



wwPDB EM Validation Summary Report ⓘ

Nov 7, 2022 – 10:44 AM JST

PDB ID : 5GL1
EMDB ID : EMD-9521
Title : Structure of RyR1 in an open state
Authors : Bai, X.C.; Yan, Z.; Wu, J.P.; Yan, N.
Deposited on : 2016-07-07
Resolution : 5.70 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

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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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

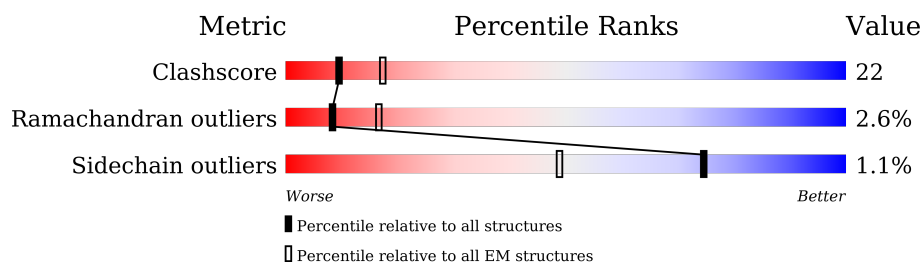
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.70 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	C	5037	
1	E	5037	
1	G	5037	
2	B	108	
2	D	108	
2	F	108	
2	H	108	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 110704 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	3645	Total	C	N	O	S	0	0
			26843	17063	4667	4956	157		
1	C	3645	Total	C	N	O	S	0	0
			26843	17063	4667	4956	157		
1	E	3645	Total	C	N	O	S	0	0
			26843	17063	4667	4956	157		
1	G	3645	Total	C	N	O	S	0	0
			26843	17063	4667	4956	157		

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	107	Total	C	N	O	S	0	0
			832	527	146	155	4		
2	D	107	Total	C	N	O	S	0	0
			832	527	146	155	4		
2	F	107	Total	C	N	O	S	0	0
			832	527	146	155	4		
2	H	107	Total	C	N	O	S	0	0
			832	527	146	155	4		

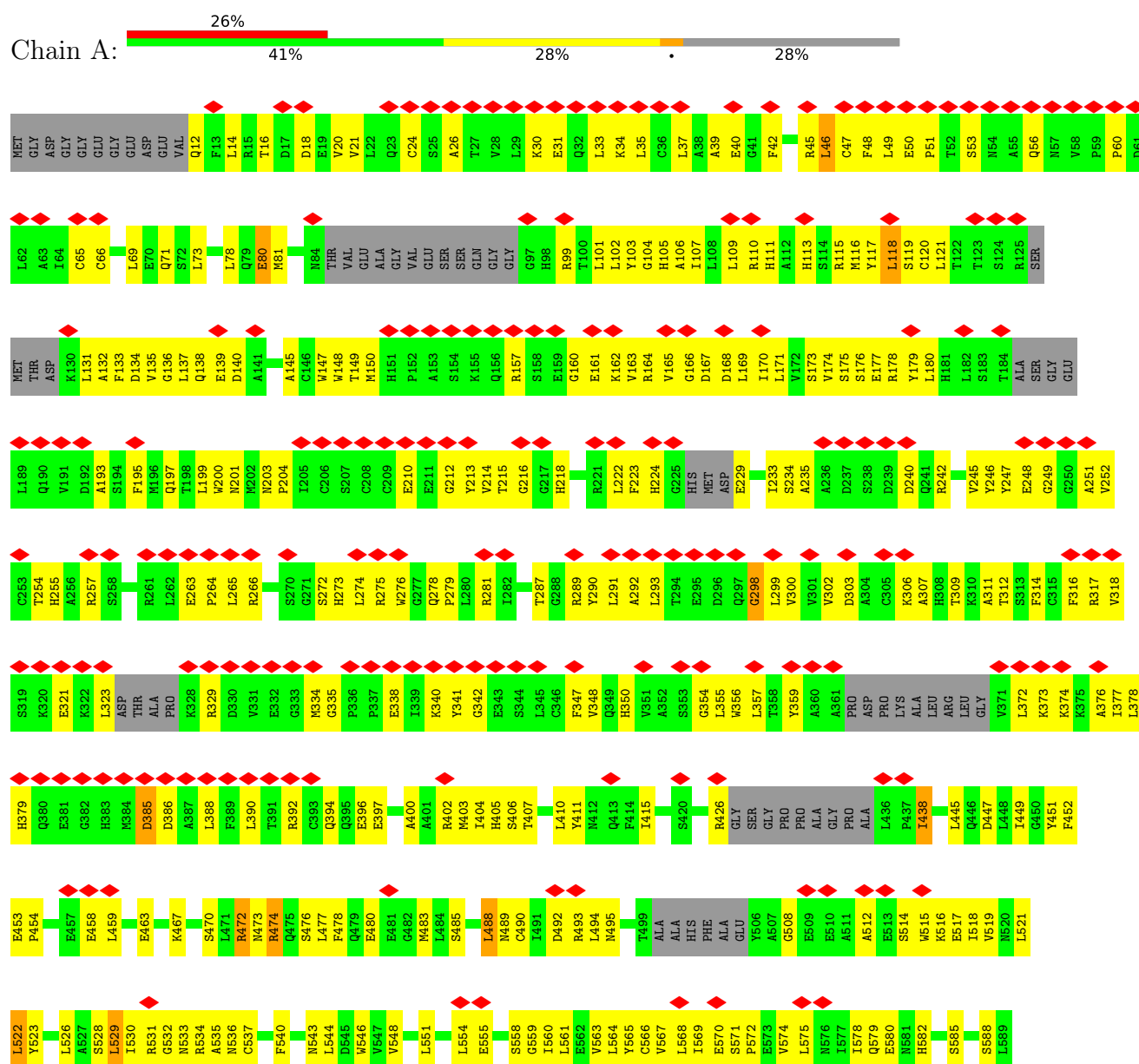
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	
3	C	1	Total	Zn	0
			1	1	
3	E	1	Total	Zn	0
			1	1	
3	G	1	Total	Zn	0
			1	1	

