



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:38 PM UTC

PDB ID : 7T65 / pdb_00007t65
EMDB ID : EMD-25710
Title : Rabbit RyR1 disease mutant Y523S in complex with FKBP12.6 embedded in lipidic nanodisc in the open state
Authors : Iyer, K.A.; Hu, Y.; Murayama, T.; Samso, M.
Deposited on : 2021-12-13
Resolution : 4.05 Å(reported)
Based on initial model : 6WOT

This is a Full wwPDB EM Validation 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:

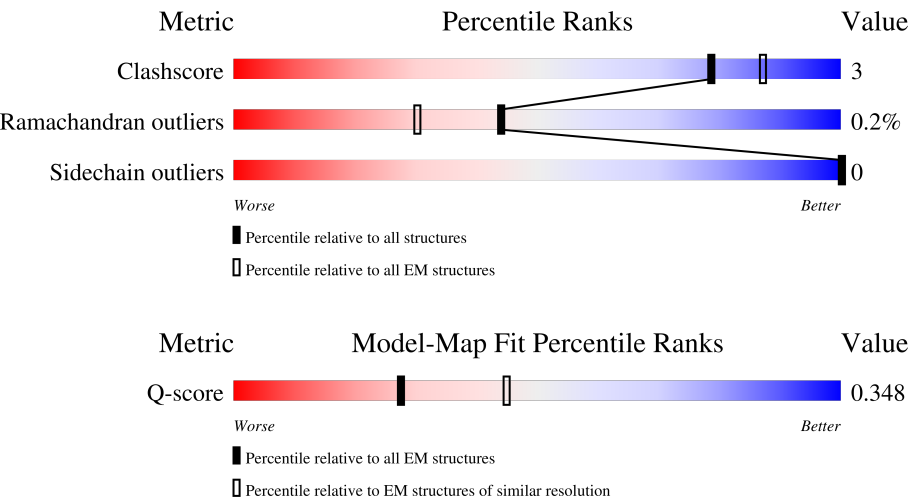
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.05 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.



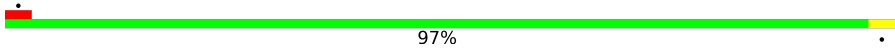
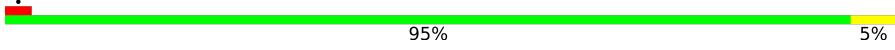
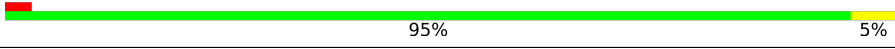
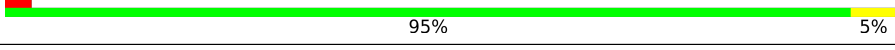
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6569 (3.55 - 4.55)

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	17% 78% 6% 16%
1	B	5037	18% 78% 6% 16%
1	C	5037	17% 78% 6% 16%
1	D	5037	18% 78% 6% 16%

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Mol	Chain	Length	Quality of chain
2	E	107	 97%5%
2	F	107	 95%5%
2	G	107	 95%5%
2	H	107	 95%5%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 135328 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	4252	Total	C	N	O	S	0	0
			32981	20992	5666	6114	209		
1	B	4252	Total	C	N	O	S	0	0
			32981	20992	5666	6114	209		
1	C	4252	Total	C	N	O	S	0	0
			32981	20992	5666	6114	209		
1	D	4252	Total	C	N	O	S	0	0
			32981	20992	5666	6114	209		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	523	SER	TYR	engineered mutation	UNP P11716
B	523	SER	TYR	engineered mutation	UNP P11716
C	523	SER	TYR	engineered mutation	UNP P11716
D	523	SER	TYR	engineered mutation	UNP P11716

- Molecule 2 is a protein called 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		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total Ca 1 1	0
4	B	1	Total Ca 1 1	0
4	C	1	Total Ca 1 1	0
4	D	1	Total Ca 1 1	0

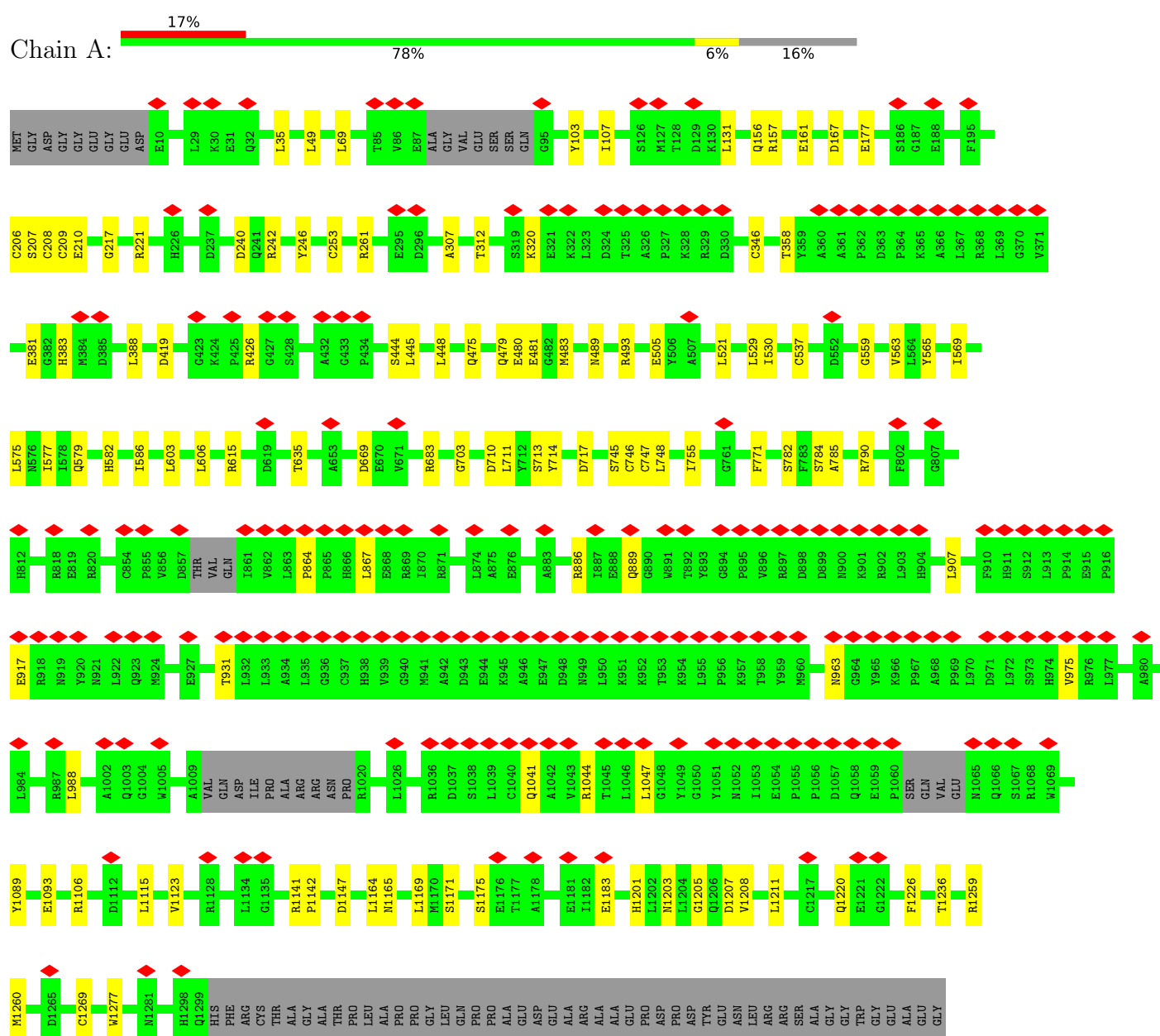
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

