Primary map



X Index: 200

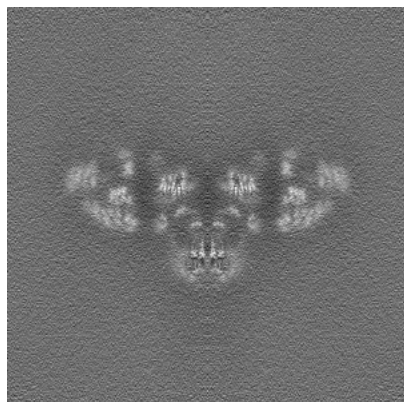


Y Index: 200

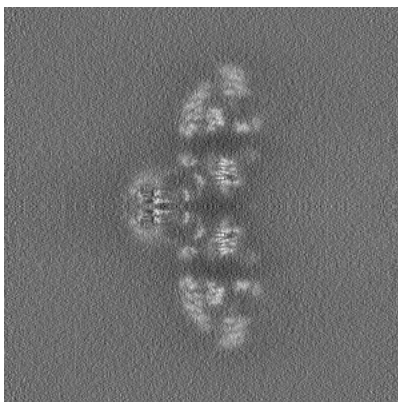


Z Index: 200

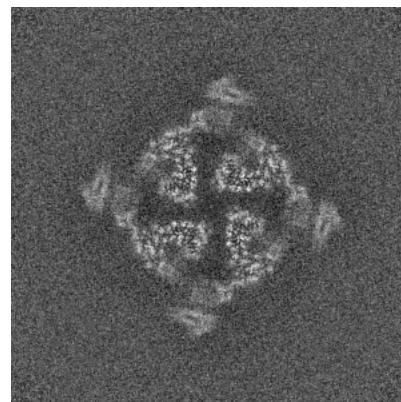
6.2.2 Raw map



X Index: 200



Y Index: 200



Z Index: 200

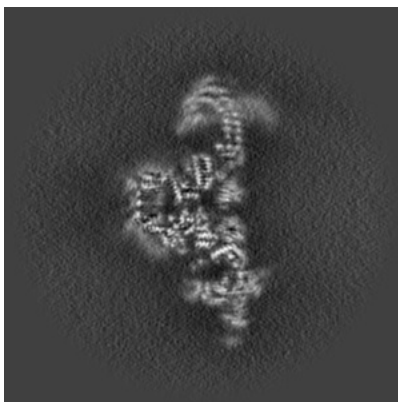
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