3 Residue-property plots

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

• Molecule 1: Ryanodine receptor 1







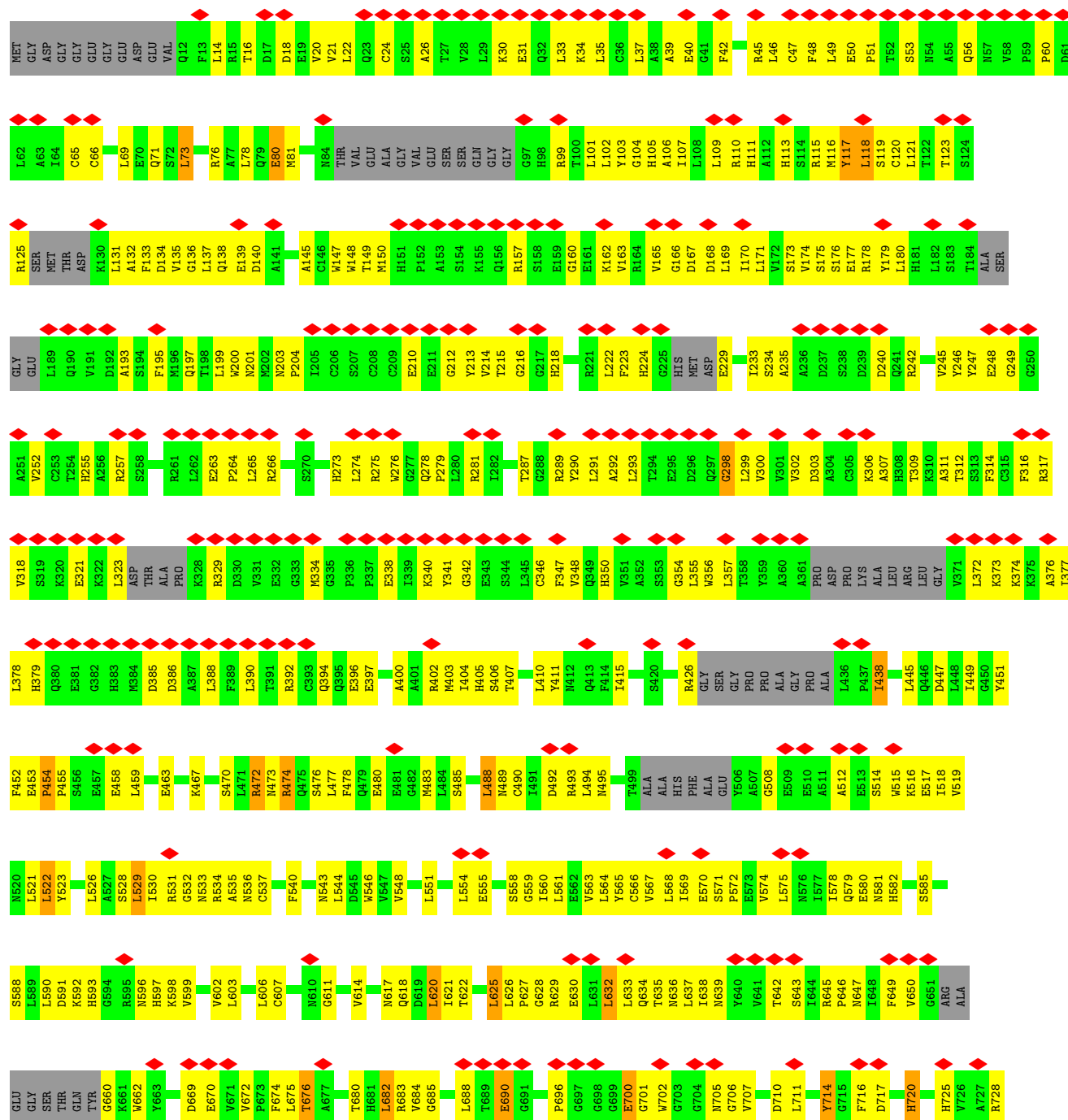








Molecule 1: Ryanodine receptor 1







LEU	GLY	T3273	L3274	P3275	M3276	C3278	Y3280	S3279	L3281	P3282	R3283	W3284	H3285	R3287	C3288	P3289																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
ARG	SER	F3095	F3096	F3097	S3098	A3099	S3100	I3103	E3104	K3105	M3106	V3107	E3108	N3109	L3110	R3111	L3112	G3113	K3114	V3115	S3116	G3118	A3184	K3185	L3186	R3187	P3188	A3195	R3196	L3197	A3198	A3199	A3200	MET	PRO	VAL	A3204	F3205	L3206	P3208	Q3209	L3210	A3215	C3216	S3217	VAL	TYR	THR	THR	THR	THR	VAL	ARG	GLU	ALA	ALA	ILE																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
H3030	A3031	S3032	N3033	K3034	E3035	K3036	E3037	M3038	I3039	THR	SER	SER	VAL	VAL	SER	SER	GLY	ARG	VAL	GLU	VAL	F3043	L3046	A3047	A3048	L3049	V3050	R3051	H3052	R3053	V3054	S3055	L3056	F3057	D3060	A3061	P3062	ALA	VAL	VAL	ASN	ASN	CYS	L3068	H3069	I3070	L3071	A3072	R3073	S3074	L3075	D3076	A3077	R3078	T3079	V3080	M3081	K3082	S3083	G3084	F3085	E3086	I3087	A3090	GLY	LEU																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
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Q3162	V3163	S3164	S3164	C3165	Y3166	R3167	T3168	L3169	C3170	S3171	T3172	Y3173	S3174	L3175	G3176	T3177	L3178	LYS	ASN	THR	TYR	V3183	E3184	K3185	L3186	R3187	P3188	A3195	R3196	L3197	A3198	A3199	A3200	MET	PRO	VAL	A3204	F3205	L3206	E3207	P3208	Q3209	L3210	A3215	C3216	S3217	VAL	TYR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	





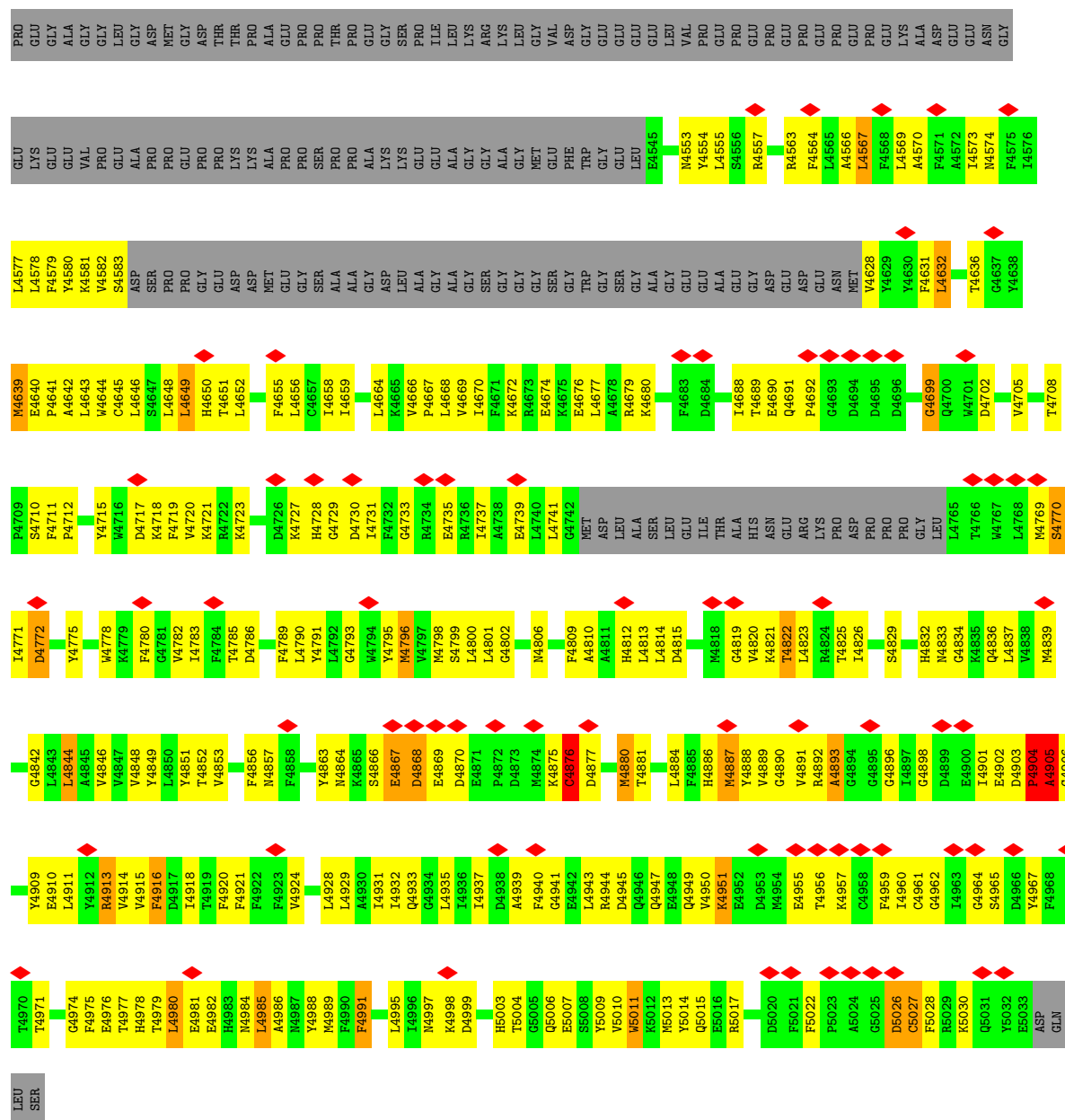
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T731	S732	F733	G734	L737	L738	A739	E741	D742	G746	G747	L748	L749	L750	S751	V752	P753	S754	I755	S756	F757	R758	G761	G762	V763	V764	V767	F768	E769	A770	F771	M772	L773	D774	G775	L776	F777	F778	P779	V780	V781	F783	S784	A785	G786	V787	K788	V789	R790	F791	L792	L793	G794						
ARG	ALA	GLU	GLY	SER	THR	GLN	TYR	G660	R661	W662	Y663	D669	E670	V671	P672	P673	P674	L675	T676	A677	L682	R683	V684	G685	L688	T689	E690	G691	P696	G697	G698	G699	E700	G701	W702	G703	G704	N705	G706	V707	D710	L711	Y714	G715	F716	D717	H720	H725	V726	A727	R728							