3 Residue-property plots [i](#)

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

• Molecule 1: Ryanodine receptor 1



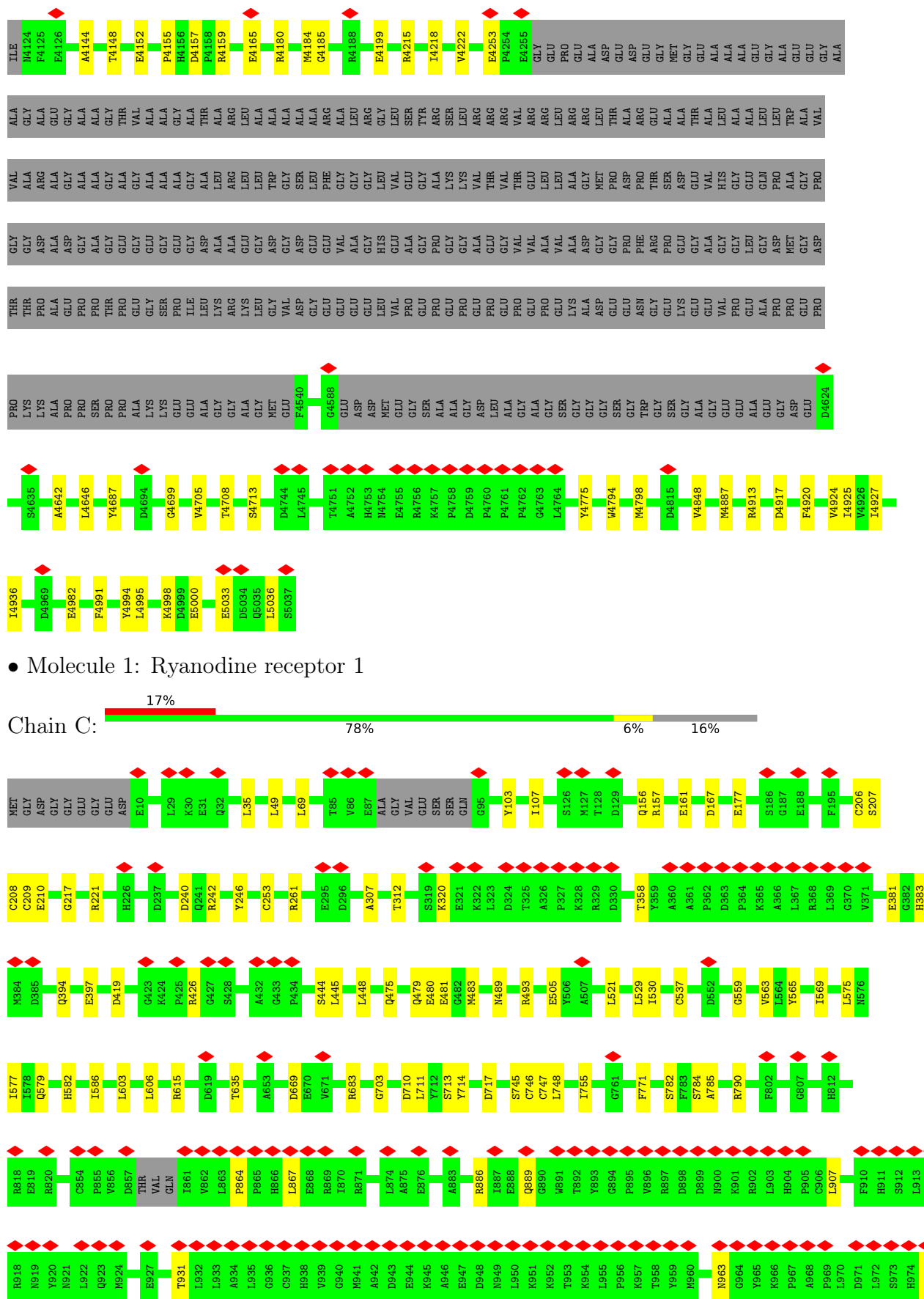






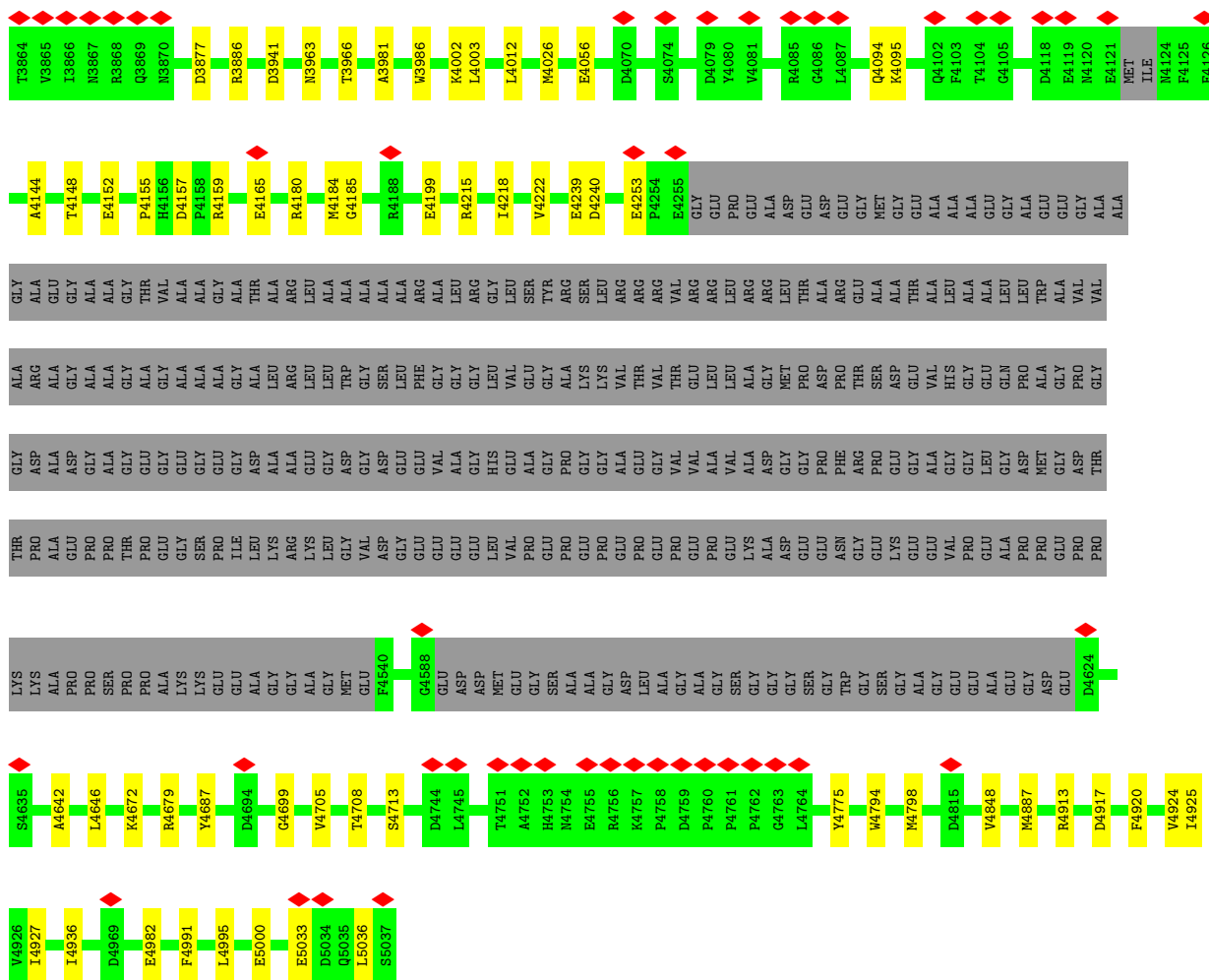




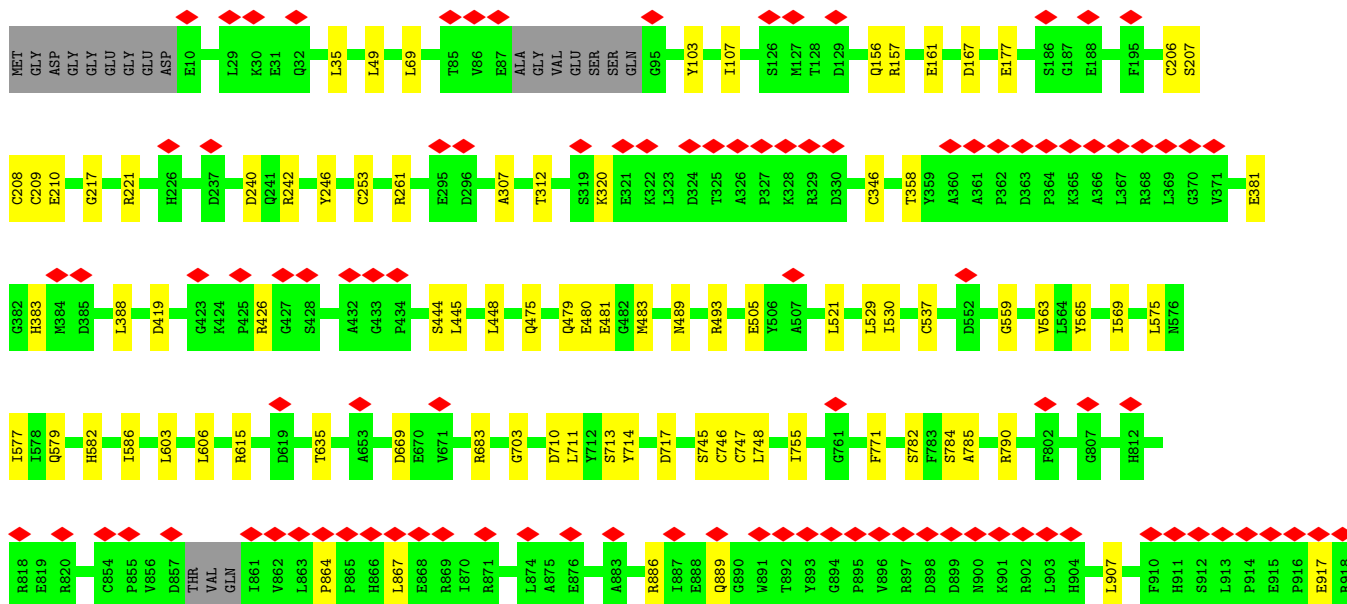
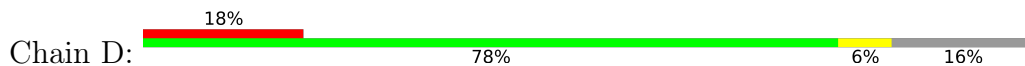




T3664	E3665	D3666	H3667	E3682	Q3683	E3684	E3685	E3686	E3687	E3688	E3689	V3690	E3691	E3692	H3734	L3735	E3736	E3737	G3738	G3739	E3740	ASN	GLY	GLU	ALA	GLU	GLU	E3748	V3749	E3750	Q3767	T3772	C3786	I3802	S3803	I3804	L3805	N3806	K3815	S3831	S3840	G3857	H3858	V3859	N3860	E3861	D3862	G3863												
K3562	V3563	E3564	G3565	L3575	Y3576	R3577	G3578	L3579	P3580	G3581	R3582	E3583	E3584	D3585	A3586	D3587	L3588	P3589	K3590	K3591	I3592	Q3597	E3598	E3610	H3611	P3612	TYR	LYS	SER	LYS	LYS	ALA	VAL	TRP	HIS	LYS	LEU	LEU	SER	LYS	GLN	ARG	ARG	ALA	VAL	VAL	ALA	CYS	PHE	N3859	N3860	E3861	D3862	G3863						
SER	ASP	GLN	GLU	ARG	THR	LYS	LYS	ARG	GLY	ASP	ARG	TYR	VAL	Q3506	T3507	S3508	L3509	I3510	T3513	L3514	K3515	K3516	M3517	G3521	L3522	N3523	D3531	L3536	T3538	R3539	Y3540	A3541	L3542	K3543	D3544	T3545	D3546	E3547	E3548	V3549	F3552	L3553	Q3554	N3555	N3556	L3557	H3558	L3559	Q3560	G3561										
Y3416	D3417	N3418	N3419	R3420	A3421	K3422	V3423	L3424	A3429	E3433	L3434	F3435	R3436	M3437	E3440	W3445	K3447	F3451	K3452	E3454	E3455	Q3456	N3457	Q3461	N3462	E3463	I3464	N3465	N3466	K3467	S3468	F3469	L3470	THR	ALA	ASP	SER	LYS	LYS	MET	ALA	LYS	N3556	ASP	GLY	ALA	SER	GLY												
R3348	A3349	R3350	P3351	E3352	L3353	L3354	H3355	S3356	H3357	F3358	I3362	K3363	R3364	L3365	R3366	K3367	R3368	A3369	G3370	E3375	E3376	E3377	Q3378	L3379	R3380	L3381	GLU	ALA	LYS	ALA	GLU	ALA	E3388	E3389	G3390	E3391	L3392	L3393	V3394	R3395	D3396	E3397	V3400	R3403	D3404	L3405	Y3406	A3407	L3408	Y3409	I3413	R3414	Y3415							
P3282	R3283	W3284	G3288	P3289	E3290	A3291	P3292	P3293	PRO	ALA	LEU	PRO	ALA	A3300	P3301	P3302	P3303	C3304	T3305	V3307	T3308	D3310	H3311	L3312	N3313	S3314	L3315	L3316	I3319	L3320	R3321	I3322	N3325	G3328	I3329	D3330	E3331	W3334	M3335	K3336	R3337	L3338	A3339	V3340	F3341	A3342	Q3343	P3344	I3345	V3346	S3347									
V3218	Y3219	T3220	T3221	G3222	S3223	P3224	R3225	A3228	ILE	LEU	GLY	PRO	N3234	S3235	V3236	E3237	E3238	M3239	C3240	P3241	D3242	I3243	P3244	V3245	L3246	D3247	R3248	L3249	D3252	I3253	G3254	G3255	L3256	A3257	E3258	S3259	G3260	Y3263	THR	GLU	MET	P3267	H3268	S3269	I3270	E3271	I3272	T3273	L3274	L3277	C3278	S3279	Y3280	L3281						
H3150	Q3151	F3152	G3153	D3154	D3155	Y3156	T3157	L3158	D3159	Y3166	R3167	T3168	L3169	C3170	S3171	T3172	Y3173	S3174	L3175	Q3176	T3177	T3178	K3179	N3180	T3181	VAL	GLU	K3185	L3186	R3187	P3188	A3189	C3193	L3194	L3197	A3198	A3199	A3200	M3201	P3202	V3203	A3204	A3205	L3206	E3207	P3208	Q3209	L3210	N3211	E3212	Y3213	A3215	C3216	SER						
R3073	S3074	L3075	ASP	ALA	R3078	T3079	V3080	M3081	LYS	S3083	G3084	A3090	R3093	E3101	K3105	E3108	M3109	L3110	R3111	L3112	G3113	LYS	VAL	SER	GLY	ALA	GLN	ARG	THR	GLN	VAL	LYS	V3125	G3126	Q3127	M3128	L3129	T3130	T3133	V3134	A3135	L3136	L3137	P3138	V3139	L3140	T3141	T3142	Q3145	A3148	Q3149									
E2915	K2916	A2917	R2918	D2919	R2920	E2921	K2922	A2923	Q2924	E2925	L2926	L2927	K2928	Y2929	L2930	Q2931	M2932	N2933	G2934	T2935	A2936	V2937	T2938	R2939	G2940	L2941	K2942	D2943	M2944	E2945	T2946	G2947	T2948	S2949	S2950	T2951	E2952	K2953	R2954	T2955	A2956	F2959	W2966	F2973	I2974	A2975	H2976	L2977	E2978	ALA	VAL	VAL	SER	GLY	ARG					
Y2855	N2856	P2857	Q2858	P2859	P2860	D2861	L2862	S2863	G2864	V2865	L2866	L2867	S2868	R2869	E2870	L2871	Q2872	L2813	K2814	A2815	M2816	L2817	Q2877	L2878	A2879	E2880	W2881	T2882	H2883	N2884	T2885	T2886	G2887	R2887	R2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	A2896	R2897	G2898	G2899	G2900	T2901	H2902	P2903	L2904	L2905	V2906	P2907	Y2908	D2909	L2910	L2911	L2912	K2914
K2796	T2796	F2797	S2798	E2799	K2800	D2801	K2802	E2803	L2804	Y2805	R2806	W2807	P2808	I2809	K2810	E2811	S2812	L2813	K2814	A2815	M2816	L2817	Q2877	L2878	A2879	E2880	W2881	T2882	H2883	N2884	T2885	T2886	G2887	R2887	R2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	A2896	R2897	G2898	G2899	G2900	T2901	H2902	P2903	L2904	L2905	V2906	P2907	Y2908	D2909	L2910	L2911	L2912	K2914