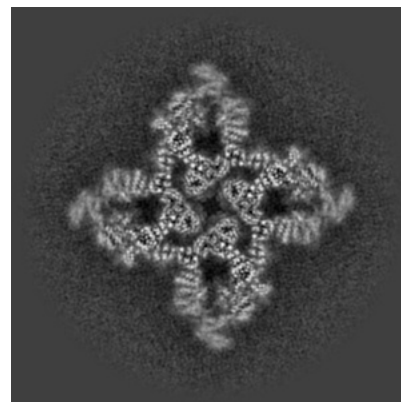
6.3.1 Primary map



X Index: 182

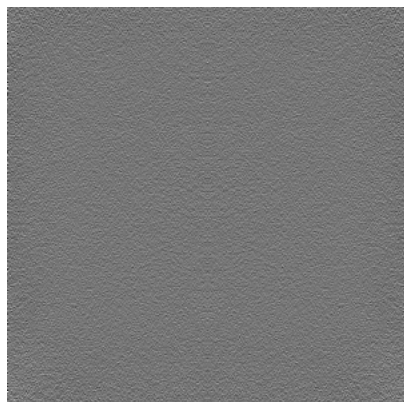


Y Index: 182

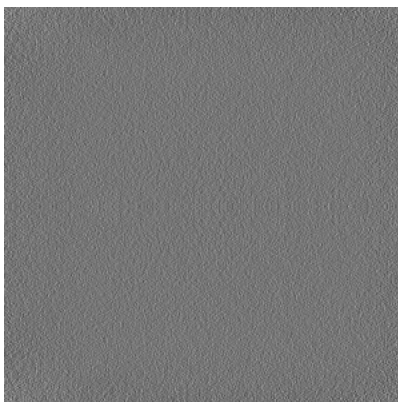


Z Index: 225

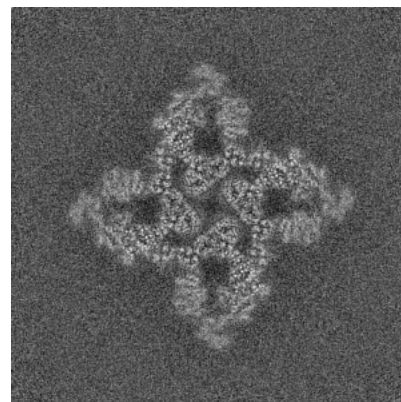
6.3.2 Raw map



X Index: 0



Y Index: 0

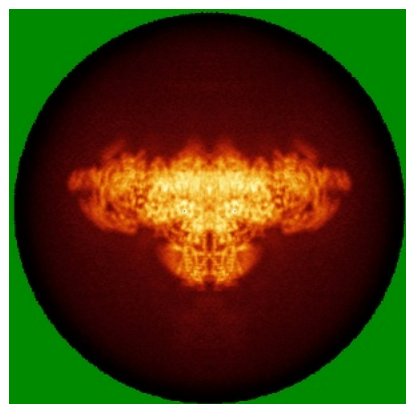


Z Index: 224

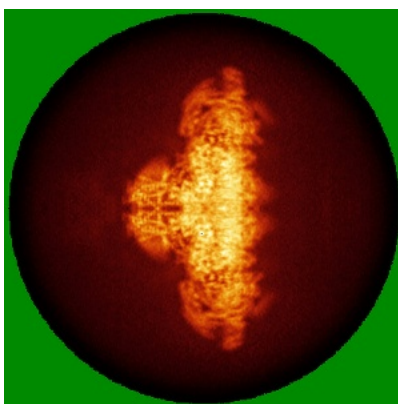
The images above show the largest variance slices of the map in three orthogonal directions.