S588	L589	L590	D591	K592	H593	G594	R595	N596	H597	K598	V599	V602	L603	L606	C607	N610	G611	V614	N617	O618	P619	L620	T621	T622	E623	A556	S557	S558	G559	T560	L561	S562	V563	L564	Y565	C566	L568	I569	E570	S571	P572	E573	V574	L575	S576	R577	G578	Q579	N580	N581	H582	S585						
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L378	H379	Q380	E381	G382	H383	K384	D385	D386	A387	L388	F389	L390	T391	R392	C393	Q394	Q395	E396	E397	A400	A401	R402	M403	L404	H405	S406	T407	L410	Y411	N412	Q413	F414	L415	S420	R426	GLY	SER	PRD	PRD	ALA	ALA	PRD	GLY	PRD	PRD	ALA	L436	P437	T438	L445	Q446	D447	L448	T449	G450	Y451		
V518	S519	K520	E521	K522	L523	ASP	THR	ALA	PRD	K328	R329	D330	V331	E332	G333	K334	G335	P336	P337	E338	T339	K340	Y341	G342	E343	S344	L345	C346	F347	V348	Q349	H350	V351	A352	S353	G354	L355	W356	T358	Y359	A360	A361	PRD	ASP	PRD	LYS	ALA	LEU	ARG	LEU	GLY	V371	L372	K373	K374	K375	A376	I377
A251	V252	C253	T254	H255	A256	R257	S258	R261	L262	E263	P264	L265	R266	S270	H273	L274	R275	W276	G277	Q278	P279	L280	G281	R282	L282	T287	G288	R289	Y290	L291	A292	L293	T294	E295	D296	Q297	G298	L299	V300	V302	D303	A304	C305	K306	A307	H308	T309	K310	A311	T312	S313	F314	C315	F316	R317			
GLY	GLU	L189	Q190	V191	D192	A193	S194	F195	H196	Q197	T198	L199	W200	N201	H202	N203	P204	I205	C206	S207	L208	C209	E210	G212	Y213	W214	T215	G216	G217	H218	G219	R221	L222	F223	H224	G225	HIS	MET	ASP	E229	I233	S234	A235	A236	D237	A304	S238	D239	Q241	R242	V245	Y246	E248	G249	G250			
R125	SER	MET	THR	ASP	K130	L131	A132	F133	D134	G136	Q138	E139	D140	A141	A145	C146	W147	V148	T149	M150	H151	P152	A153	S154	K155	Q156	R157	S158	R159	G160	E161	K162	F163	R164	V165	G166	D167	D168	L169	I170	L171	V172	S173	V174	S175	S176	E177	R178	Y179	L180	H181	L182	S183	T184	ALA	SER		
A63	I64	C65	C66	F67	T68	L69	E70	Q71	L73	R76	A77	L78	Q79	E80	M81	N84	THR	VAL	GLU	ALA	VAL	P152	A153	S154	K155	Q156	R157	S158	R159	T100	L101	L102	Y103	G104	H105	A106	I107	L108	L109	R110	H111	H113	S114	R115	M116	Y117	L118	S119	C120	L121	T122	T123	S124					
MET	GLY	ASP	GLY	GLY	GLU	GLY	GLU	ASP	GLU	VAL	Q12	F13	L14	D17	D18	E19	V20	V21	L22	Q23	C24	S25	A26	T27	V28	L29	K30	G31	Q32	L33	K34	L35	C36	A38	A39	E40	G41	F42	R45	L46	C47	F48	L49	E50	P51	T52	S53	N54	A55	Q56	N57	V58	P59	P60	D61	L62		