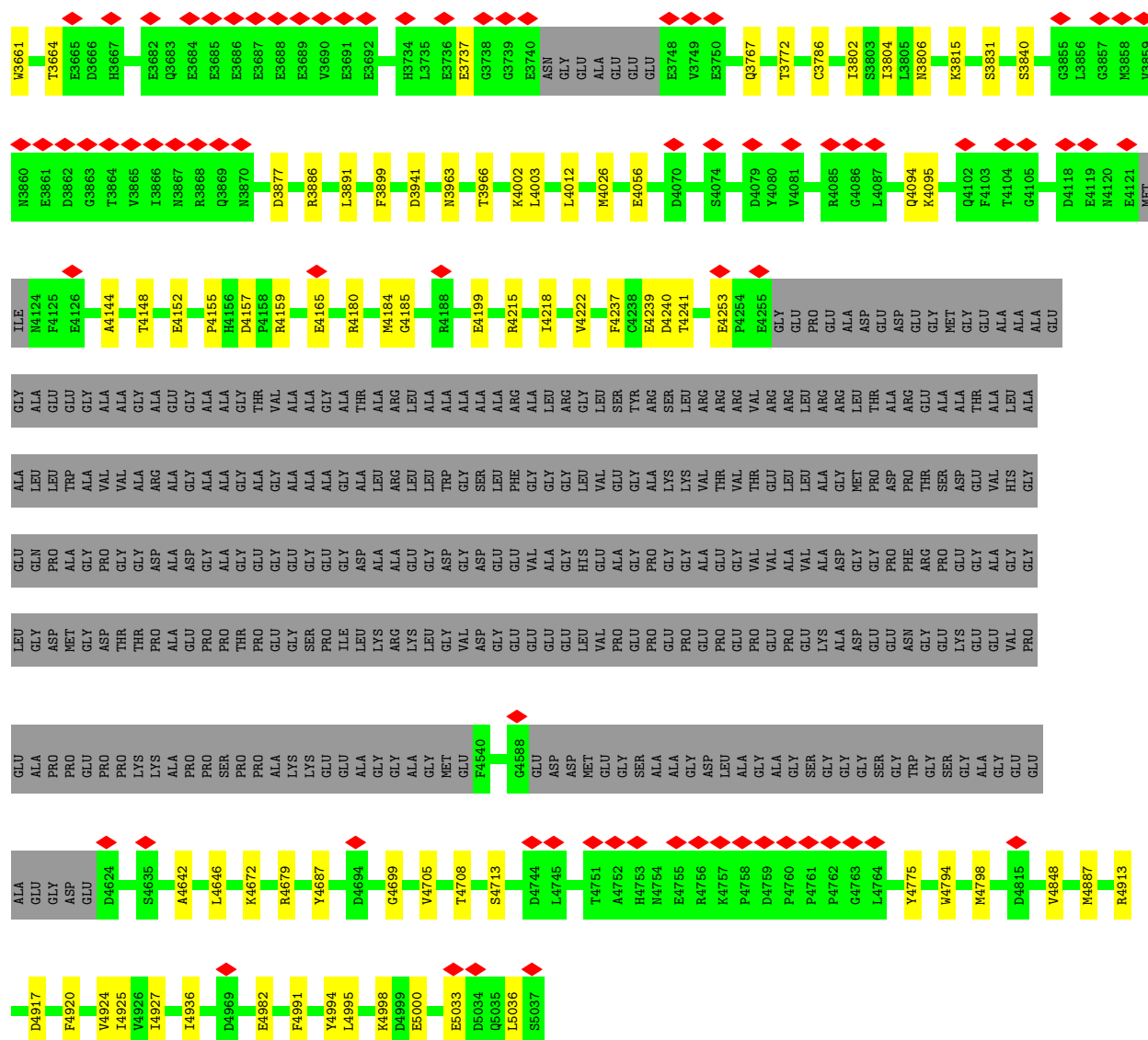


- Molecule 1: Ryanodine receptor 1



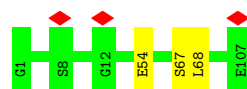


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GLY	SER	ASP	GLN	GLU	ARG	THR	LYS	LYS	ARG	ARG	GLY	ASP	THR	SER	VAL	Q3506	T3507	S3508	L3509	I3510	T3513	L3514	K3515	K3516	M3517	G3521	L3522	N3523	D3531	L3535	T3538	L3539	Y3540	A3541	L3542	L3543	D3544	L3545	L3546	E3547	E3548	V3549	F3552	L3553	Q3554	N3555	L3556	L3557	H3558	L3559													
V3346	S3347	R3348	A3349	R3350	P3351	E3352	L3353	H3354	H3355	S3356	H3357	F3358	I3362	G3363	R3364	L3365	R3366	K3367	R3368	A3369	G3370	K3371	E3375	E3376	E3377	Q3378	L3379	R3380	L3381	GLU	ALA	LYS	ALA	GLU	ALA	E3388	E3389	G3390	E3391	L3392	L3393	V3394	R3395	D3396	E3397	V3400	R3403	D3404	L3405	Y3406	A3407	L3408	Y3409	I3413									
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S3279	Y3280	L3281	P3282	R3283	W3284	G3288	P3289	E3290	A3291	P3292	P3293	PRO	ALA	LEU	PRO	ALA	A3300	P3301	P3302	P3303	C3304	T3305	ALA	V3307	D3310	H3311	L3312	S3313	L3314	L3315	L3316	I3319	L3320	R3321	I3322	N3325	G3328	I3329	D3330	E3331	W3334	N3335	K3336	R3337	L3338	A3339	V3340	F3341	A3342	Q3343	P3344	I3345											
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A3148	Q3149	H3150	Q3151	F3152	G3153	D3154	D3155	V3156	L3157	D3158	D3159	Y3166	R3167	T3168	L3169	C3170	S3171	I3172	Y3173	S3174	L3175	G3176	T3177	T3178	K3179	N3180	T3181	Y3182	VAL	GLU	K3185	L3186	R3187	P3188	A3189	C3193	L3194	L3197	A3198	A3199	A3200	M3201	P3202	V3203	A3204	F3205	L3206	E3207	P3208	L3210	N3211	E3212	N3214										
A3215	C3216	SER	V3218	Y3219	T3220	T3221	K3222	S3223	P3224	R3225	A3228	ILE	LEU	GLY	LEU	PRO	N3234	S3235	V3236	E3237	E3238	H3239	C3240	P3241	D3242	I3243	P3244	V3245	L3246	D3247	R3248	L3249	D3252	I3253	G3254	G3255	L3256	A3257	E3258	S3259	G3260	Y3263	THR	GLU	MET	P3267	H3268	V3269	I3270	E3271	L3272	T3273	L3274	L3277	C3278								
S3279	Y3280	L3281	P3282	R3283	W3284	G3288	P3289	E3290	A3291	P3292	P3293	PRO	ALA	LEU	PRO	ALA	A3300	P3301	P3302	P3303	C3304	T3305	ALA	V3307	D3310	H3311	L3312	S3313	L3314	L3315	L3316	I3319	L3320	R3321	I3322	N3325	G3328	I3329	D3330	E3331	W3334	N3335	K3336	R3337	L3338	A3339	V3340	F3341	A3342	Q3343	P3344	I3345											
V3346	S3347	R3348	A3349	R3350	P3351	E3352	L3353	H3354	H3355	S3356	H3357	F3358	I3362	G3363	R3364	L3365	R3366	K3367	R3368	A3369	G3370	K3371	E3375	E3376	E3377	Q3378	L3379	R3380	L3381	GLU	ALA	LYS	ALA	GLU	ALA	E3388	E3389	G3390	E3391	L3392	L3393	V3394	R3395	D3396	E3397	V3400	R3403	D3404	L3405	Y3406	A3407	L3408	Y3409	I3413									
R3414	Y3415	V3416	D3417	N3418	N3419	R3420	A3421	H3422	W3423	L3424	A3429	E3433	L3434	F3435	R3436	R3437	E3440	W3445	S3446	K3447	F3451	K3452	R3453	E3454	E3455	Q3456	N3457	Q3461	N3462	E3463	I3464	N3465	N3466	N3467	S3468	F3469	L3470	THR	ALA	ASP	SER	LYS	SER	LYS	MET	ALA	LYS	ALA	GLY	ASP	GLN	SER											
GLY	GLY	SER	ASP	GLN	GLU	ARG	THR	LYS	LYS	ARG	ARG	GLY	ASP	THR	SER	VAL	Q3506	T3507	S3508	L3509	I3510	T3513	L3514	K3515	K3516	M3517	G3521	L3522	N3523	D3531	L3535	T3538	L3539	Y3540	A3541	L3542	L3543	D3544	L3545	L3546	E3547	E3548	V3549	F3552	L3553	Q3554	N3555	L3556	L3557	H3558	L3559												
Q3560	G3561	K3562	V3563	E3564	Q3565	L3575	Y3576	R3577	R3578	L3579	P3580	G3581	R3582	E3583	E3584	D3585	A3586	D3587	P3588	P3589	E3590	K3591	I3592	Q3597	E3598	E3610	H3611	P3612	T3612	L3635	T3638	L3639	Y3640	A3641	L3642	L3643	L3644	L3645	L3646	L3647	S3648	L3649	L3650	L3651	L3652	L3653	Q3654	N3655	L3656	L3657	H3658	L3659	T3639										
GLU	GLY	N2734	F2735	D2736	F2737	R2738	P2739	V2740	E2741	T2742	L2743	N2744	V2745	L2746	L2747	P2748	E2749	K2750	L2751	D2752	S2753	F2754	L2755	N2756	K2757	F2758	A2759	E2760	Y2761	T2762	L2763	E2764	K2765	N2766	A2767	F2768	D2769	K2770	L2771	Q2772	W2773	N2774	W2775	S2776	L2777	Q2778	E2779	W2780	V2781	D2782	E2783	E2784	L2785	K2786	T2787	P2789	L2790	L2791					
R2792	P2793	Y2794	K2795	T2796	F2797	S2798	E2799	D2800	L2801	K2802	E2803	L2804	V2805	L2806	W2807	P2808	L2809	K2810	E2811	L2812	S2813	K2814	A2815	M2816	L2817	A2818	W2819	E2820	W2821	T2822	L2823	E2824	K2825	A2826	R2827	F2828	D2829	E2830	GLU	GLU	ARG	THR	GLU	LYS	LYS	THR	ARG	LYS	ILE	SER	GLN	THR	ALA	GLN	THR	ASP	PRO						
ARG	GLU	GLY	Y2855	N2856	P2857	Q2858	P2859	P2860	D2861	L2862	S2863	G2864	V2865	L2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	N2881	Y2882	L2883	N2884	T2885	W2886	R2887	R2888	K2889	K2890	K2891	Q2892	E2893	K2894	L2894	E2895	A2896	K2897	Q2898	Q2899	G2900	T2901	L2902	H2902	P2903	L2904	L2905	V2906	P2907	Y2908	D2909	L2910	L2911		
T2912	A2913	K2914	E2915	K2916	A2917	R2918	D2919	K2920	E2921	K2922	A2923	Q2924	E2925	L2926	L2927	K2928	F2929	L2930	Q2931	M2932	N2933	G2934	Y2935	A2936	V2937	T2938	R2939	G2940	L2941	K2942	D2943	M2944	E2945	L2946	D2947	T2948	S2949	S2950	L2951	E2952	K2953	R2954	F2955	A2956	F2959	T2973	L2974	A2975	H2976	P2903	L2904	E2978	ALA	VAL	VAL	SER	GLY						
ARG	VAL	LYS	SER	PRO	H2991	E2992	I2995	G3153	R3078	T3079	V3080	K3081	LYS	S3083	G3084	A3090	R3093	E3101	K3105	E3108	N3109	L3110	L3111	R3112	G3113	LYS	VAL	SER	GLN	ALA	THR	GLN	VAL	LYS	V3125	G3126	Q3127	N3128	L3129	T3130	T3133	V3134	A3135	L3136	L3137	P3138	V3139	L3140	T3141	T3142	Q3145												