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

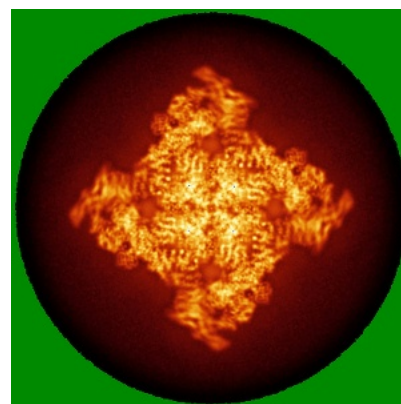
6.4.1 Primary map



X

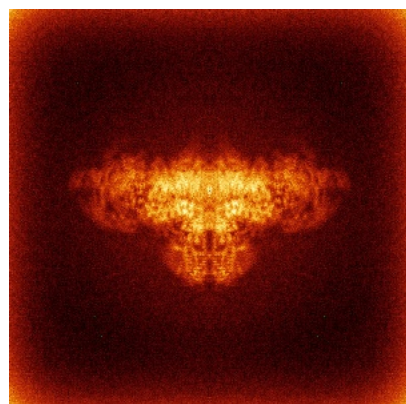


Y

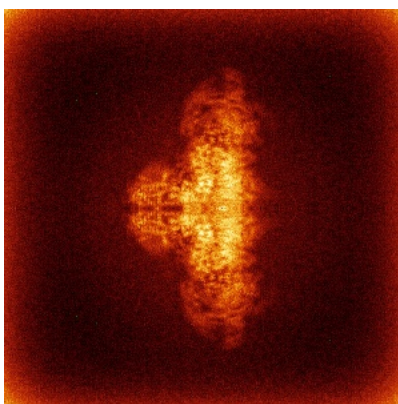


Z

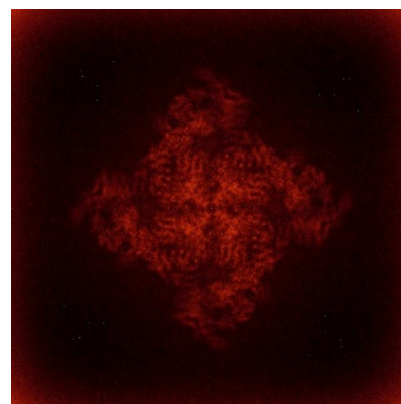
6.4.2 Raw map



X



Y

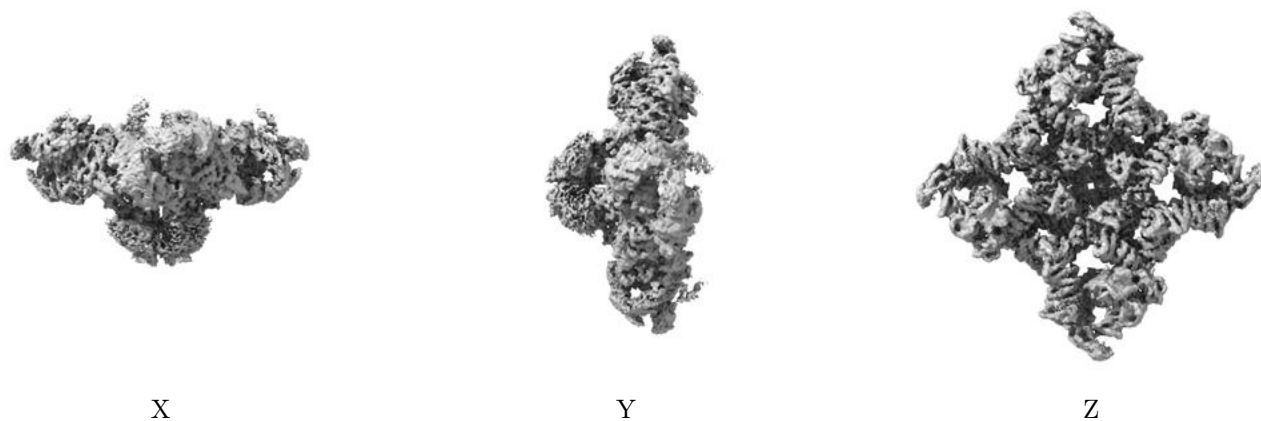


Z

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.

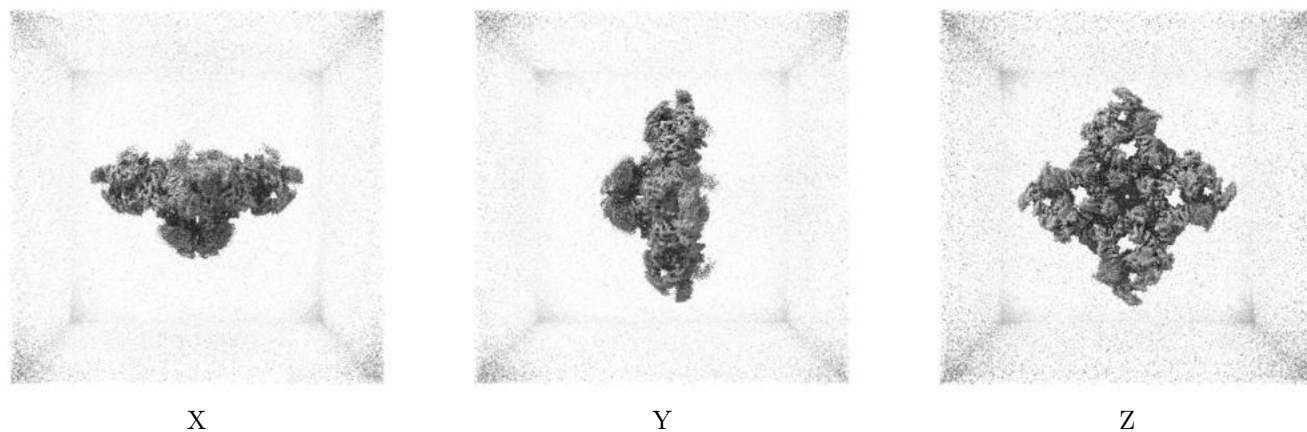
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.305. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