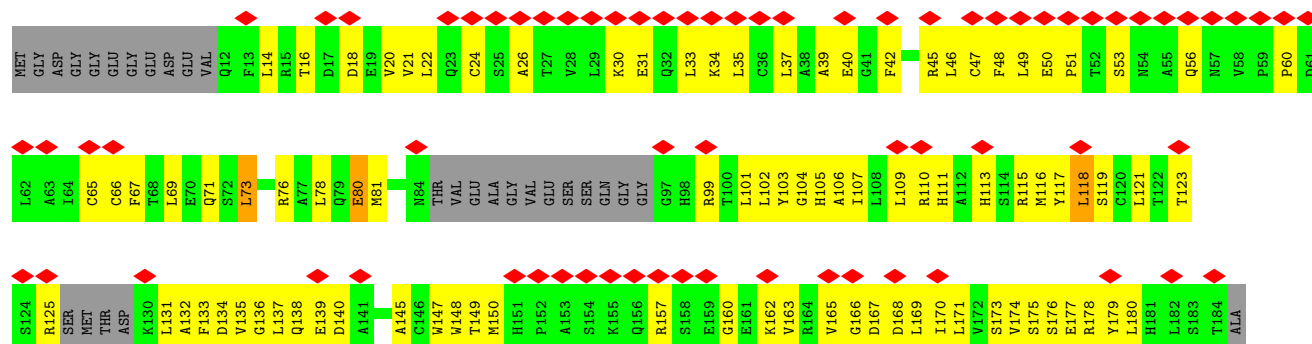








• Molecule 1: Ryanodine receptor 1



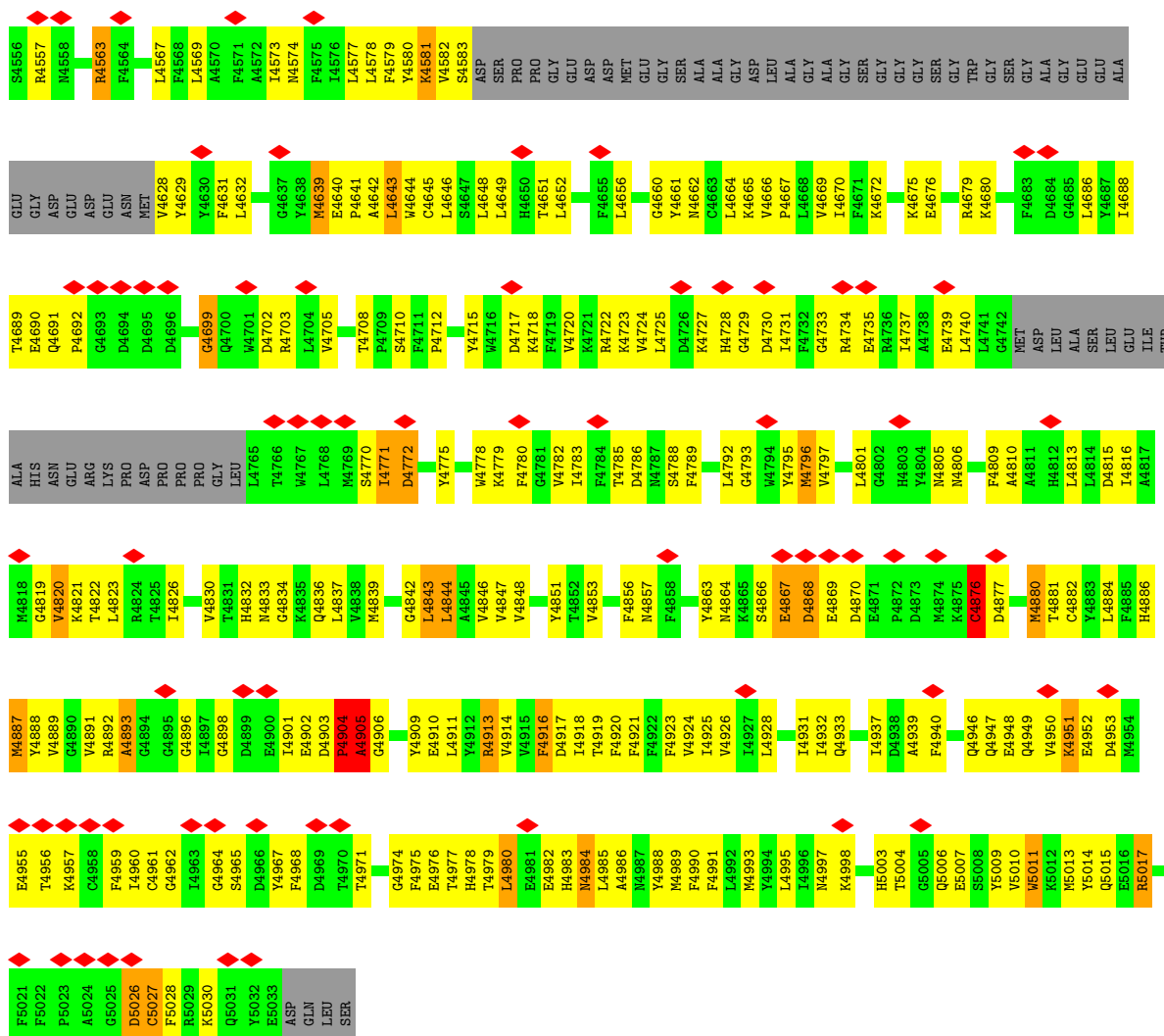




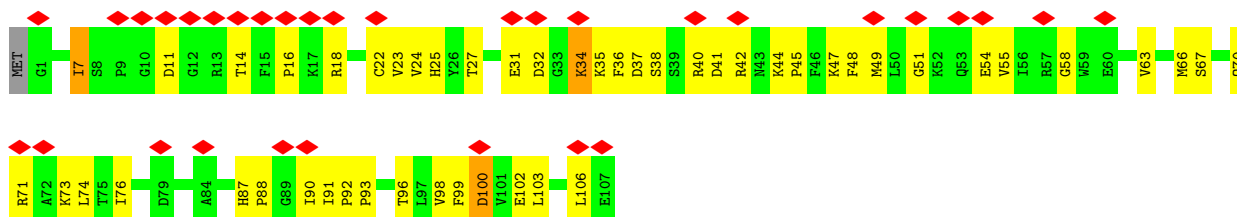
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THR	ASP	GLU	GLU	V3549	R3550	F3551	R3552	L3553	R3554	R3555	N3556	L3557	H3558	L3559	Q3560	G3561	D3501	K3562	V3503	S3504	VAL	GLN	THR	SER	LEU	ILE	VAL	ALA	T3513	L3514	K3515	K3516	G3517	L3518	P3519	I3520	G3521	L3522	N3523	M3524	C3525	A3526	P3527	THR	ASP	GLN	ASP	LEU	LEU	ILE	VAL	ARG	ARG	VAL	GLN	ASP	VAL	GLU	THR	ALA	VAL	THR	HIS
D3483	A3484	Q3485	Q3486	G3487	G3488	S3489	G3490	Q3491	GLU	ARG	T3494	K3495	K3496	K3497	D3501	R3562	Y3503	S3504	VAL	GLN	THR	S3568	L3569	R3570	W3571	Q3572	T3513	L3514	K3515	K3516	G3517	L3518	P3519	I3520	G3521	L3522	N3523	M3524	C3525	A3526	P3527	THR	ASP	GLN	ASP	LEU	LEU	ILE	VAL	ARG	ARG	VAL	GLN	ASP	VAL	GLU	THR	ALA	VAL	THR	HIS		
P3410	L3411	L3412	L3413	R3414	Y3415	V3416	D3417	N3418	N3419	R3420	A3421	H3422	W3423	L3424	THR	GLU	P3427	N3428	A3429	N3430	A3431	E3432	E3433	L3434	F3435	ARG	M3437	V3438	R3439	E3440	T3441	F3442	W3445	S3446	K3447	S3448	H3449	N3450	E3455	N3457	S3468	F3469	L3470	THR	ALA	ASP	SER	SER	LYS	LYS	N3478	A3479	K3480	A3481	G3482								
S3347	R3348	A3349	R3350	P3351	E3352	L3353	L3354	H3355	S3356	H3357	F3358	I3359	P3360	T3361	I3362	G3363	ARG	ARG	K3367	R3368	A3369	G3370	K3371	V3372	V3373	A3374	E3375	E3376	E3377	Q3378	L3379	R3380	L3381	E3382	A3383	A3387	E3388	E3389	G3390	E3391	V3394	R3395	D3396	E3397	PHE	SER	VAL	LEU	VAL	C3402	R3403	D3404	L3405	Y3406	A3407	L3408	Y3409						
W3284	W3285	E3286	R3287	G3288	E3290	ALA	PRO	PRO	P3294	A3295	L3296	P3297	A3298	G3299	P3301	P3302	Y3303	C3304	T3305	A3306	V3307	T3308	S3309	D3310	H3311	L3312	N3313	SER	GLY	ALA	G3317	N3318	I3319	L3320	R3321	I3322	T3323	V3324	N3325	N3326	L3327	E3331	A3332	T3333	W3334	R3337	L3338	A3339	VAL	PHE	ALA	GLN	PRO	PRO	ILE	V3346							
PRO	ARG	GLU	ARG	ALA	ILE	LEU	GLY	LEU	PRO	ASN	SER	VAL	GLU	GLU	MET	CYS	ASP	ILE	PRO	VAL	VAL	ASP	ARG	GLY	GLY	LEU	ALA	GLU	SER	GLY	ALA	GLY	THR	GLY	VAL	GLN	ASN	THR	THR	T3273	L3274	P3275	M3276	L3277	E3207	Q3208	Q3209	L3210	A3215	C3216	S3217	VAL	TYR	THR	THR	LYS	SER						
L3158	D3159	D3160	V3161	Q3162	V3163	S3164	C3165	Y3166	R3167	T3168	L3169	C3170	S3171	I3172	Y3173	L3175	G3176	T3177	L3178	LYS	ASN	THR	TYR	V3183	E3184	K3185	L3186	R3187	P3188	A3189	L3190	L3194	A3195	A3198	A3199	A3200	PRO	VAL	A3204	F3205	L3206	E3207	P3208	Q3209	L3210	A3215	C3216	S3217	VAL	TYR	THR	THR	LYS	SER									
E3086	I3087	A3090	GLY	LEU	ARG	SER	F3095	F3096	E3097	S3098	A3099	T3103	E3104	K3105	M3106	V3107	E3108	N3109	L3110	R3111	L3112	G3113	K3114	V3115	S3116	ALA	ARG	THR	GLN	VAL	GLY	VAL	VAL	GLY	GLN	ASN	THR	THR	T3132	T3133	L3137	L3140	H3146	T3147	Q3151	F3152	GLY	ASP	ASP	VAL	ILE												
V3024	L3025	G3026	S3027	G3028	G3029	H3030	A3031	S3032	N3033	K3034	E3035	K3036	E3037	M3038	I3039	THR	SER	VAL	GLY	GLU	LYS	SER	PRO	HIS	GLN	GLU	ILE	L3046	A3047	A3048	L3049	V3050	R3051	H3052	R3053	V3054	S3055	L3056	F3057	G3058	T3059	D3060	A3061	P3062	ALA	VAL	VAL	ASN	CYS	L3068	H3069	I3070	L3071	A3072	R3073	L3075	A3077	R3078	T3079	V3080	S3083	G3084	P3085
L2904	L2905	V2906	P2907	Y2908	D2909	T2910	L2911	T2912	T2913	K2914	E2915	L2916	A2917	R2918	D2919	E2920	R2921	K2922	A2923	Q2924	E2925	L2926	L2927	R2928	P2929	L2930	Q2931	A2932	M2933	L2934	Y2935	E2936	V2937	T2938	R2939	E2940	LEU	LYS	ASP	MET	GLU	LEU	ASP	THR	SER	SER	ILE	GLU	LYS	ARG	PHE	ALA	PHE	GLY	PHE	A2895	A2896	L2897	G2898	G2899	T2901	H2902	P2903
E2784	L2785	K2786	T2787	H2788	P2789	R2790	L2791	R2792	R2793	Y2794	K2795	T2796	T2797	S2798	E2799	K2800	D2801	K2802	E2803	I2804	Y2805	R2806	W2807	P2808	E2809	L2810	E2811	S2812	L2813	K2814	A2815	L2816	T2817	A2818	W2819	E2820	W2821	T2822	I2823	K2825	A2826	R2827	E2828	G2829	E2830	GLU	GLU	ARG	THR	GLU	LYS	LYS	THR	ARG	LYS	ILE	SER						

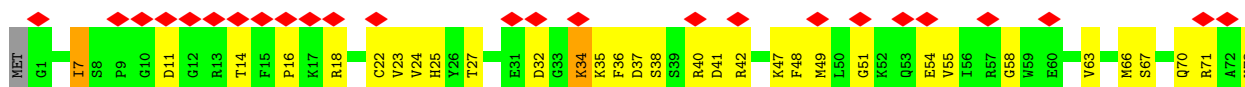


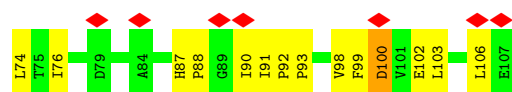


• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

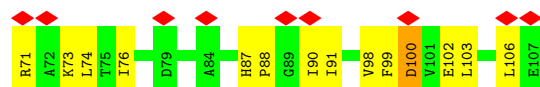
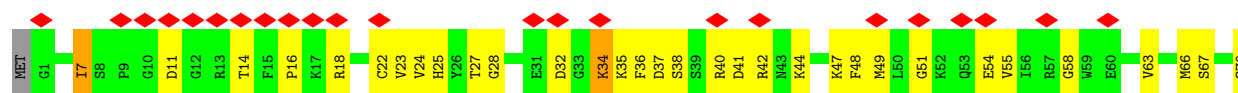


• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

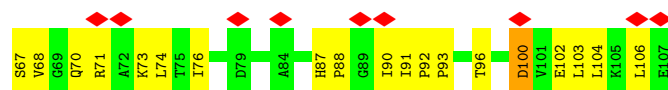
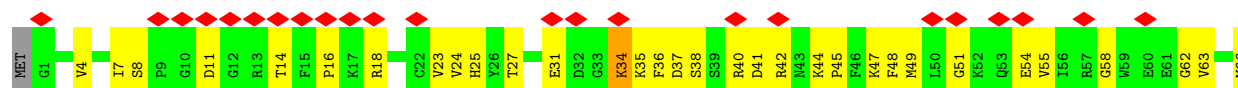




- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	30000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.243	Depositor
Minimum map value	-0.085	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.075	Depositor
Map size (Å)	482.40002, 482.40002, 482.40002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	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

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	1.21	41/27312 (0.2%)	1.12	151/37004 (0.4%)
1	C	1.20	39/27312 (0.1%)	1.12	154/37004 (0.4%)
1	E	1.21	35/27312 (0.1%)	1.12	158/37004 (0.4%)
1	G	1.21	38/27312 (0.1%)	1.11	145/37004 (0.4%)
2	B	0.91	1/851 (0.1%)	0.93	2/1146 (0.2%)
2	D	0.91	1/851 (0.1%)	0.92	2/1146 (0.2%)
2	F	0.91	1/851 (0.1%)	0.92	2/1146 (0.2%)
2	H	0.93	1/851 (0.1%)	0.90	0/1146
All	All	1.20	157/112652 (0.1%)	1.11	614/152600 (0.4%)

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	36
1	C	0	35
1	E	0	36
1	G	0	34
All	All	0	141

The worst 5 of 157 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	80	GLU	CG-CD	11.12	1.68	1.51
1	G	3661	TRP	CB-CG	10.06	1.68	1.50
1	A	3661	TRP	CB-CG	9.81	1.68	1.50
1	G	1976	ARG	NE-CZ	9.78	1.45	1.33
1	A	741	GLU	CG-CD	9.74	1.66	1.51

The worst 5 of 614 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	80	GLU	OE1-CD-OE2	-10.92	110.20	123.30
1	A	1212	ARG	NE-CZ-NH1	10.39	125.49	120.30
1	G	4796	MET	CG-SD-CE	10.33	116.73	100.20
1	G	1976	ARG	CD-NE-CZ	10.23	137.93	123.60
1	C	1212	ARG	NE-CZ-NH1	10.17	125.39	120.30

There are no chirality outliers.

5 of 141 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	31	GLU	Peptide,Mainchain
1	A	329	ARG	Peptide,Mainchain
1	A	734	GLY	Peptide
1	A	841	GLY	Peptide,Mainchain
1	A	894	GLY	Mainchain

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	26843	0	24428	1190	0
1	C	26843	0	24428	1200	0
1	E	26843	0	24428	1194	0
1	G	26843	0	24427	1209	0
2	B	832	0	831	58	0
2	D	832	0	831	54	0
2	F	832	0	831	58	0
2	H	832	0	831	58	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
All	All	110704	0	101035	4733	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 22.

The worst 5 of 4733 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:4880:MET:HA	1:G:4578:LEU:HD11	1.26	1.17
1:A:4578:LEU:HD11	1:C:4880:MET:HA	1.18	1.17
1:E:4578:LEU:HD11	1:G:4880:MET:HA	1.25	1.16
1:C:4578:LEU:HD11	1:E:4880:MET:HA	1.17	1.10
1:A:4822:THR:HG22	1:C:4839:MET:SD	1.93	1.08

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	3483/5037 (69%)	3132 (90%)	258 (7%)	93 (3%)	5	31
1	C	3483/5037 (69%)	3133 (90%)	254 (7%)	96 (3%)	5	30
1	E	3483/5037 (69%)	3134 (90%)	255 (7%)	94 (3%)	5	31
1	G	3483/5037 (69%)	3137 (90%)	252 (7%)	94 (3%)	5	31
2	B	105/108 (97%)	95 (90%)	9 (9%)	1 (1%)	15	54
2	D	105/108 (97%)	95 (90%)	9 (9%)	1 (1%)	15	54
2	F	105/108 (97%)	96 (91%)	8 (8%)	1 (1%)	15	54
2	H	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
All	All	14352/20580 (70%)	12919 (90%)	1053 (7%)	380 (3%)	8	31

5 of 380 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	806	PRO
1	A	900	ASN
1	A	914	PRO

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Mol	Chain	Res	Type
1	A	916	PRO
1	A	971	ASP

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	2502/4276 (58%)	2472 (99%)	30 (1%)	71	83
1	C	2504/4276 (59%)	2476 (99%)	28 (1%)	73	84
1	E	2501/4276 (58%)	2472 (99%)	29 (1%)	71	83
1	G	2501/4276 (58%)	2474 (99%)	27 (1%)	73	84
2	B	89/90 (99%)	88 (99%)	1 (1%)	73	84
2	D	89/90 (99%)	88 (99%)	1 (1%)	73	84
2	F	89/90 (99%)	88 (99%)	1 (1%)	73	84
2	H	89/90 (99%)	88 (99%)	1 (1%)	73	84
All	All	10364/17464 (59%)	10246 (99%)	118 (1%)	74	84

5 of 118 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	4207	MET
1	G	2555	CYS
1	E	1211	LEU
1	G	2518	LEU
1	G	978	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 155 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	4947	GLN
1	G	3809	ASN
1	G	224	HIS

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Mol	Chain	Res	Type
1	G	1130	GLN
1	G	4728	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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.

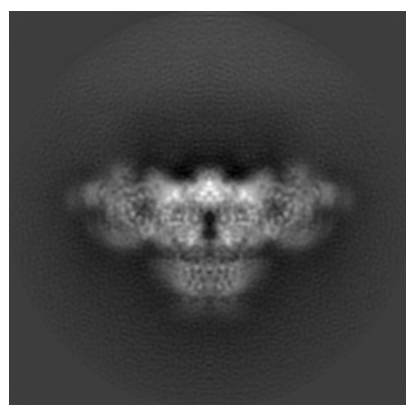
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9521. These allow visual inspection of the internal detail of the map and identification of artifacts.

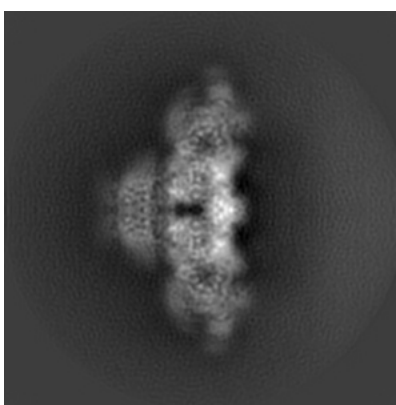
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

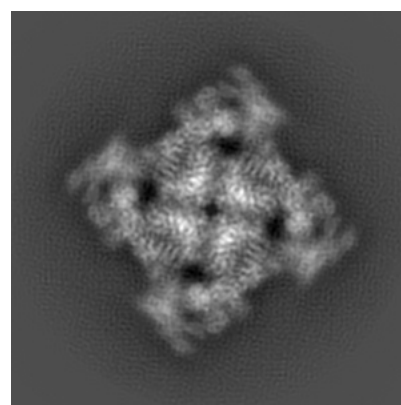
6.1.1 Primary map



X



Y

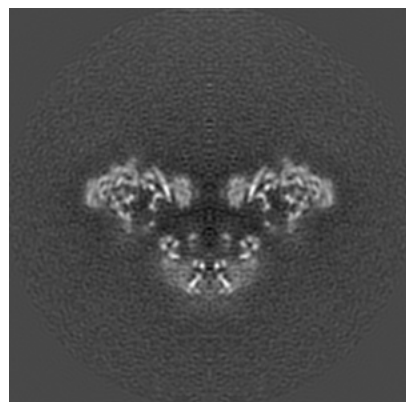


Z

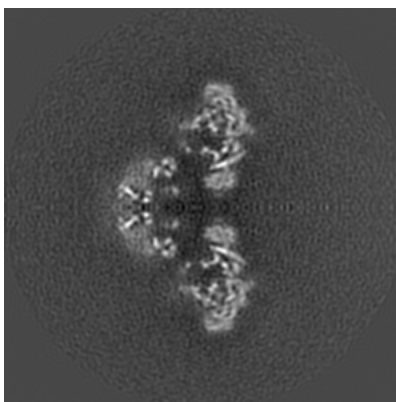
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