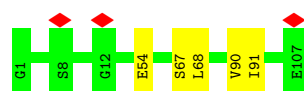
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E: 97%

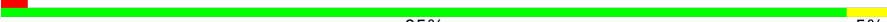


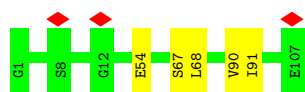
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F: 95%



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

Chain G:  95% 5%



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

Chain H:  95% 5%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	84954	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	53.19	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.769	Depositor
Minimum map value	-0.355	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.038	Depositor
Recommended contour level	0.176	Depositor
Map size ($\text{\AA}$)	463.54004, 463.54004, 463.54004	wwPDB
Map dimensions	430, 430, 430	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0780001, 1.0780001, 1.0780001	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: ATP, CA, 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	0.29	1/33703 (0.0%)	0.53	1/45746 (0.0%)
1	B	0.29	1/33703 (0.0%)	0.53	1/45746 (0.0%)
1	C	0.29	1/33703 (0.0%)	0.53	1/45746 (0.0%)
1	D	0.29	1/33703 (0.0%)	0.53	1/45746 (0.0%)
2	E	0.25	0/834	0.53	0/1123
2	F	0.25	0/834	0.53	0/1123
2	G	0.25	0/834	0.53	0/1123
2	H	0.25	0/834	0.53	0/1123
All	All	0.29	4/138148 (0.0%)	0.53	4/187476 (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	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1652	GLU	C-O	-8.13	1.13	1.24
1	D	1652	GLU	C-O	-8.08	1.13	1.24
1	B	1652	GLU	C-O	-8.02	1.13	1.24
1	A	1652	GLU	C-O	-7.96	1.14	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2955	PHE	N-CA-CB	-5.25	102.64	110.10
1	C	2955	PHE	N-CA-CB	-5.25	102.64	110.10
1	A	2955	PHE	N-CA-CB	-5.22	102.69	110.10
1	D	2955	PHE	N-CA-CB	-5.22	102.69	110.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	4253	GLU	Peptide
1	B	4253	GLU	Peptide
1	C	4253	GLU	Peptide
1	D	4253	GLU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32981	0	31923	186	0
1	B	32981	0	31923	187	0
1	C	32981	0	31923	190	0
1	D	32981	0	31923	189	0
2	E	818	0	824	2	0
2	F	818	0	824	3	0
2	G	818	0	824	3	0
2	H	818	0	824	3	0
3	A	31	0	12	1	0
3	B	31	0	12	1	0
3	C	31	0	12	1	0
3	D	31	0	12	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	135328	0	131036	750	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 3.