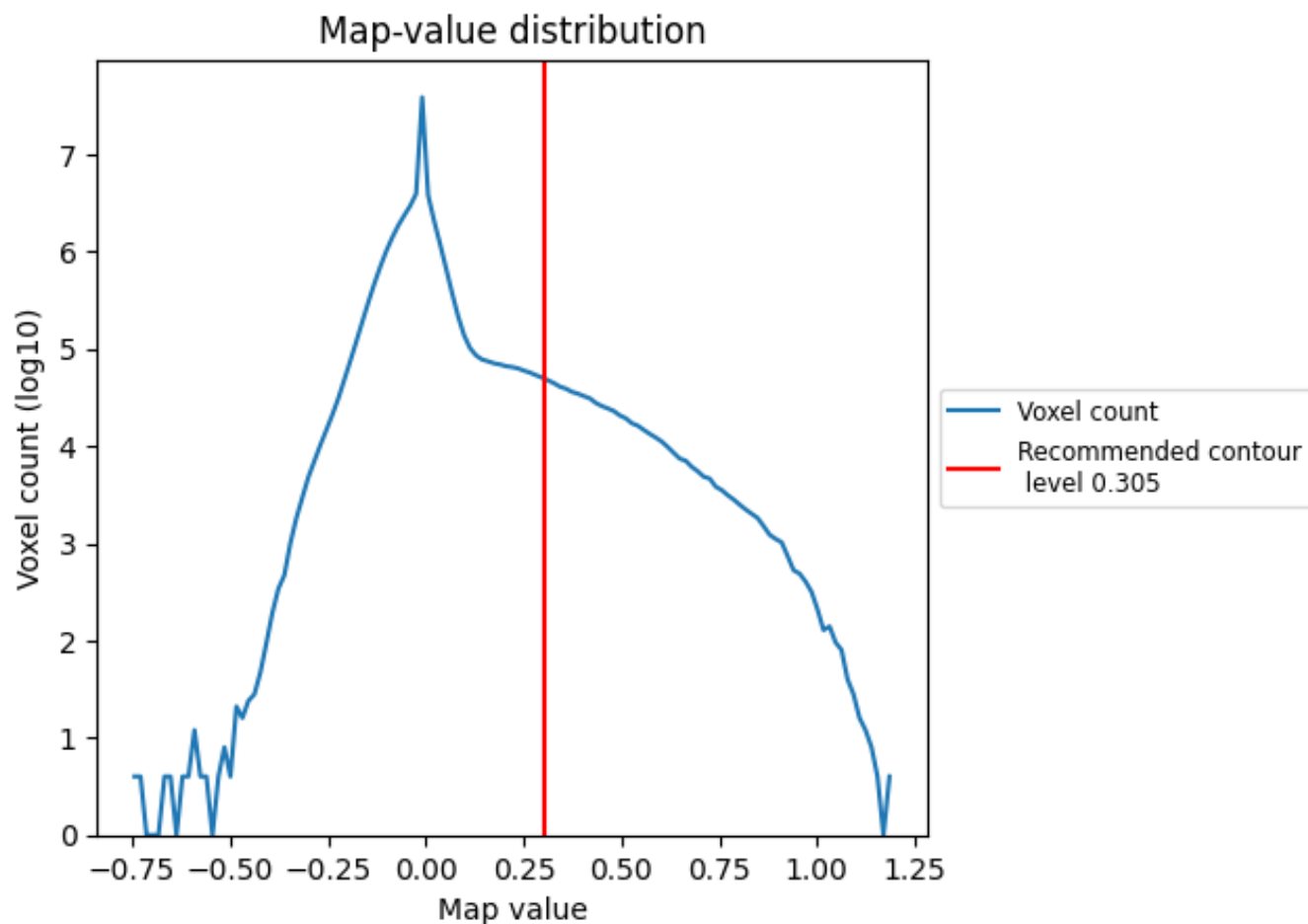
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

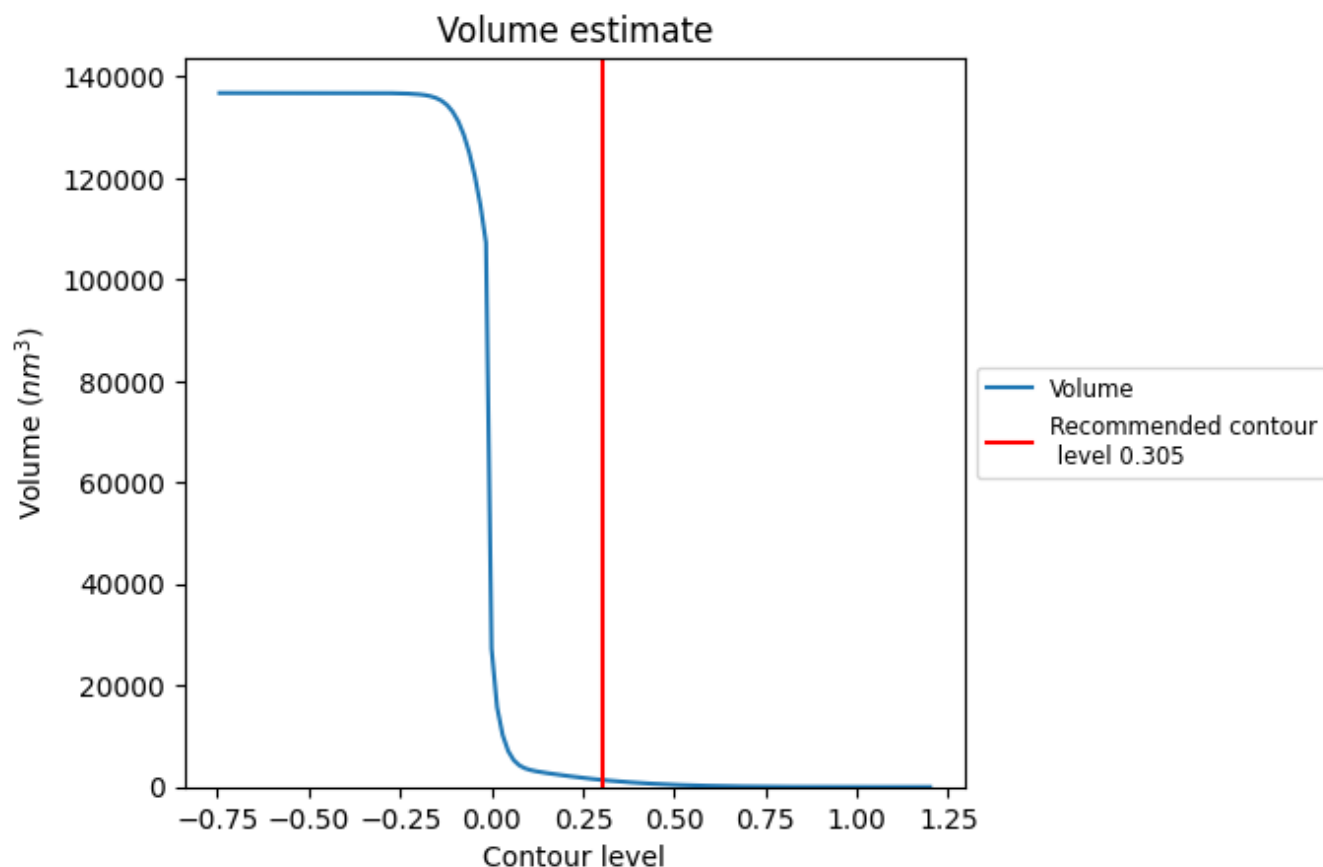
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