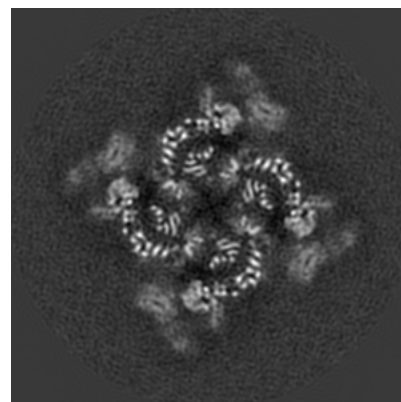
6.2.1 Primary map



X Index: 180



Y Index: 180

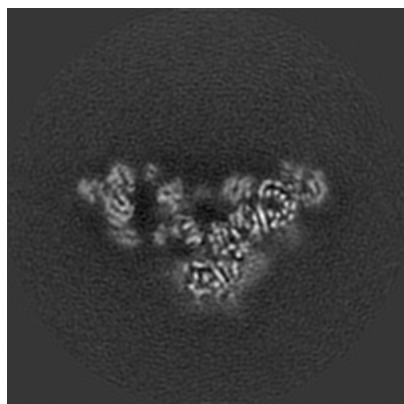


Z Index: 180

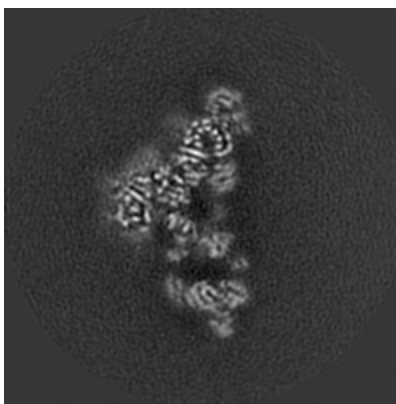
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

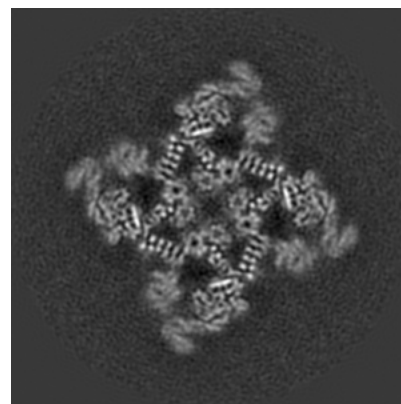
6.3.1 Primary map



X Index: 169



Y Index: 191



Z Index: 190

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

6.4 Orthogonal surface views [i](#)

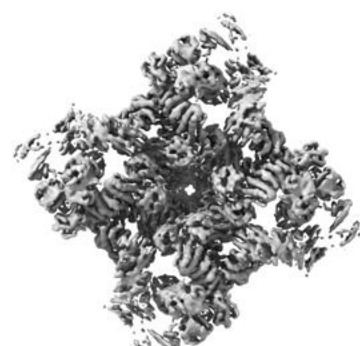
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.075. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