All (750) 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:4913:ARG:NH1	1:C:4917:ASP:OD2	2.23	0.72
1:B:4913:ARG:NH1	1:B:4917:ASP:OD2	2.22	0.72
1:A:4913:ARG:NH1	1:A:4917:ASP:OD2	2.22	0.72
1:D:4913:ARG:NH1	1:D:4917:ASP:OD2	2.22	0.71
1:A:3540:TYR:OH	1:A:3597:GLN:OE1	2.11	0.69
1:B:3540:TYR:OH	1:B:3597:GLN:OE1	2.11	0.69
1:C:3540:TYR:OH	1:C:3597:GLN:OE1	2.11	0.68
1:D:3540:TYR:OH	1:D:3597:GLN:OE1	2.11	0.68
1:A:615:ARG:NH2	1:A:1677:GLY:O	2.28	0.67
1:C:615:ARG:NH2	1:C:1677:GLY:O	2.28	0.67
1:B:426:ARG:NH2	1:B:505:GLU:O	2.28	0.67
1:A:426:ARG:NH2	1:A:505:GLU:O	2.28	0.67
1:D:426:ARG:NH2	1:D:505:GLU:O	2.28	0.67
1:D:615:ARG:NH2	1:D:1677:GLY:O	2.28	0.67
1:C:426:ARG:NH2	1:C:505:GLU:O	2.28	0.67
1:B:615:ARG:NH2	1:B:1677:GLY:O	2.28	0.67
1:C:710:ASP:O	1:C:713:SER:OG	2.13	0.67
1:C:489:ASN:OD1	1:C:493:ARG:NH2	2.29	0.66
1:D:710:ASP:O	1:D:713:SER:OG	2.13	0.66
1:B:489:ASN:OD1	1:B:493:ARG:NH2	2.29	0.66
1:C:746:CYS:SG	1:C:747:CYS:N	2.69	0.66
1:B:746:CYS:SG	1:B:747:CYS:N	2.69	0.66
1:A:710:ASP:O	1:A:713:SER:OG	2.13	0.66
1:B:1259:ARG:NH2	1:B:1591:CYS:SG	2.70	0.65
1:D:746:CYS:SG	1:D:747:CYS:N	2.69	0.65
1:B:710:ASP:O	1:B:713:SER:OG	2.13	0.65
1:A:1259:ARG:NH2	1:A:1591:CYS:SG	2.69	0.65
1:A:746:CYS:SG	1:A:747:CYS:N	2.69	0.65
1:A:1450:VAL:HG11	1:A:1454:THR:HG21	1.79	0.65
1:D:489:ASN:OD1	1:D:493:ARG:NH2	2.29	0.65
1:C:1450:VAL:HG11	1:C:1454:THR:HG21	1.79	0.65
1:D:1753:LYS:O	1:D:1758:ARG:NH1	2.30	0.65
1:A:489:ASN:OD1	1:A:493:ARG:NH2	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1753:LYS:O	1:C:1758:ARG:NH1	2.30	0.65
1:B:1450:VAL:HG11	1:B:1454:THR:HG21	1.79	0.65
1:C:1259:ARG:NH2	1:C:1591:CYS:SG	2.69	0.65
1:A:577:ILE:O	1:A:579:GLN:NE2	2.31	0.64
1:B:475:GLN:NE2	1:B:529:LEU:O	2.30	0.64
1:B:1753:LYS:O	1:B:1758:ARG:NH1	2.30	0.64
1:D:1259:ARG:NH2	1:D:1591:CYS:SG	2.70	0.64
1:A:475:GLN:NE2	1:A:529:LEU:O	2.30	0.64
1:C:475:GLN:NE2	1:C:529:LEU:O	2.30	0.64
1:D:577:ILE:O	1:D:579:GLN:NE2	2.31	0.64
1:A:1753:LYS:O	1:A:1758:ARG:NH1	2.30	0.64
1:D:1450:VAL:HG11	1:D:1454:THR:HG21	1.79	0.64
1:A:3941:ASP:O	1:A:4002:LYS:NZ	2.31	0.63
1:B:577:ILE:O	1:B:579:GLN:NE2	2.30	0.63
1:B:3510:ILE:O	1:B:3513:THR:OG1	2.17	0.63
1:D:475:GLN:NE2	1:D:529:LEU:O	2.30	0.63
1:D:3941:ASP:O	1:D:4002:LYS:NZ	2.32	0.63
1:C:3510:ILE:O	1:C:3513:THR:OG1	2.17	0.63
1:C:3941:ASP:O	1:C:4002:LYS:NZ	2.31	0.63
1:C:577:ILE:O	1:C:579:GLN:NE2	2.31	0.62
1:C:1269:CYS:HG	1:C:1473:THR:HG1	1.36	0.62
1:D:1171:SER:OG	1:D:1175:SER:O	2.14	0.62
1:B:3941:ASP:O	1:B:4002:LYS:NZ	2.32	0.62
1:A:2355:ARG:O	1:A:2359:ARG:NH1	2.33	0.62
1:C:2355:ARG:O	1:C:2359:ARG:NH1	2.33	0.62
1:B:2355:ARG:O	1:B:2359:ARG:NH1	2.33	0.62
1:D:2355:ARG:O	1:D:2359:ARG:NH1	2.33	0.62
1:A:1269:CYS:SG	1:A:1473:THR:OG1	2.54	0.61
1:A:3510:ILE:O	1:A:3513:THR:OG1	2.17	0.61
1:A:221:ARG:NH1	1:A:253:CYS:O	2.34	0.61
1:B:1171:SER:OG	1:B:1175:SER:O	2.14	0.61
1:D:221:ARG:NH1	1:D:253:CYS:O	2.34	0.61
1:D:3510:ILE:O	1:D:3513:THR:OG1	2.17	0.61
1:C:3445:TRP:O	1:C:3452:LYS:NZ	2.33	0.61
1:B:221:ARG:NH1	1:B:253:CYS:O	2.34	0.60
1:D:4920:PHE:O	1:D:4924:VAL:HG12	2.01	0.60
1:B:4920:PHE:O	1:B:4924:VAL:HG12	2.01	0.60
1:B:669:ASP:OD2	1:B:790:ARG:NH2	2.34	0.60
1:C:221:ARG:NH1	1:C:253:CYS:O	2.34	0.60
1:A:1171:SER:OG	1:A:1175:SER:O	2.14	0.60
1:C:1171:SER:OG	1:C:1175:SER:O	2.14	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:669:ASP:OD2	1:A:790:ARG:NH2	2.34	0.60
1:A:4920:PHE:O	1:A:4924:VAL:HG12	2.01	0.60
1:B:3445:TRP:O	1:B:3452:LYS:NZ	2.33	0.60
1:B:1269:CYS:HG	1:B:1473:THR:HG1	1.36	0.60
1:C:669:ASP:OD2	1:C:790:ARG:NH2	2.35	0.60
1:A:3445:TRP:O	1:A:3452:LYS:NZ	2.33	0.60
1:A:103:TYR:OH	1:A:167:ASP:OD2	2.20	0.59
1:B:103:TYR:OH	1:B:167:ASP:OD2	2.20	0.59
1:C:103:TYR:OH	1:C:167:ASP:OD2	2.20	0.59
1:D:419:ASP:OD1	1:D:493:ARG:NH1	2.35	0.59
1:A:1500:PHE:O	1:A:1534:LYS:NZ	2.30	0.59
1:C:4920:PHE:O	1:C:4924:VAL:HG12	2.01	0.59
1:A:3963:ASN:O	1:A:3966:THR:OG1	2.18	0.59
1:A:2101:MET:SD	1:A:2104:ARG:NH2	2.76	0.59
1:D:1269:CYS:SG	1:D:1473:THR:OG1	2.54	0.59
1:D:2101:MET:SD	1:D:2104:ARG:NH2	2.76	0.59
1:B:683:ARG:NH1	1:B:717:ASP:OD2	2.36	0.59
1:B:3963:ASN:O	1:B:3966:THR:OG1	2.18	0.59
1:C:2101:MET:SD	1:C:2104:ARG:NH2	2.76	0.59
1:D:103:TYR:OH	1:D:167:ASP:OD2	2.20	0.59
1:D:669:ASP:OD2	1:D:790:ARG:NH2	2.34	0.59
1:A:419:ASP:OD1	1:A:493:ARG:NH1	2.35	0.59
1:B:4687:TYR:OH	1:B:4699:GLY:O	2.20	0.59
1:C:683:ARG:NH1	1:C:717:ASP:OD2	2.36	0.59
1:B:419:ASP:OD1	1:B:493:ARG:NH1	2.35	0.59
1:C:419:ASP:OD1	1:C:493:ARG:NH1	2.35	0.59
1:D:1106:ARG:NH2	1:D:1183:GLU:O	2.36	0.59
1:B:2101:MET:SD	1:B:2104:ARG:NH2	2.76	0.59
1:B:1106:ARG:NH2	1:B:1183:GLU:O	2.36	0.58
1:A:1106:ARG:NH2	1:A:1183:GLU:O	2.36	0.58
1:D:1500:PHE:O	1:D:1534:LYS:NZ	2.30	0.58
1:C:1106:ARG:NH2	1:C:1183:GLU:O	2.36	0.58
1:D:683:ARG:NH1	1:D:717:ASP:OD2	2.36	0.58
1:C:2759:ALA:O	1:C:2762:THR:OG1	2.22	0.58
1:A:683:ARG:NH1	1:A:717:ASP:OD2	2.36	0.58
1:D:4687:TYR:OH	1:D:4699:GLY:O	2.20	0.58
1:B:2759:ALA:O	1:B:2762:THR:OG1	2.22	0.57
1:A:4687:TYR:OH	1:A:4699:GLY:O	2.20	0.57
1:D:3274:LEU:HD21	1:D:3319:ILE:HD12	1.87	0.57
1:C:3274:LEU:HD21	1:C:3319:ILE:HD12	1.87	0.57
1:A:2149:VAL:O	1:A:2152:THR:OG1	2.23	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3274:LEU:HD21	1:B:3319:ILE:HD12	1.87	0.57
1:B:1089:TYR:O	1:B:1226:PHE:N	2.38	0.57
1:C:4687:TYR:OH	1:C:4699:GLY:O	2.20	0.57
1:A:3274:LEU:HD21	1:A:3319:ILE:HD12	1.87	0.56
1:D:2759:ALA:O	1:D:2762:THR:OG1	2.22	0.56
1:C:1089:TYR:O	1:C:1226:PHE:N	2.38	0.56
1:D:240:ASP:OD2	1:D:246:TYR:OH	2.23	0.56
1:D:4240:ASP:OD2	1:D:4672:LYS:NZ	2.33	0.56
1:D:3445:TRP:O	1:D:3452:LYS:NZ	2.33	0.56
1:B:2149:VAL:O	1:B:2152:THR:OG1	2.23	0.56
1:C:2149:VAL:O	1:C:2152:THR:OG1	2.23	0.56
1:A:1089:TYR:O	1:A:1226:PHE:N	2.38	0.56
1:A:2759:ALA:O	1:A:2762:THR:OG1	2.22	0.56
1:D:2149:VAL:O	1:D:2152:THR:OG1	2.23	0.56
1:A:1201:HIS:NE2	1:A:1203:ASN:OD1	2.39	0.56
1:B:1500:PHE:O	1:B:1534:LYS:NZ	2.30	0.56
1:C:1269:CYS:SG	1:C:1473:THR:OG1	2.54	0.56
1:C:3963:ASN:O	1:C:3966:THR:OG1	2.18	0.56
1:C:3269:VAL:O	1:C:3273:THR:OG1	2.17	0.56
1:D:3377:GLU:OE2	1:D:3378:GLN:NE2	2.39	0.56
1:B:1201:HIS:NE2	1:B:1203:ASN:OD1	2.39	0.56
1:C:1201:HIS:NE2	1:C:1203:ASN:OD1	2.39	0.56
1:D:1201:HIS:NE2	1:D:1203:ASN:OD1	2.39	0.56
1:A:3377:GLU:OE2	1:A:3378:GLN:NE2	2.39	0.55
1:B:1690:ASP:OD2	1:B:1693:GLN:NE2	2.40	0.55
1:D:1089:TYR:O	1:D:1226:PHE:N	2.38	0.55
1:C:1690:ASP:OD2	1:C:1693:GLN:NE2	2.40	0.55
1:A:635:THR:OG1	1:A:1693:GLN:OE1	2.17	0.55
1:C:3377:GLU:OE2	1:C:3378:GLN:NE2	2.39	0.55
1:D:3963:ASN:O	1:D:3966:THR:OG1	2.18	0.55
1:C:240:ASP:OD2	1:C:246:TYR:OH	2.23	0.55
1:C:3840:SER:OG	1:C:3877:ASP:OD2	2.23	0.55
1:B:206:CYS:SG	1:B:207:SER:N	2.80	0.55
1:B:240:ASP:OD2	1:B:246:TYR:OH	2.23	0.55
1:B:975:VAL:HG13	1:B:1047:LEU:HD23	1.89	0.55
1:B:3377:GLU:OE2	1:B:3378:GLN:NE2	2.39	0.55
1:B:3840:SER:OG	1:B:3877:ASP:OD2	2.23	0.55
1:D:975:VAL:HG13	1:D:1047:LEU:HD23	1.89	0.55
1:A:2663:ASN:O	1:A:2667:THR:OG1	2.21	0.54
1:A:240:ASP:OD2	1:A:246:TYR:OH	2.23	0.54
1:A:3840:SER:OG	1:A:3877:ASP:OD2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:CYS:SG	1:C:207:SER:N	2.80	0.54
1:A:1690:ASP:OD2	1:A:1693:GLN:NE2	2.40	0.54
1:B:3786:CYS:O	1:B:3831:SER:OG	2.22	0.54
1:D:3661:TRP:O	1:D:3664:THR:OG1	2.22	0.54
1:A:206:CYS:SG	1:A:207:SER:N	2.80	0.54
1:A:4240:ASP:OD2	1:A:4672:LYS:NZ	2.33	0.54
1:C:4713:SER:OG	1:C:4775:TYR:OH	2.26	0.54
1:C:4705:VAL:O	1:C:4708:THR:OG1	2.26	0.54
1:A:1863:LEU:HD21	1:A:1870:VAL:CG1	2.38	0.54