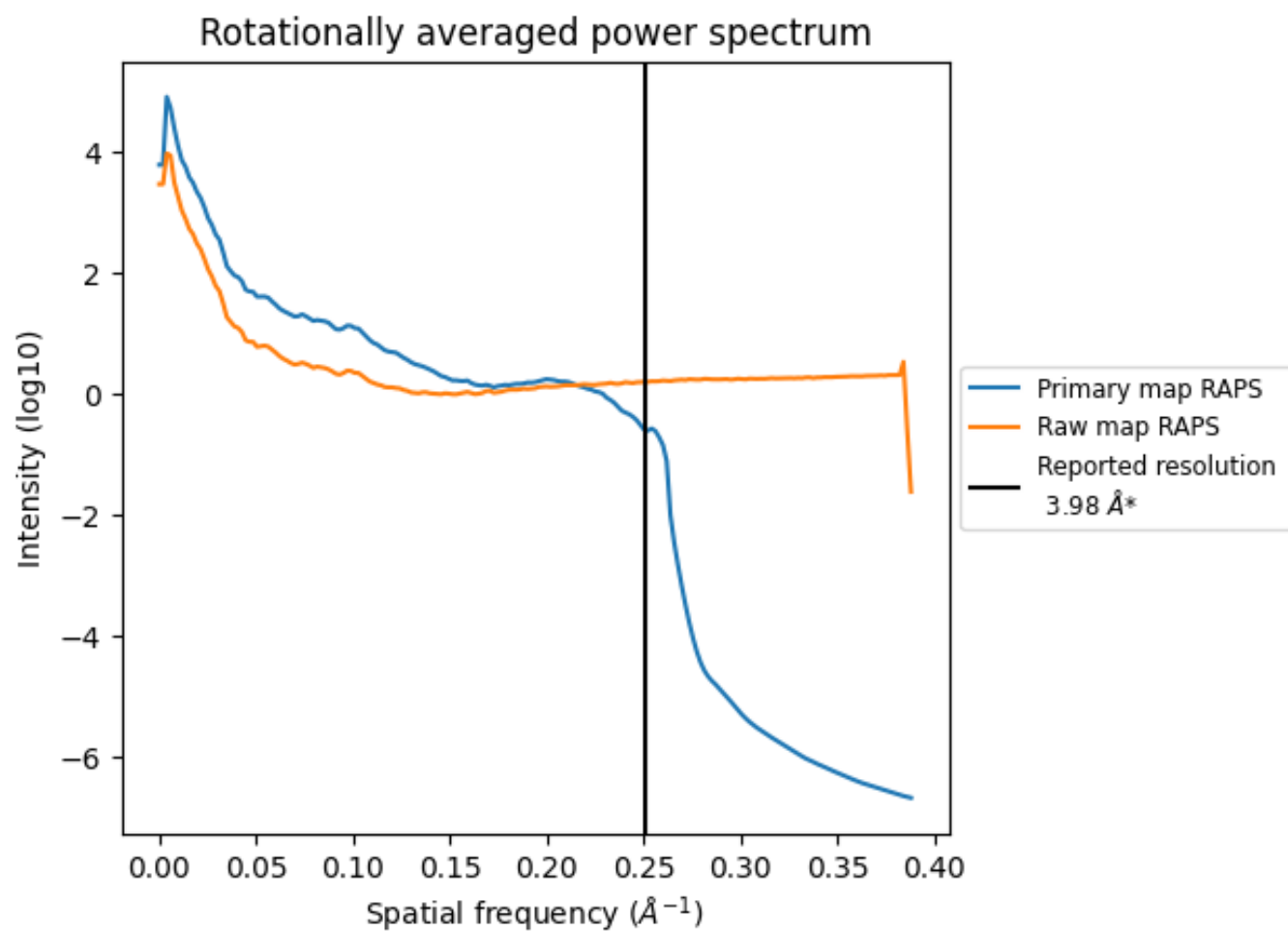
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1365 nm^3 ; this corresponds to an approximate mass of 1233 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 ⓘ