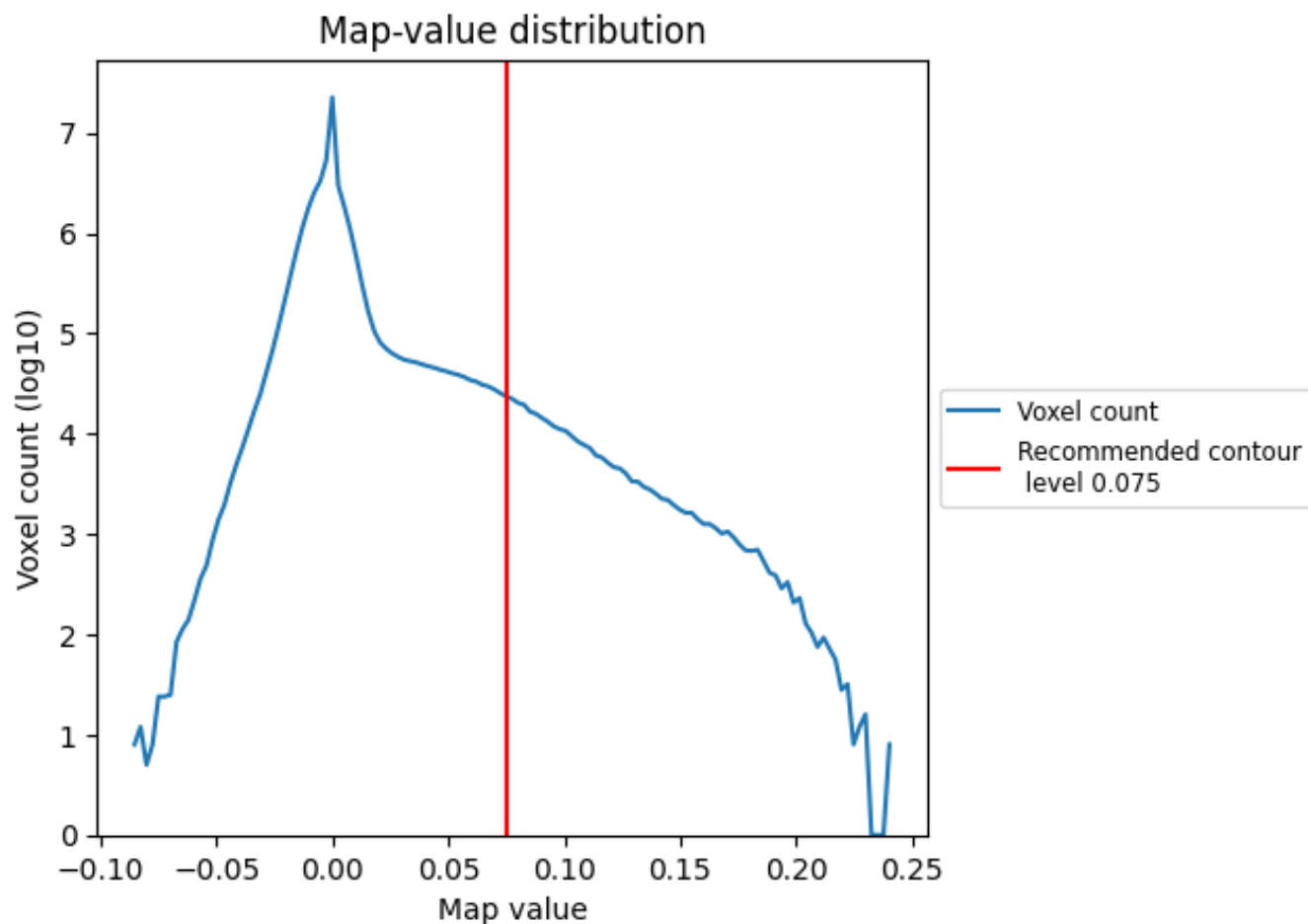
6.5 Mask visualisation

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

7 Map analysis [i](#)

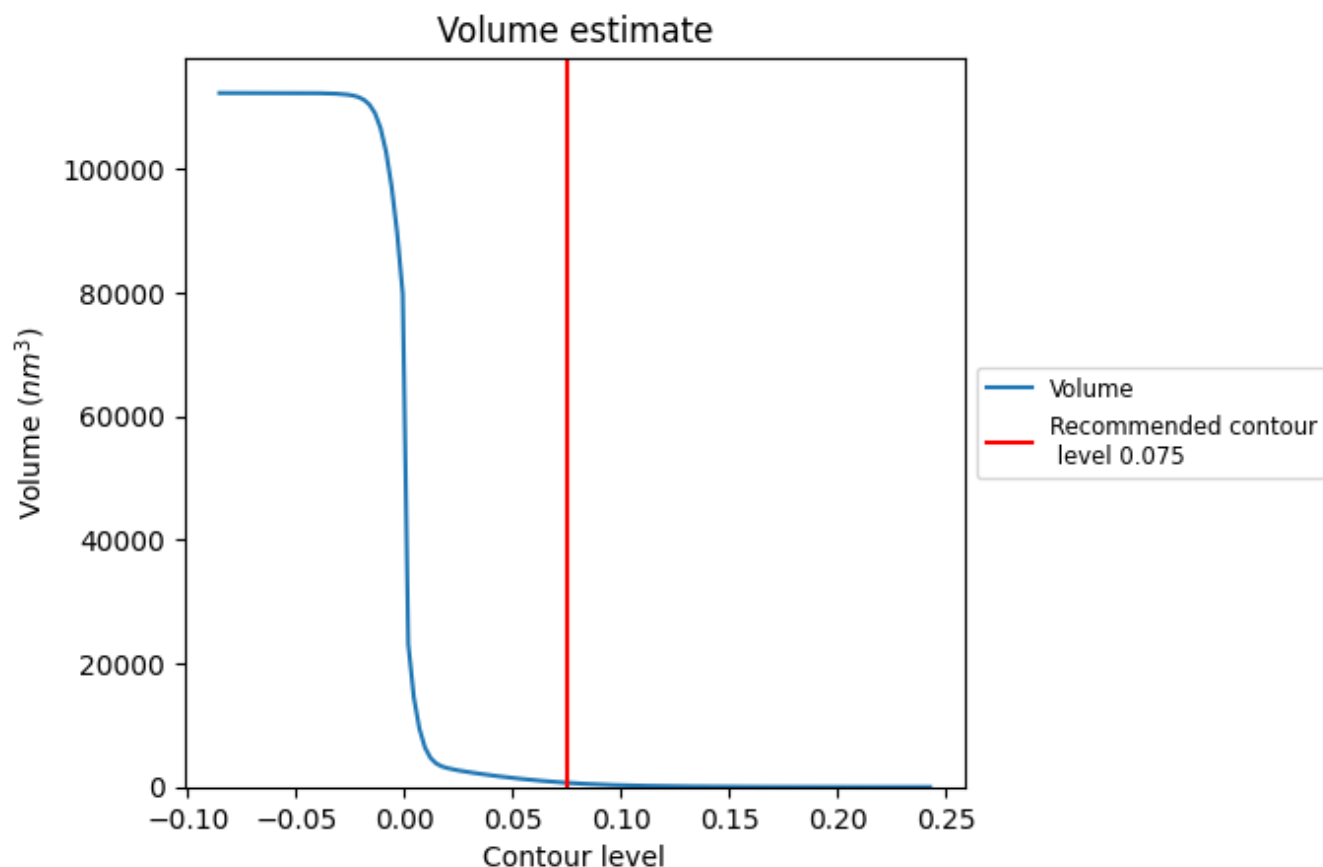
This section contains the results of statistical analysis of the map.

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.

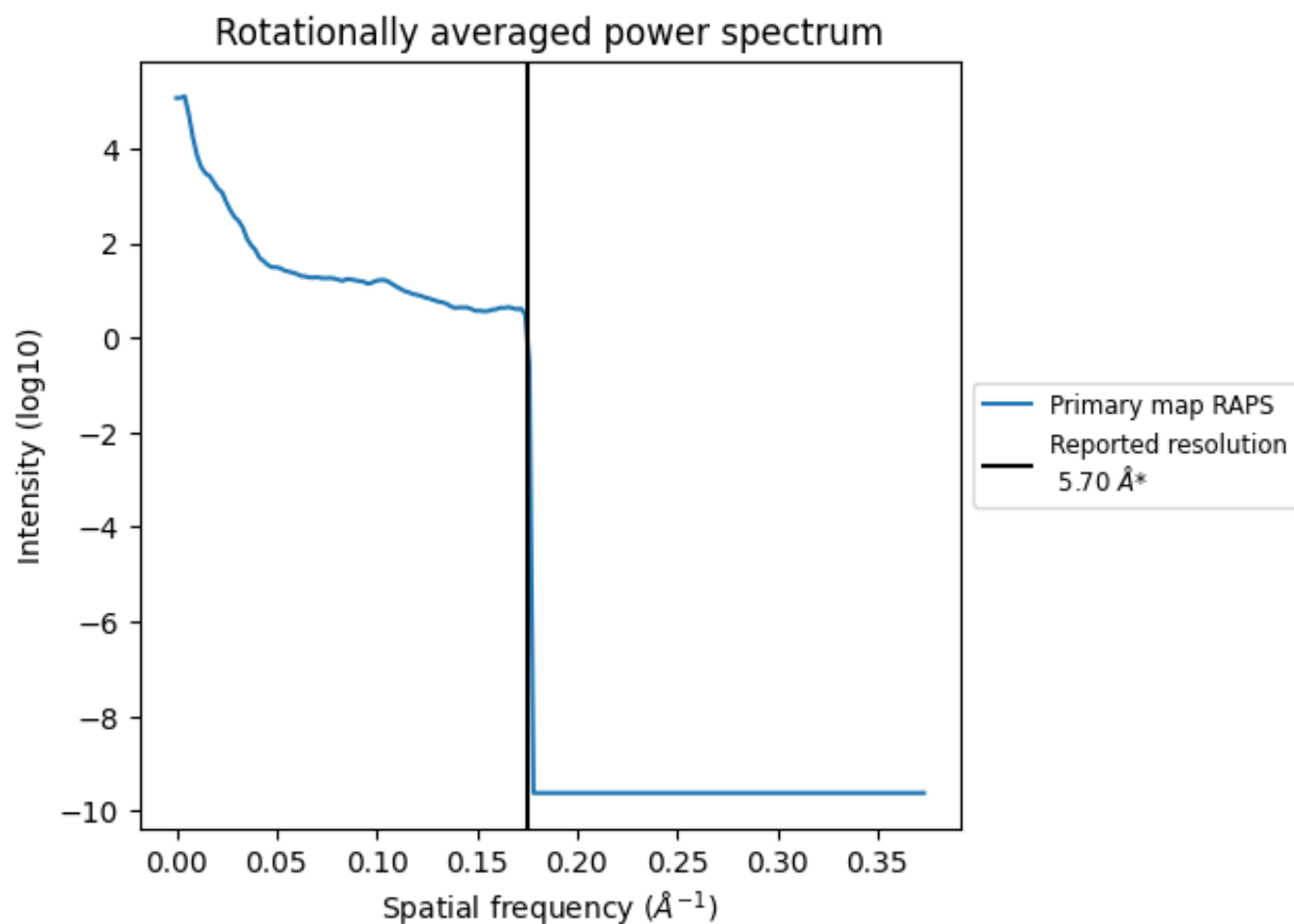
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 679 nm^3 ; this corresponds to an approximate mass of 613 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 0.175 Å⁻¹

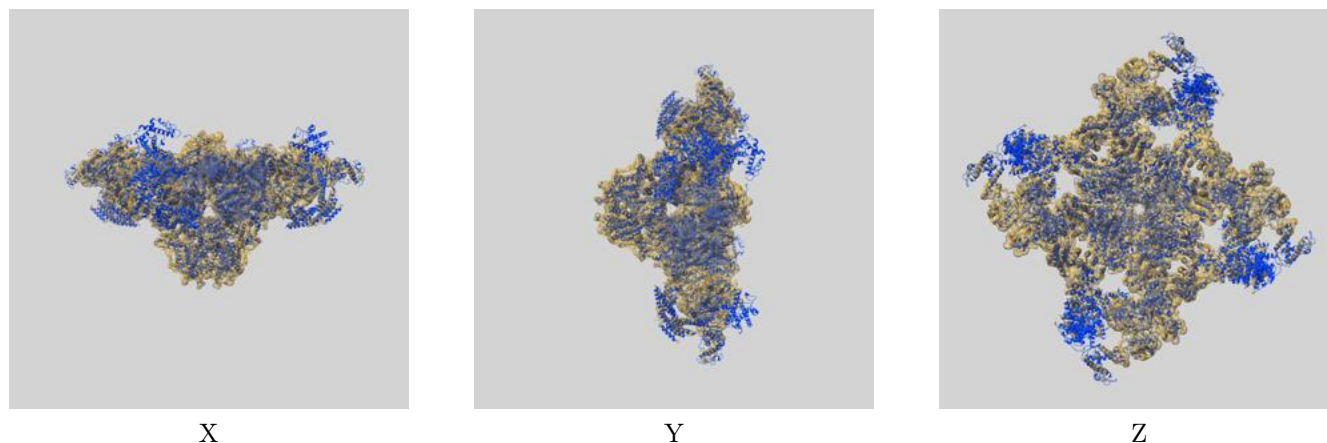
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