1:B:3271:GLU:OE2	1:B:3337:ARG:NH1	2.41	0.54
1:C:4936:ILE:HD11	1:D:4927:ILE:HD12	1.90	0.54
1:D:4705:VAL:O	1:D:4708:THR:OG1	2.26	0.54
1:D:4713:SER:OG	1:D:4775:TYR:OH	2.26	0.54
1:A:4991:PHE:O	1:A:4995:LEU:HD23	2.08	0.53
1:B:4184:MET:SD	1:B:4185:GLY:N	2.81	0.53
1:A:975:VAL:HG13	1:A:1047:LEU:HD23	1.89	0.53
1:D:4991:PHE:O	1:D:4995:LEU:HD23	2.08	0.53
1:D:4184:MET:SD	1:D:4185:GLY:N	2.81	0.53
1:A:3737:GLU:OE1	1:A:3806:ASN:ND2	2.42	0.53
1:A:3786:CYS:O	1:A:3831:SER:OG	2.22	0.53
1:C:4184:MET:SD	1:C:4185:GLY:N	2.81	0.53
1:B:1269:CYS:SG	1:B:1473:THR:OG1	2.54	0.53
1:B:4705:VAL:O	1:B:4708:THR:OG1	2.26	0.53
1:C:683:ARG:N	1:C:782:SER:OG	2.42	0.53
1:C:1863:LEU:HD21	1:C:1870:VAL:CG1	2.38	0.53
1:D:1863:LEU:HD21	1:D:1870:VAL:CG1	2.38	0.53
1:B:745:SER:OG	1:B:746:CYS:N	2.42	0.53
1:D:1690:ASP:OD2	1:D:1693:GLN:NE2	2.40	0.53
1:C:975:VAL:HG13	1:C:1047:LEU:HD23	1.89	0.53
1:A:4184:MET:SD	1:A:4185:GLY:N	2.81	0.53
1:B:1164:LEU:HD12	1:B:1169:LEU:HD13	1.91	0.53
1:D:1164:LEU:HD12	1:D:1169:LEU:HD13	1.91	0.53
1:B:3661:TRP:O	1:B:3664:THR:OG1	2.22	0.53
1:B:4936:ILE:HD11	1:C:4927:ILE:HD12	1.91	0.53
1:D:3271:GLU:OE2	1:D:3337:ARG:NH1	2.41	0.53
1:D:4794:TRP:NE1	1:D:4798:MET:HE1	2.24	0.53
1:A:307:ALA:HB1	1:A:312:THR:HG21	1.91	0.53
1:A:4705:VAL:O	1:A:4708:THR:OG1	2.26	0.53
1:B:3737:GLU:OE1	1:B:3806:ASN:ND2	2.42	0.53
1:B:4794:TRP:NE1	1:B:4798:MET:HE1	2.24	0.53
1:D:3737:GLU:OE1	1:D:3806:ASN:ND2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3271:GLU:OE2	1:A:3337:ARG:NH1	2.41	0.52
1:C:1500:PHE:O	1:C:1534:LYS:NZ	2.30	0.52
1:D:931:THR:HB	1:D:988:LEU:HD22	1.90	0.52
1:A:683:ARG:N	1:A:782:SER:OG	2.42	0.52
1:A:4936:ILE:HD11	1:B:4927:ILE:HD12	1.91	0.52
1:C:4794:TRP:NE1	1:C:4798:MET:HE1	2.24	0.52
1:A:745:SER:OG	1:A:746:CYS:N	2.42	0.52
1:A:4982:GLU:N	1:A:4982:GLU:OE1	2.43	0.52
1:B:3046:LEU:O	1:B:3050:VAL:HG12	2.09	0.52
1:C:307:ALA:HB1	1:C:312:THR:HG21	1.91	0.52
1:C:4991:PHE:O	1:C:4995:LEU:HD23	2.08	0.52
1:D:206:CYS:SG	1:D:207:SER:N	2.80	0.52
1:D:683:ARG:N	1:D:782:SER:OG	2.42	0.52
1:D:1663:HIS:O	1:D:1666:THR:OG1	2.25	0.52
1:A:586:ILE:HG21	1:A:603:LEU:HD21	1.92	0.52
1:A:931:THR:HB	1:A:988:LEU:HD22	1.90	0.52
1:B:1863:LEU:HD21	1:B:1870:VAL:CG1	2.38	0.52
1:C:1164:LEU:HD12	1:C:1169:LEU:HD13	1.91	0.52
1:C:3271:GLU:OE2	1:C:3337:ARG:NH1	2.41	0.52
1:D:307:ALA:HB1	1:D:312:THR:HG21	1.91	0.52
1:C:745:SER:OG	1:C:746:CYS:N	2.42	0.52
1:D:586:ILE:HG21	1:D:603:LEU:HD21	1.92	0.52
1:A:1164:LEU:HD12	1:A:1169:LEU:HD13	1.91	0.52
1:B:683:ARG:N	1:B:782:SER:OG	2.42	0.52
1:C:931:THR:HB	1:C:988:LEU:HD22	1.90	0.52
1:C:3046:LEU:O	1:C:3050:VAL:HG12	2.09	0.52
1:C:3737:GLU:OE1	1:C:3806:ASN:ND2	2.42	0.52
1:A:4927:ILE:HD12	1:D:4936:ILE:HD11	1.92	0.52
1:B:907:LEU:O	1:B:963:ASN:ND2	2.42	0.52
1:B:4991:PHE:O	1:B:4995:LEU:HD23	2.08	0.52
1:C:907:LEU:O	1:C:963:ASN:ND2	2.42	0.52
1:D:745:SER:OG	1:D:746:CYS:N	2.42	0.52
1:D:907:LEU:O	1:D:963:ASN:ND2	2.42	0.52
1:D:3246:LEU:HD13	1:D:3281:LEU:HD21	1.91	0.52
2:E:54:GLU:N	2:E:54:GLU:OE1	2.43	0.52
2:G:54:GLU:N	2:G:54:GLU:OE1	2.43	0.52
1:A:907:LEU:O	1:A:963:ASN:ND2	2.42	0.52
1:A:4794:TRP:NE1	1:A:4798:MET:HE1	2.24	0.52
1:B:565:TYR:CZ	1:B:569:ILE:HD11	2.45	0.52
1:B:586:ILE:HG21	1:B:603:LEU:HD21	1.92	0.52
1:B:4713:SER:HG	1:B:4775:TYR:HH	1.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3786:CYS:O	1:C:3831:SER:OG	2.22	0.52
1:A:3284:TRP:HB3	1:A:3305:THR:HG21	1.92	0.52
1:D:4982:GLU:N	1:D:4982:GLU:OE1	2.43	0.52
1:A:565:TYR:CZ	1:A:569:ILE:HD11	2.45	0.51
1:A:4155:PRO:CG	1:A:5036:LEU:HD23	2.41	0.51
1:B:307:ALA:HB1	1:B:312:THR:HG21	1.91	0.51
1:D:4155:PRO:CG	1:D:5036:LEU:HD23	2.41	0.51
2:H:54:GLU:OE1	2:H:54:GLU:N	2.43	0.51
1:A:3246:LEU:HD13	1:A:3281:LEU:HD21	1.91	0.51
1:B:156:GLN:OE1	1:B:157:ARG:NH1	2.44	0.51
1:B:4155:PRO:CG	1:B:5036:LEU:HD23	2.41	0.51
1:C:586:ILE:HG21	1:C:603:LEU:HD21	1.92	0.51
1:C:4982:GLU:N	1:C:4982:GLU:OE1	2.43	0.51
1:D:3046:LEU:O	1:D:3050:VAL:HG12	2.09	0.51
1:D:3284:TRP:HB3	1:D:3305:THR:HG21	1.92	0.51
2:F:54:GLU:N	2:F:54:GLU:OE1	2.43	0.51
1:A:156:GLN:OE1	1:A:157:ARG:NH1	2.44	0.51
1:A:3046:LEU:O	1:A:3050:VAL:HG12	2.09	0.51
1:A:3575:LEU:HD13	1:B:1208:VAL:HG11	1.93	0.51
1:B:931:THR:HB	1:B:988:LEU:HD22	1.90	0.51
1:C:156:GLN:OE1	1:C:157:ARG:NH1	2.44	0.51
1:C:3246:LEU:HD13	1:C:3281:LEU:HD21	1.91	0.51
1:B:3246:LEU:HD13	1:B:3281:LEU:HD21	1.91	0.51
1:B:4982:GLU:OE1	1:B:4982:GLU:N	2.43	0.51
1:C:207:SER:OG	1:C:208:CYS:N	2.43	0.51
1:D:3840:SER:OG	1:D:3877:ASP:OD2	2.23	0.51
1:A:1141:ARG:NH1	1:A:1142:PRO:O	2.44	0.51
1:B:1147:ASP:OD1	1:B:1165:ASN:N	2.44	0.51
1:C:4155:PRO:CG	1:C:5036:LEU:HD23	2.41	0.51
1:D:886:ARG:NH2	1:D:889:GLN:OE1	2.44	0.51
1:B:207:SER:OG	1:B:208:CYS:N	2.43	0.51
1:B:886:ARG:NH2	1:B:889:GLN:OE1	2.44	0.51
1:B:3284:TRP:HB3	1:B:3305:THR:HG21	1.92	0.51
1:D:1141:ARG:NH1	1:D:1142:PRO:O	2.44	0.51
1:A:4713:SER:OG	1:A:4775:TYR:OH	2.26	0.51
1:C:1663:HIS:O	1:C:1666:THR:OG1	2.25	0.51
1:D:1147:ASP:OD1	1:D:1165:ASN:N	2.44	0.51
1:C:565:TYR:CZ	1:C:569:ILE:HD11	2.45	0.51
1:A:703:GLY:N	1:A:1647:CYS:SG	2.84	0.51
1:A:886:ARG:NH2	1:A:889:GLN:OE1	2.44	0.51
1:B:1141:ARG:NH1	1:B:1142:PRO:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:703:GLY:N	1:C:1647:CYS:SG	2.84	0.51
2:H:67:SER:OG	2:H:68:LEU:N	2.44	0.51
1:C:4056:GLU:OE1	1:C:4056:GLU:N	2.44	0.50
1:A:1147:ASP:OD1	1:A:1165:ASN:N	2.44	0.50
1:A:4056:GLU:OE1	1:A:4056:GLU:N	2.44	0.50
1:B:864:PRO:HD2	1:B:867:LEU:HD12	1.94	0.50
1:C:1147:ASP:OD1	1:C:1165:ASN:N	2.44	0.50
1:B:575:LEU:HD11	1:B:606:LEU:O	2.12	0.50
1:C:864:PRO:HD2	1:C:867:LEU:HD12	1.94	0.50
1:D:320:LYS:NZ	1:D:383:HIS:O	2.42	0.50
1:D:635:THR:OG1	1:D:1693:GLN:OE1	2.17	0.50
1:A:864:PRO:HD2	1:A:867:LEU:HD12	1.94	0.50
1:C:886:ARG:NH2	1:C:889:GLN:OE1	2.44	0.50
1:C:1141:ARG:NH1	1:C:1142:PRO:O	2.44	0.50
1:D:575:LEU:HD11	1:D:606:LEU:O	2.12	0.50
1:D:703:GLY:N	1:D:1647:CYS:SG	2.84	0.50
1:A:207:SER:OG	1:A:208:CYS:N	2.43	0.50
1:B:703:GLY:N	1:B:1647:CYS:SG	2.84	0.50
1:A:575:LEU:HD11	1:A:606:LEU:O	2.12	0.50
1:D:320:LYS:NZ	1:D:381:GLU:O	2.43	0.50
1:D:3772:THR:O	1:D:3815:LYS:NZ	2.42	0.50
1:A:711:LEU:HD13	1:A:1532:ASN:HB3	1.94	0.50
1:C:320:LYS:NZ	1:C:383:HIS:O	2.42	0.50
1:C:575:LEU:HD11	1:C:606:LEU:O	2.12	0.50
1:D:156:GLN:OE1	1:D:157:ARG:NH1	2.44	0.50
1:B:711:LEU:HD13	1:B:1532:ASN:HB3	1.94	0.50
1:C:711:LEU:HD13	1:C:1532:ASN:HB3	1.94	0.49
1:D:864:PRO:HD2	1:D:867:LEU:HD12	1.94	0.49
1:A:714:TYR:CE1	1:A:1514:LEU:HD13	2.47	0.49
1:A:4920:PHE:CZ	1:A:4924:VAL:HG11	2.47	0.49
1:C:3661:TRP:O	1:C:3664:THR:OG1	2.22	0.49
1:D:565:TYR:CZ	1:D:569:ILE:HD11	2.45	0.49
1:D:3786:CYS:O	1:D:3831:SER:OG	2.22	0.49
2:G:67:SER:OG	2:G:68:LEU:N	2.44	0.49
1:B:714:TYR:CE1	1:B:1514:LEU:HD13	2.47	0.49
1:C:3284:TRP:HB3	1:C:3305:THR:HG21	1.92	0.49
1:D:4920:PHE:CZ	1:D:4924:VAL:HG11	2.47	0.49
1:C:4199:GLU:OE1	1:C:4199:GLU:N	2.45	0.49
1:D:2663:ASN:O	1:D:2667:THR:OG1	2.21	0.49
1:A:4199:GLU:N	1:A:4199:GLU:OE1	2.45	0.49
1:B:4056:GLU:N	1:B:4056:GLU:OE1	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:711:LEU:HD13	1:D:1532:ASN:HB3	1.94	0.49
1:D:4199:GLU:N	1:D:4199:GLU:OE1	2.45	0.49
1:C:714:TYR:CE1	1:C:1514:LEU:HD13	2.47	0.49
1:C:4920:PHE:CZ	1:C:4924:VAL:HG11	2.47	0.49
1:D:1450:VAL:CG1	1:D:1454:THR:HG21	2.43	0.49
1:A:1973:GLN:OE1	1:A:1976:ARG:NH1	2.46	0.49
1:A:2736:ASP:OD1	1:A:2736:ASP:N	2.46	0.49
1:A:3376:GLU:OE1	1:A:3376:GLU:N	2.45	0.49
1:D:5033:GLU:OE1	1:D:5033:GLU:N	2.46	0.49