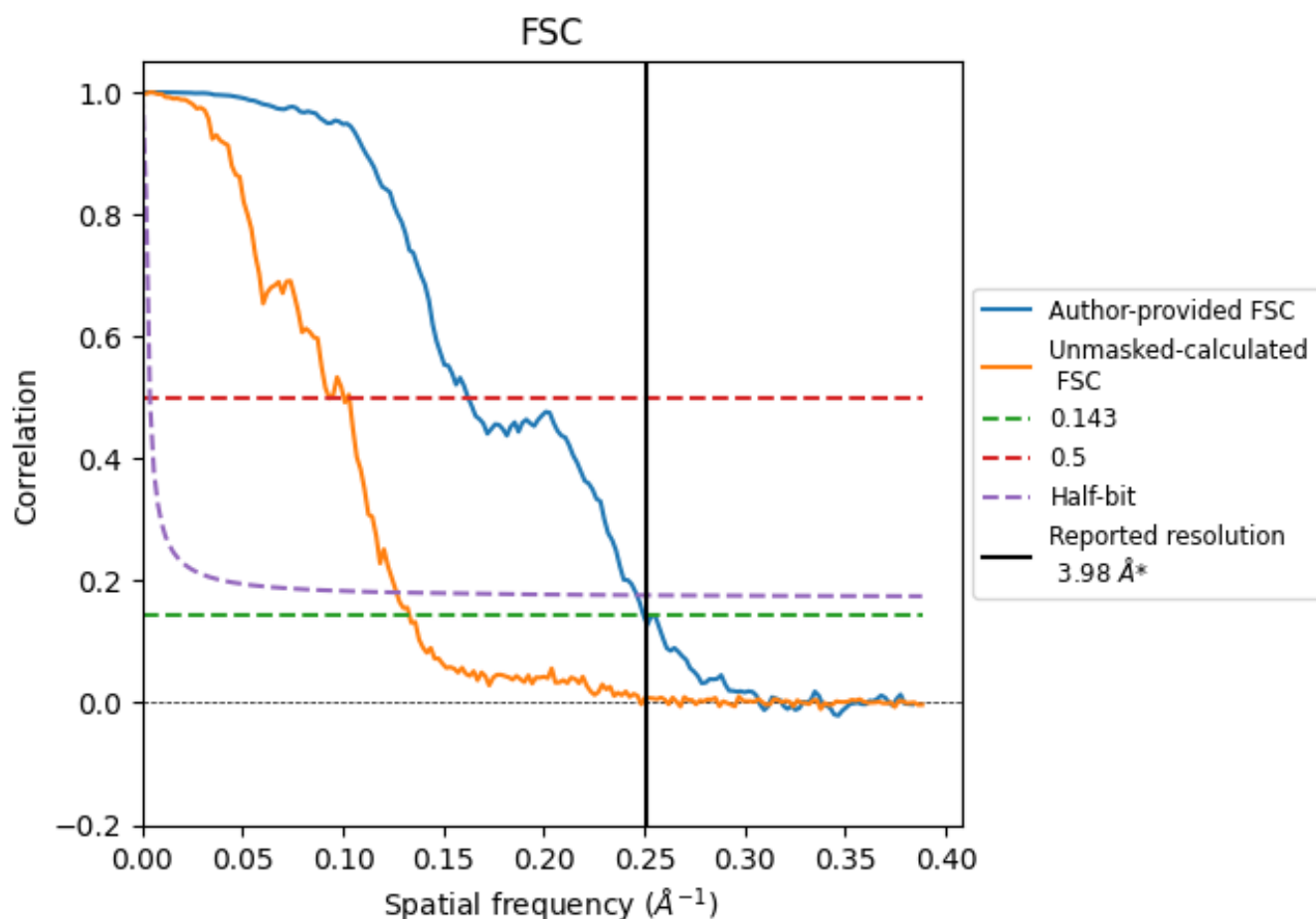


*Reported resolution corresponds to spatial frequency of 0.251 $\text{\AA}^{-1}$

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

8.2 Resolution estimates [i](#)

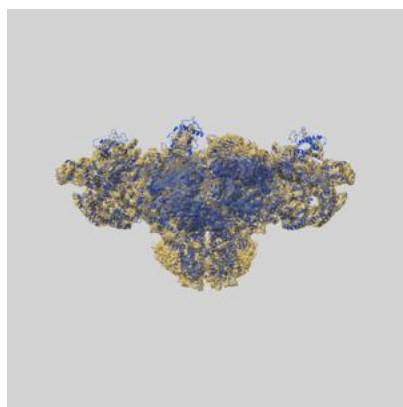
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.98	-	-
Author-provided FSC curve	4.01	6.17	4.06
Unmasked-calculated*	7.52	10.75	7.91