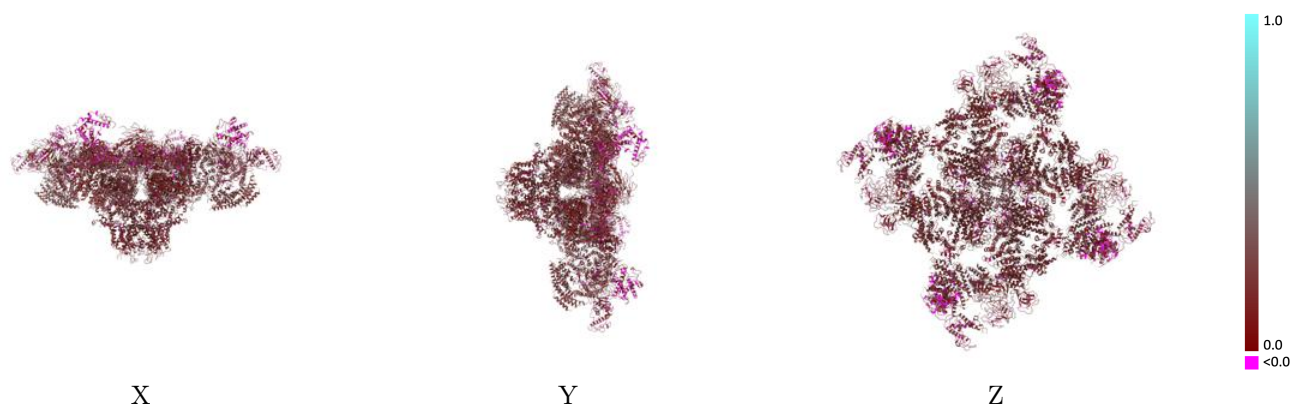
This section contains information regarding the fit between EMDB map EMD-9521 and PDB model 5GL1. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



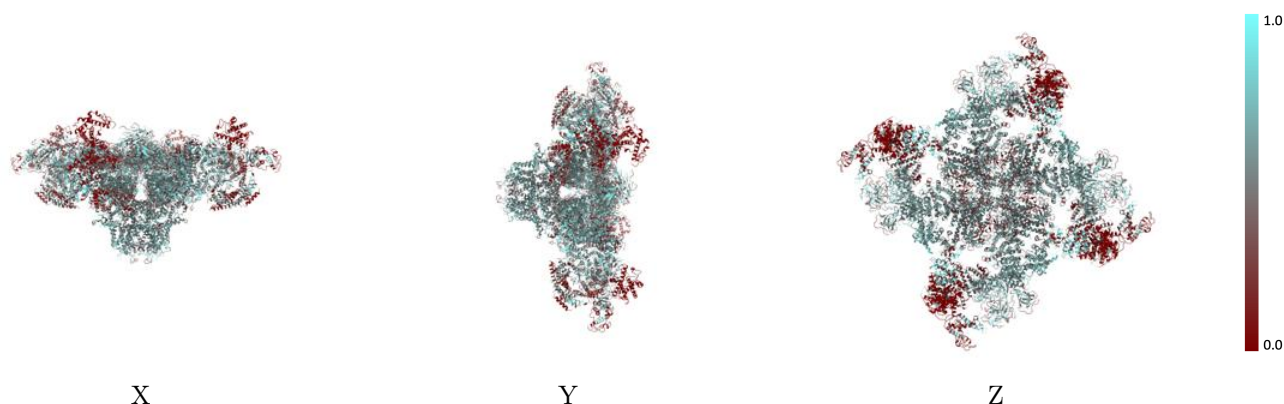
The images above show the 3D surface view of the map at the recommended contour level 0.075 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



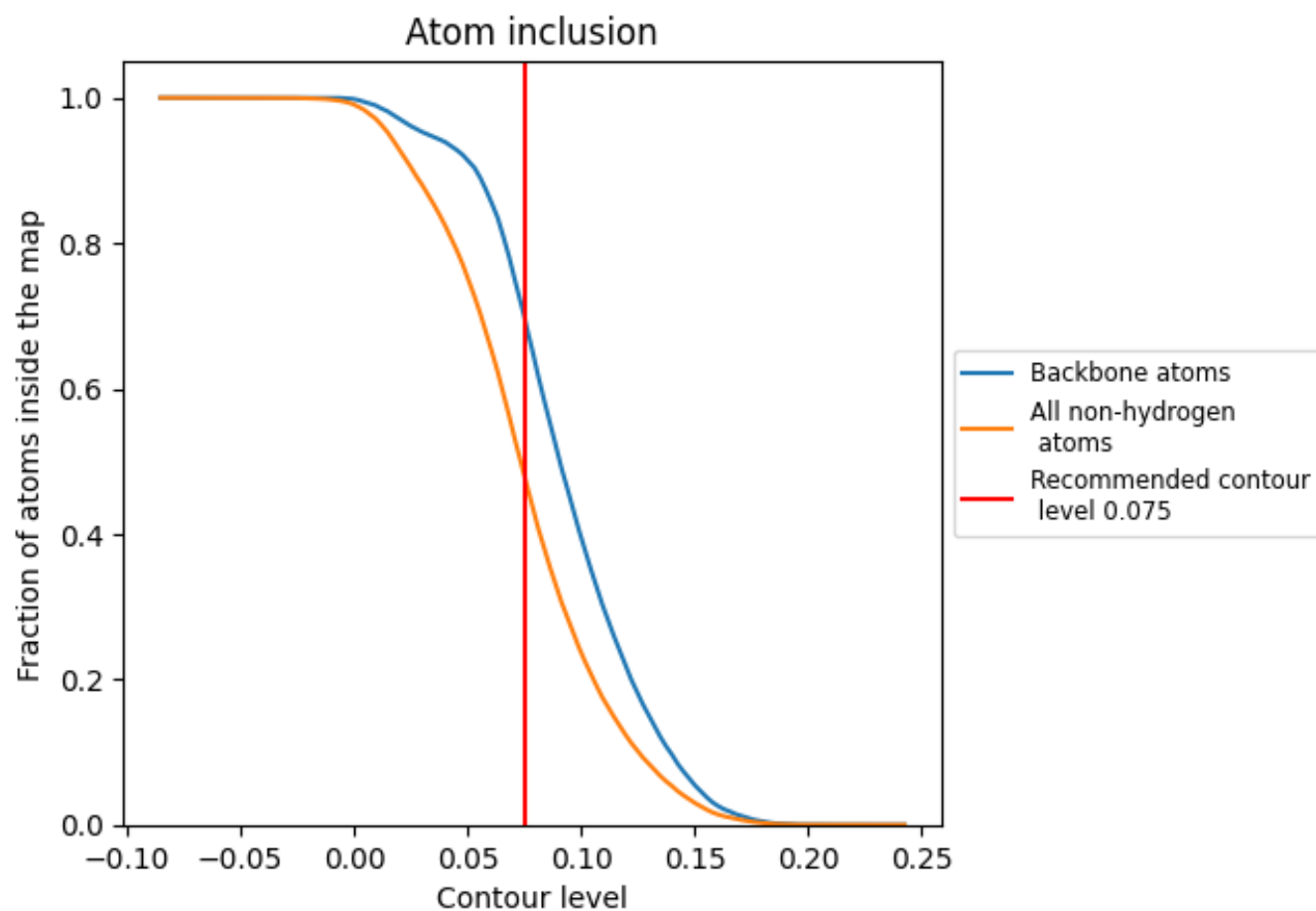
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.075).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 48% 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 (0.075) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4829	<div></div> 0.2010
A	<div></div> 0.4823	<div></div> 0.2020
B	<div></div> 0.4988	<div></div> 0.2060
C	<div></div> 0.4824	<div></div> 0.2010
D	<div></div> 0.4988	<div></div> 0.2080
E	<div></div> 0.4823	<div></div> 0.2010
F	<div></div> 0.5000	<div></div> 0.2050
G	<div></div> 0.4824	<div></div> 0.2010
H	<div></div> 0.4975	<div></div> 0.2040