1:C:917:GLU:OE1	1:C:917:GLU:N	2.46	0.49
1:C:1490:SER:OG	1:C:1491:ASN:N	2.46	0.49
1:D:714:TYR:CE1	1:D:1514:LEU:HD13	2.47	0.49
1:A:559:GLY:O	1:A:563:VAL:HG23	2.13	0.49
1:B:917:GLU:N	1:B:917:GLU:OE1	2.46	0.49
1:B:3802:ILE:HD12	1:B:3886:ARG:HG3	1.94	0.49
1:A:2452:ARG:NH1	1:B:177:GLU:OE2	2.45	0.49
1:C:559:GLY:O	1:C:563:VAL:HG23	2.13	0.49
1:D:2587:TYR:O	1:D:2590:SER:N	2.46	0.49
2:E:67:SER:OG	2:E:68:LEU:N	2.44	0.49
1:A:3274:LEU:HD21	1:A:3319:ILE:CD1	2.43	0.48
1:B:559:GLY:O	1:B:563:VAL:HG23	2.13	0.48
1:D:559:GLY:O	1:D:563:VAL:HG23	2.13	0.48
1:D:2736:ASP:OD1	1:D:2736:ASP:N	2.46	0.48
1:A:320:LYS:NZ	1:A:381:GLU:O	2.43	0.48
1:B:4199:GLU:N	1:B:4199:GLU:OE1	2.45	0.48
1:A:3802:ILE:HD12	1:A:3886:ARG:HG3	1.94	0.48
1:D:1857:GLU:OE1	1:D:1857:GLU:N	2.46	0.48
1:C:3802:ILE:HD12	1:C:3886:ARG:HG3	1.94	0.48
1:D:3802:ILE:HD12	1:D:3886:ARG:HG3	1.94	0.48
1:B:3274:LEU:HD21	1:B:3319:ILE:CD1	2.43	0.48
1:D:1973:GLN:OE1	1:D:1976:ARG:NH1	2.46	0.48
1:C:3259:SER:OG	1:C:3260:GLY:N	2.47	0.48
1:C:3376:GLU:OE1	1:C:3376:GLU:N	2.45	0.48
1:A:1490:SER:OG	1:A:1491:ASN:N	2.46	0.48
1:A:2830:GLU:N	1:A:2830:GLU:OE1	2.47	0.48
1:B:1973:GLN:OE1	1:B:1976:ARG:NH1	2.46	0.48
1:B:3575:LEU:HD13	1:C:1208:VAL:HG11	1.95	0.48
1:C:1207:ASP:N	1:C:1207:ASP:OD1	2.47	0.48
1:D:1490:SER:OG	1:D:1491:ASN:N	2.46	0.48
1:D:3376:GLU:OE1	1:D:3376:GLU:N	2.45	0.48
1:A:2587:TYR:O	1:A:2590:SER:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4920:PHE:CZ	1:B:4924:VAL:HG11	2.47	0.48
1:C:2587:TYR:O	1:C:2590:SER:N	2.46	0.48
1:D:917:GLU:N	1:D:917:GLU:OE1	2.46	0.48
1:B:320:LYS:NZ	1:B:383:HIS:O	2.42	0.48
1:B:1260:MET:N	1:B:1269:CYS:O	2.47	0.48
1:B:1490:SER:OG	1:B:1491:ASN:N	2.46	0.48
1:B:1663:HIS:O	1:B:1666:THR:OG1	2.25	0.48
1:B:5033:GLU:OE1	1:B:5033:GLU:N	2.46	0.48
1:C:1450:VAL:CG1	1:C:1454:THR:HG21	2.43	0.48
1:C:4713:SER:HG	1:C:4775:TYR:HH	1.59	0.48
1:D:2830:GLU:OE1	1:D:2830:GLU:N	2.47	0.48
1:A:3259:SER:OG	1:A:3260:GLY:N	2.46	0.47
1:A:5000:GLU:OE1	1:A:5000:GLU:N	2.47	0.47
1:B:2126:ARG:NE	1:B:2133:GLU:OE2	2.47	0.47
1:B:2587:TYR:O	1:B:2590:SER:N	2.46	0.47
1:B:2830:GLU:OE1	1:B:2830:GLU:N	2.47	0.47
1:C:1973:GLN:OE1	1:C:1976:ARG:NH1	2.46	0.47
1:D:530:ILE:HD11	1:D:537:CYS:HA	1.96	0.47
1:D:1260:MET:N	1:D:1269:CYS:O	2.47	0.47
1:C:5000:GLU:OE1	1:C:5000:GLU:N	2.47	0.47
1:D:2126:ARG:NE	1:D:2133:GLU:OE2	2.47	0.47
1:A:917:GLU:N	1:A:917:GLU:OE1	2.46	0.47
1:A:1663:HIS:O	1:A:1666:THR:OG1	2.25	0.47
1:B:3772:THR:O	1:B:3815:LYS:NZ	2.42	0.47
1:D:2042:CYS:SG	1:D:2043:GLY:N	2.87	0.47
1:D:2115:GLU:OE1	1:D:2115:GLU:N	2.47	0.47
1:D:5000:GLU:N	1:D:5000:GLU:OE1	2.47	0.47
1:A:1260:MET:N	1:A:1269:CYS:O	2.47	0.47
1:A:3772:THR:O	1:A:3815:LYS:NZ	2.42	0.47
1:A:5033:GLU:OE1	1:A:5033:GLU:N	2.46	0.47
1:B:1450:VAL:CG1	1:B:1454:THR:HG21	2.43	0.47
1:C:635:THR:OG1	1:C:1693:GLN:OE1	2.17	0.47
1:C:2126:ARG:NE	1:C:2133:GLU:OE2	2.47	0.47
1:C:2830:GLU:N	1:C:2830:GLU:OE1	2.47	0.47
1:D:3274:LEU:HD21	1:D:3319:ILE:CD1	2.43	0.47
1:A:530:ILE:HD11	1:A:537:CYS:HA	1.96	0.47
1:B:2452:ARG:NH1	1:C:177:GLU:OE2	2.47	0.47
1:B:3259:SER:OG	1:B:3260:GLY:N	2.47	0.47
1:B:5000:GLU:N	1:B:5000:GLU:OE1	2.47	0.47
1:B:1857:GLU:N	1:B:1857:GLU:OE1	2.46	0.47
1:B:2663:ASN:O	1:B:2667:THR:OG1	2.21	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4713:SER:OG	1:B:4775:TYR:OH	2.26	0.47
1:C:2115:GLU:OE1	1:C:2115:GLU:N	2.47	0.47
1:C:2452:ARG:NH1	1:D:177:GLU:OE2	2.47	0.47
1:A:69:LEU:CD2	1:A:107:ILE:HD11	2.45	0.47
1:B:2736:ASP:N	1:B:2736:ASP:OD1	2.46	0.47
1:C:1857:GLU:N	1:C:1857:GLU:OE1	2.46	0.47
1:C:2042:CYS:SG	1:C:2043:GLY:N	2.87	0.47
1:C:3274:LEU:HD21	1:C:3319:ILE:CD1	2.43	0.47
1:D:69:LEU:CD2	1:D:107:ILE:HD11	2.45	0.47
1:B:2770:LYS:O	1:B:2774:ASN:N	2.48	0.47
1:D:2770:LYS:O	1:D:2774:ASN:N	2.48	0.47
1:D:3259:SER:OG	1:D:3260:GLY:N	2.47	0.47
1:A:161:GLU:N	1:A:161:GLU:OE1	2.48	0.47
1:A:1207:ASP:N	1:A:1207:ASP:OD1	2.47	0.47
1:A:2042:CYS:SG	1:A:2043:GLY:N	2.87	0.47
1:A:2126:ARG:NE	1:A:2133:GLU:OE2	2.47	0.47
1:C:161:GLU:N	1:C:161:GLU:OE1	2.48	0.47
1:C:445:LEU:HD23	1:C:521:LEU:HB3	1.97	0.47
1:C:5033:GLU:OE1	1:C:5033:GLU:N	2.46	0.47
1:A:2770:LYS:O	1:A:2774:ASN:N	2.48	0.47
1:C:2736:ASP:OD1	1:C:2736:ASP:N	2.46	0.47
1:D:161:GLU:N	1:D:161:GLU:OE1	2.48	0.47
1:A:177:GLU:OE2	1:D:2452:ARG:NH1	2.48	0.46
1:A:3344:PRO:O	1:A:3348:ARG:NH1	2.48	0.46
1:A:4237:PHE:O	1:A:4241:THR:OG1	2.28	0.46
1:B:69:LEU:CD2	1:B:107:ILE:HD11	2.45	0.46
1:D:3344:PRO:O	1:D:3348:ARG:NH1	2.48	0.46
1:A:320:LYS:NZ	1:A:383:HIS:O	2.42	0.46
1:A:3552:PHE:O	1:A:3556:ASN:ND2	2.47	0.46
1:C:3173:TYR:OH	1:C:3242:ASP:O	2.20	0.46
1:C:3344:PRO:O	1:C:3348:ARG:NH1	2.48	0.46
1:C:3575:LEU:HD13	1:D:1208:VAL:HG11	1.96	0.46
1:C:3772:THR:O	1:C:3815:LYS:NZ	2.42	0.46
1:D:207:SER:OG	1:D:208:CYS:N	2.43	0.46
1:A:1857:GLU:OE1	1:A:1857:GLU:N	2.46	0.46
1:B:2042:CYS:SG	1:B:2043:GLY:N	2.87	0.46
1:B:3376:GLU:N	1:B:3376:GLU:OE1	2.45	0.46
1:D:445:LEU:HD23	1:D:521:LEU:HB3	1.97	0.46
1:D:1207:ASP:OD1	1:D:1207:ASP:N	2.47	0.46
1:D:4056:GLU:OE1	1:D:4056:GLU:N	2.44	0.46
1:A:1456:ASP:N	1:A:1456:ASP:OD1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2115:GLU:OE1	1:A:2115:GLU:N	2.47	0.46
1:C:530:ILE:HD11	1:C:537:CYS:HA	1.96	0.46
1:C:2770:LYS:O	1:C:2774:ASN:N	2.48	0.46
1:B:2347:GLU:N	1:B:2347:GLU:OE1	2.49	0.46
1:B:4003:LEU:HD21	1:B:4012:LEU:HD23	1.98	0.46
1:D:1608:MET:SD	1:D:1608:MET:N	2.88	0.46
1:D:4152:GLU:OE1	1:D:4180:ARG:NH2	2.49	0.46
1:A:4144:ALA:O	1:A:4148:THR:OG1	2.24	0.46
1:B:530:ILE:HD11	1:B:537:CYS:HA	1.96	0.46
1:B:1456:ASP:OD1	1:B:1456:ASP:N	2.49	0.46
1:C:69:LEU:CD2	1:C:107:ILE:HD11	2.45	0.46
1:C:1260:MET:N	1:C:1269:CYS:O	2.47	0.46
1:B:3344:PRO:O	1:B:3348:ARG:NH1	2.48	0.46
1:C:2347:GLU:N	1:C:2347:GLU:OE1	2.49	0.46
2:F:67:SER:OG	2:F:68:LEU:N	2.44	0.46
1:A:1093:GLU:O	1:A:1201:HIS:N	2.49	0.46
1:A:1450:VAL:CG1	1:A:1454:THR:HG21	2.43	0.46
1:B:445:LEU:HD23	1:B:521:LEU:HB3	1.97	0.46
1:B:2351:ASN:O	1:B:2355:ARG:NE	2.49	0.46
1:C:1456:ASP:N	1:C:1456:ASP:OD1	2.49	0.46
1:D:1093:GLU:O	1:D:1201:HIS:N	2.49	0.46
1:D:3173:TYR:OH	1:D:3242:ASP:O	2.20	0.46
1:D:4157:ASP:OD2	1:D:4159:ARG:NH1	2.49	0.46
1:A:3453:ARG:NH1	1:A:3456:GLN:OE1	2.49	0.46
1:A:4157:ASP:OD2	1:A:4159:ARG:NH1	2.49	0.46
1:B:1207:ASP:OD1	1:B:1207:ASP:N	2.47	0.46
1:B:2115:GLU:N	1:B:2115:GLU:OE1	2.47	0.46
1:A:445:LEU:HD23	1:A:521:LEU:HB3	1.98	0.45
1:A:755:ILE:HD11	1:A:771:PHE:HZ	1.81	0.45
1:C:242:ARG:NH1	1:C:481:GLU:OE2	2.50	0.45
1:C:3141:THR:HG22	1:C:3193:CYS:HA	1.98	0.45
1:A:4003:LEU:HD21	1:A:4012:LEU:HD23	1.98	0.45
1:A:4152:GLU:OE1	1:A:4180:ARG:NH2	2.49	0.45
1:B:635:THR:OG1	1:B:1693:GLN:OE1	2.17	0.45
1:B:3166:TYR:OH	1:B:3243:ILE:HD12	2.16	0.45
1:C:3552:PHE:O	1:C:3556:ASN:ND2	2.47	0.45
1:C:4152:GLU:OE1	1:C:4180:ARG:NH2	2.49	0.45
1:A:2347:GLU:OE1	1:A:2347:GLU:N	2.49	0.45
1:D:1456:ASP:OD1	1:D:1456:ASP:N	2.49	0.45
1:A:3166:TYR:OH	1:A:3243:ILE:HD12	2.16	0.45
1:B:161:GLU:OE1	1:B:161:GLU:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:755:ILE:HD11	1:B:771:PHE:HZ	1.81	0.45
1:B:2439:GLU:O	1:B:2508:ARG:NH2	2.50	0.45
1:B:4152:GLU:OE1	1:B:4180:ARG:NH2	2.49	0.45
1:B:4157:ASP:OD2	1:B:4159:ARG:NH1	2.49	0.45
1:C:3166:TYR:OH	1:C:3243:ILE:HD12	2.16	0.45
1:D:3453:ARG:NH1	1:D:3456:GLN:OE1	2.49	0.45
1:B:1608:MET:SD	1:B:1608:MET:N	2.88	0.45
1:C:2663:ASN:O	1:C:2667:THR:OG1	2.21	0.45
1:D:242:ARG:NH1	1:D:481:GLU:OE2	2.50	0.45
1:D:748:LEU:HD12	1:D:755:ILE:HD12	1.99	0.45
1:D:755:ILE:HD11	1:D:771:PHE:HZ	1.81	0.45