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.52 differs from the reported value 3.98 by more than 10 %

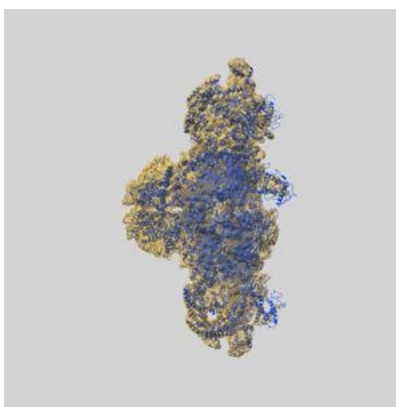
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-40427 and PDB model 8SES. Per-residue inclusion information can be found in section [3](#) on page [9](#).

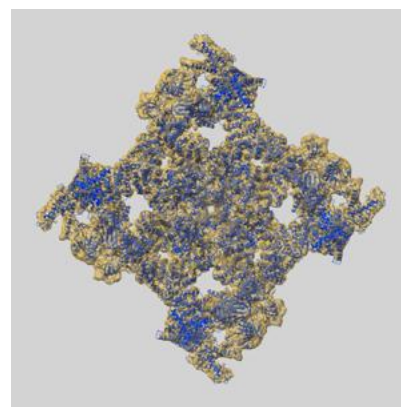
9.1 Map-model overlay [i](#)



X



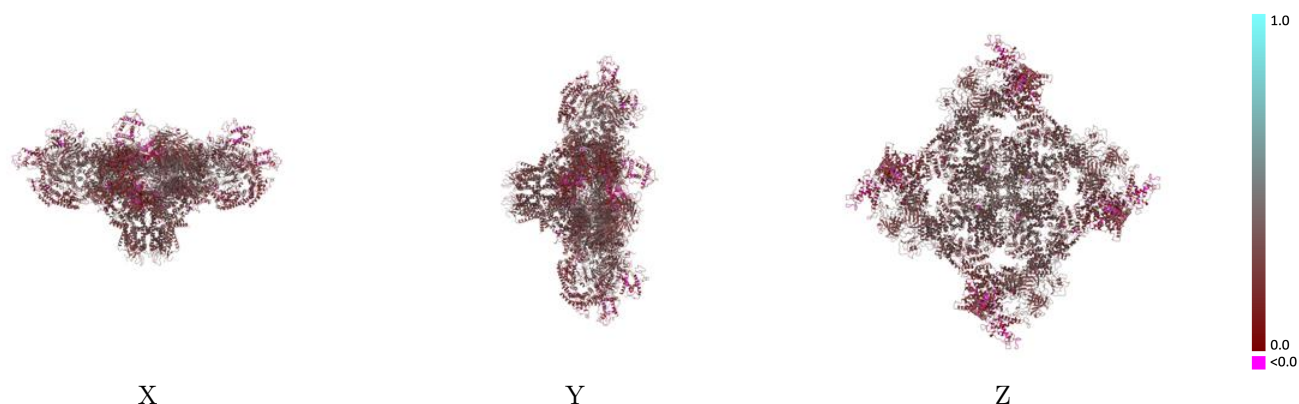
Y



Z

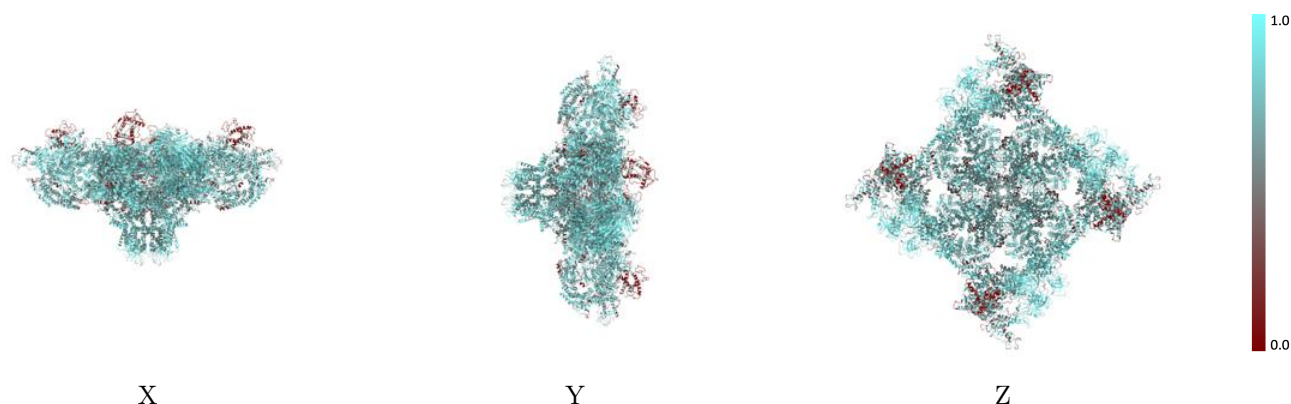
The images above show the 3D surface view of the map at the recommended contour level 0.305 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



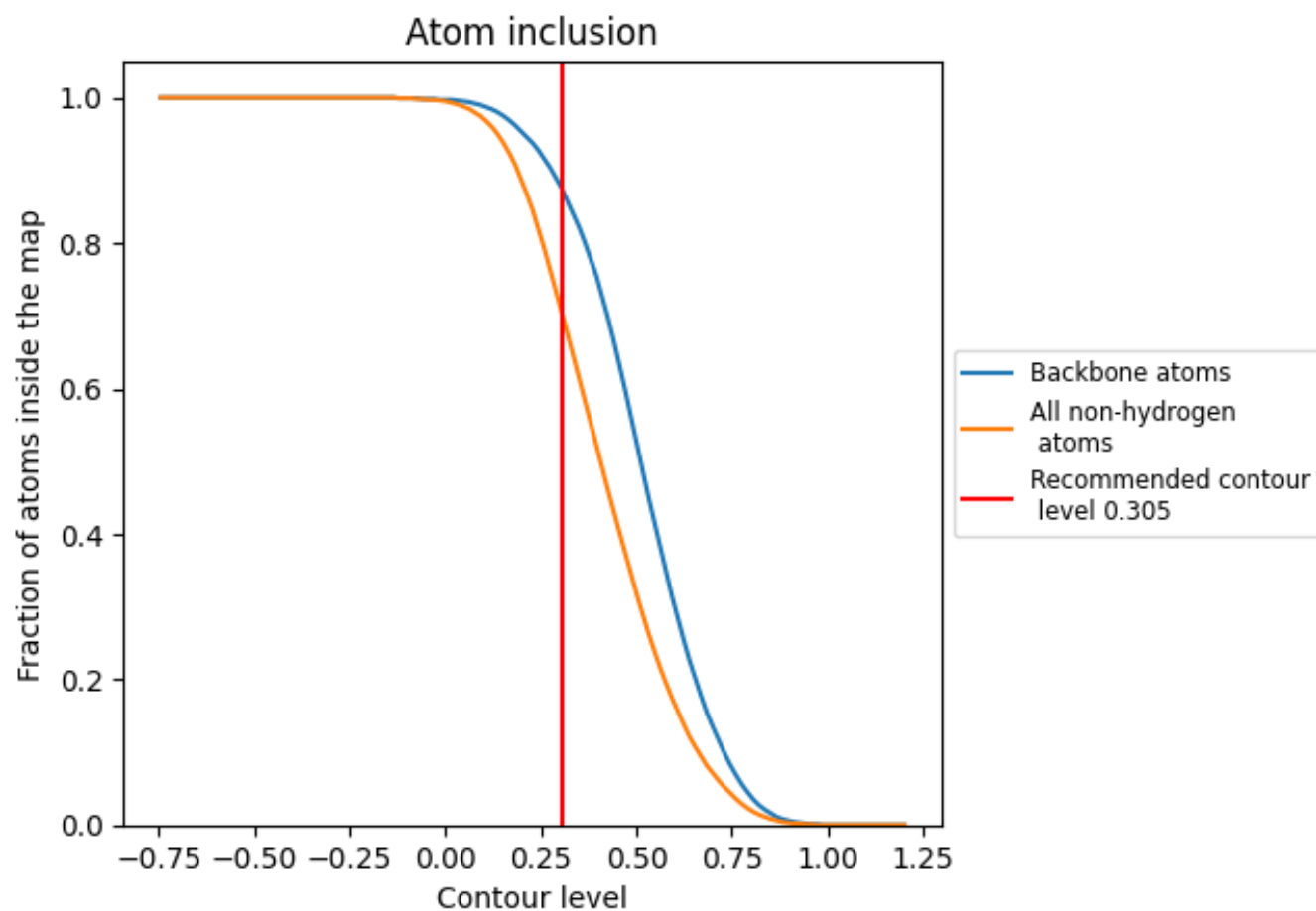
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.305).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 70% 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 (0.305) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7040	0.2840
A	0.7000	0.2820
B	0.7010	0.2820
C	0.7010	0.2820
D	0.7010	0.2830
E	0.8610	0.3440
F	0.8610	0.3430
G	0.8610	0.3420
H	0.8610	0.3450

1.0

0.0

<0.0