1:D:3166:TYR:OH	1:D:3243:ILE:HD12	2.16	0.45
1:D:3552:PHE:O	1:D:3556:ASN:ND2	2.47	0.45
1:A:748:LEU:HD12	1:A:755:ILE:HD12	1.99	0.45
1:B:483:MET:N	1:B:483:MET:HE2	2.32	0.45
1:C:4157:ASP:OD2	1:C:4159:ARG:NH1	2.49	0.45
1:D:307:ALA:CB	1:D:312:THR:HG21	2.47	0.45
1:D:1637:MET:SD	1:D:1637:MET:N	2.90	0.45
1:B:1041:GLN:OE1	1:B:1044:ARG:NE	2.50	0.45
1:B:3552:PHE:O	1:B:3556:ASN:ND2	2.47	0.45
1:C:2351:ASN:O	1:C:2355:ARG:NE	2.49	0.45
1:D:3141:THR:HG22	1:D:3193:CYS:HA	1.98	0.45
1:A:242:ARG:NH1	1:A:481:GLU:OE2	2.49	0.45
1:A:483:MET:HE2	1:A:483:MET:N	2.32	0.45
1:B:4924:VAL:HG13	1:B:4925:ILE:HG13	1.99	0.45
1:C:755:ILE:HD11	1:C:771:PHE:HZ	1.82	0.45
1:D:483:MET:N	1:D:483:MET:HE2	2.32	0.45
1:D:2347:GLU:OE1	1:D:2347:GLU:N	2.49	0.45
1:D:2439:GLU:O	1:D:2508:ARG:NH2	2.50	0.45
1:A:3141:THR:HG22	1:A:3193:CYS:HA	1.98	0.45
1:B:3141:THR:HG22	1:B:3193:CYS:HA	1.98	0.45
1:C:3546:ASP:O	1:C:3597:GLN:NE2	2.50	0.45
1:C:4003:LEU:HD21	1:C:4012:LEU:HD23	1.98	0.45
1:D:4003:LEU:HD21	1:D:4012:LEU:HD23	1.98	0.45
1:B:242:ARG:NH1	1:B:481:GLU:OE2	2.50	0.44
1:B:320:LYS:NZ	1:B:381:GLU:O	2.43	0.44
1:C:1093:GLU:O	1:C:1201:HIS:N	2.49	0.44
1:C:3453:ARG:NH1	1:C:3456:GLN:OE1	2.49	0.44
1:A:307:ALA:CB	1:A:312:THR:HG21	2.47	0.44
1:C:483:MET:HE2	1:C:483:MET:N	2.32	0.44
1:C:1236:THR:OG1	1:C:1608:MET:SD	2.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1639:LEU:N	1:C:1648:MET:O	2.51	0.44
1:B:1236:THR:OG1	1:B:1608:MET:SD	2.76	0.44
1:C:748:LEU:HD12	1:C:755:ILE:HD12	1.99	0.44
1:C:3981:ALA:O	1:C:3986:TRP:NE1	2.49	0.44
1:C:4239:GLU:OE2	1:C:4679:ARG:NH2	2.51	0.44
1:D:1041:GLN:OE1	1:D:1044:ARG:NE	2.50	0.44
1:D:4924:VAL:HG13	1:D:4925:ILE:HG13	1.99	0.44
1:A:2439:GLU:O	1:A:2508:ARG:NH2	2.50	0.44
1:A:3546:ASP:O	1:A:3597:GLN:NE2	2.49	0.44
1:A:4165:GLU:N	1:A:4165:GLU:OE1	2.50	0.44
1:B:307:ALA:CB	1:B:312:THR:HG21	2.47	0.44
1:B:3453:ARG:NH1	1:B:3456:GLN:OE1	2.49	0.44
1:B:4165:GLU:N	1:B:4165:GLU:OE1	2.50	0.44
1:C:2629:ASP:O	1:C:2633:LEU:N	2.51	0.44
1:A:3206:LEU:HD12	1:A:3246:LEU:HD12	2.00	0.44
1:B:358:THR:HG21	1:B:383:HIS:HB2	2.00	0.44
1:B:3767:GLN:NE2	1:B:3804:ILE:O	2.50	0.44
1:C:4144:ALA:O	1:C:4148:THR:OG1	2.24	0.44
1:D:4165:GLU:N	1:D:4165:GLU:OE1	2.50	0.44
1:A:209:CYS:SG	1:A:210:GLU:N	2.91	0.44
1:A:346:CYS:N	1:A:388:LEU:O	2.49	0.44
1:B:3206:LEU:HD12	1:B:3246:LEU:HD12	2.00	0.44
1:C:307:ALA:CB	1:C:312:THR:HG21	2.47	0.44
1:C:358:THR:HG21	1:C:383:HIS:HB2	2.00	0.44
1:D:1700:ASP:OD1	1:D:1701:ALA:N	2.51	0.44
1:D:2629:ASP:O	1:D:2633:LEU:N	2.50	0.44
1:D:3269:VAL:O	1:D:3273:THR:OG1	2.17	0.44
1:D:3546:ASP:O	1:D:3597:GLN:NE2	2.49	0.44
1:A:784:SER:OG	1:A:785:ALA:N	2.51	0.44
1:B:209:CYS:SG	1:B:210:GLU:N	2.91	0.44
1:B:3981:ALA:O	1:B:3986:TRP:NE1	2.49	0.44
1:C:444:SER:O	1:C:448:LEU:HD23	2.18	0.44
1:C:1041:GLN:OE1	1:C:1044:ARG:NE	2.50	0.44
1:C:4094:GLN:O	1:C:4095:LYS:NZ	2.39	0.44
1:C:4924:VAL:HG13	1:C:4925:ILE:HG13	1.99	0.44
1:D:1236:THR:OG1	1:D:1608:MET:SD	2.76	0.44
1:D:2351:ASN:O	1:D:2355:ARG:NE	2.49	0.44
1:A:358:THR:HG21	1:A:383:HIS:HB2	2.00	0.44
1:A:1637:MET:SD	1:A:1637:MET:N	2.90	0.44
1:B:4144:ALA:O	1:B:4148:THR:OG1	2.24	0.44
1:C:784:SER:OG	1:C:785:ALA:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1637:MET:SD	1:C:1637:MET:N	2.90	0.44
1:C:2439:GLU:O	1:C:2508:ARG:NH2	2.50	0.44
1:C:3767:GLN:NE2	1:C:3804:ILE:O	2.50	0.44
1:D:1220:GLN:OE1	1:D:1220:GLN:N	2.51	0.44
1:A:444:SER:O	1:A:448:LEU:HD23	2.18	0.44
1:A:1236:THR:OG1	1:A:1608:MET:SD	2.76	0.44
1:B:748:LEU:HD12	1:B:755:ILE:HD12	1.99	0.44
1:B:1639:LEU:N	1:B:1648:MET:O	2.51	0.44
1:A:1041:GLN:OE1	1:A:1044:ARG:NE	2.50	0.43
1:C:209:CYS:SG	1:C:210:GLU:N	2.91	0.43
1:D:346:CYS:N	1:D:388:LEU:O	2.49	0.43
1:A:1208:VAL:HG11	1:D:3575:LEU:HD13	1.99	0.43
1:A:1615:VAL:HG11	1:A:1632:ASP:H	1.83	0.43
1:A:3152:PHE:O	1:A:3156:VAL:HG22	2.18	0.43
1:A:4794:TRP:O	1:A:4798:MET:HE3	2.19	0.43
1:B:1637:MET:SD	1:B:1637:MET:N	2.90	0.43
1:C:1700:ASP:OD1	1:C:1701:ALA:N	2.51	0.43
1:C:3206:LEU:HD12	1:C:3246:LEU:HD12	2.00	0.43
1:D:444:SER:O	1:D:448:LEU:HD23	2.18	0.43
1:D:3152:PHE:O	1:D:3156:VAL:HG22	2.18	0.43
1:A:217:GLY:O	1:A:261:ARG:NE	2.51	0.43
1:A:3767:GLN:NE2	1:A:3804:ILE:O	2.50	0.43
1:C:3152:PHE:O	1:C:3156:VAL:HG22	2.18	0.43
1:C:3156:VAL:HG23	1:C:3157:ILE:HG23	2.00	0.43
1:C:4165:GLU:OE1	1:C:4165:GLU:N	2.50	0.43
1:D:209:CYS:SG	1:D:210:GLU:N	2.91	0.43
1:D:1639:LEU:N	1:D:1648:MET:O	2.51	0.43
1:D:3156:VAL:HG23	1:D:3157:ILE:HG23	2.00	0.43
1:A:1639:LEU:N	1:A:1648:MET:O	2.51	0.43
1:A:4239:GLU:OE2	1:A:4679:ARG:NH2	2.51	0.43
1:D:3206:LEU:HD12	1:D:3246:LEU:HD12	2.00	0.43
1:A:4924:VAL:HG13	1:A:4925:ILE:HG13	1.99	0.43
1:C:217:GLY:O	1:C:261:ARG:NE	2.51	0.43
1:C:1690:ASP:OD1	1:C:1692:ALA:N	2.51	0.43
1:A:3966:THR:HG22	1:A:4026:MET:HA	2.00	0.43
1:B:1205:GLY:HA2	1:B:1211:LEU:HD21	2.01	0.43
1:B:1615:VAL:HG11	1:B:1632:ASP:H	1.83	0.43
1:C:1259:ARG:NH1	1:C:1595:LEU:O	2.52	0.43
1:D:3767:GLN:NE2	1:D:3804:ILE:O	2.50	0.43
1:B:346:CYS:N	1:B:388:LEU:O	2.49	0.43
1:B:784:SER:OG	1:B:785:ALA:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2629:ASP:O	1:B:2633:LEU:N	2.51	0.43
1:D:4239:GLU:OE2	1:D:4679:ARG:NH2	2.51	0.43
1:A:1608:MET:SD	1:A:1608:MET:N	2.88	0.43
1:C:4240:ASP:OD2	1:C:4672:LYS:NZ	2.33	0.43
1:D:358:THR:HG21	1:D:383:HIS:HB2	2.00	0.43
1:A:3661:TRP:O	1:A:3664:THR:OG1	2.22	0.43
1:B:444:SER:O	1:B:448:LEU:HD23	2.18	0.43
1:B:1259:ARG:NH1	1:B:1595:LEU:O	2.52	0.43
1:B:3156:VAL:HG23	1:B:3157:ILE:HG23	2.00	0.43
1:B:3966:THR:HG22	1:B:4026:MET:HA	2.00	0.43
1:C:1205:GLY:HA2	1:C:1211:LEU:HD21	2.01	0.43
1:C:3308:THR:OG1	1:C:3311:HIS:N	2.51	0.43
1:D:1690:ASP:OD1	1:D:1692:ALA:N	2.51	0.43
1:B:1093:GLU:O	1:B:1201:HIS:N	2.49	0.43
1:B:3152:PHE:O	1:B:3156:VAL:HG22	2.18	0.43
1:C:1042:ALA:O	1:C:1045:THR:OG1	2.30	0.43
1:D:217:GLY:O	1:D:261:ARG:NE	2.51	0.43
1:A:1115:LEU:HD23	1:A:1123:VAL:HG11	2.00	0.42
1:B:4794:TRP:O	1:B:4798:MET:HE3	2.19	0.42
1:C:1515:VAL:HG22	1:C:1530:THR:HG23	2.02	0.42
1:C:3966:THR:HG22	1:C:4026:MET:HA	2.00	0.42
1:D:1115:LEU:HD23	1:D:1123:VAL:HG11	2.00	0.42
1:D:1259:ARG:NH1	1:D:1595:LEU:O	2.52	0.42
1:A:1259:ARG:NH1	1:A:1595:LEU:O	2.52	0.42
1:A:1700:ASP:OD1	1:A:1701:ALA:N	2.51	0.42
1:A:3981:ALA:O	1:A:3986:TRP:NE1	2.49	0.42
1:B:217:GLY:O	1:B:261:ARG:NE	2.51	0.42
1:C:1608:MET:SD	1:C:1608:MET:N	2.88	0.42
1:D:784:SER:OG	1:D:785:ALA:N	2.51	0.42
1:C:1615:VAL:HG11	1:C:1632:ASP:H	1.83	0.42
1:D:1515:VAL:HG22	1:D:1530:THR:HG23	2.02	0.42
1:D:1615:VAL:HG11	1:D:1632:ASP:H	1.83	0.42
1:D:3966:THR:HG22	1:D:4026:MET:HA	2.00	0.42
1:D:4094:GLN:O	1:D:4095:LYS:NZ	2.39	0.42
1:D:4237:PHE:O	1:D:4241:THR:OG1	2.28	0.42
1:A:479:GLN:NE2	1:A:480:GLU:OE1	2.53	0.42
1:A:1205:GLY:HA2	1:A:1211:LEU:HD21	2.01	0.42
1:A:2351:ASN:O	1:A:2355:ARG:NE	2.49	0.42
1:A:3156:VAL:HG23	1:A:3157:ILE:HG23	2.00	0.42
1:A:4642:ALA:O	1:A:4646:LEU:HD23	2.20	0.42
1:B:479:GLN:NE2	1:B:480:GLU:OE1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4994:TYR:O	1:B:4998:LYS:N	2.48	0.42
1:C:4642:ALA:O	1:C:4646:LEU:HD23	2.19	0.42
1:D:2650:ARG:O	1:D:2654:TYR:N	2.53	0.42
1:D:4642:ALA:O	1:D:4646:LEU:HD23	2.20	0.42
1:B:1115:LEU:HD23	1:B:1123:VAL:HG11	2.00	0.42
1:B:1700:ASP:OD1	1:B:1701:ALA:N	2.51	0.42
1:B:3308:THR:OG1	1:B:3311:HIS:N	2.51	0.42
1:C:1115:LEU:HD23	1:C:1123:VAL:HG11	2.00	0.42
1:D:4794:TRP:O	1:D:4798:MET:HE3	2.19	0.42
1:C:320:LYS:NZ	1:C:381:GLU:O	2.43	0.42
1:C:2650:ARG:O	1:C:2654:TYR:N	2.53	0.42
1:D:35:LEU:HD22	1:D:49:LEU:HD21	2.02	0.42
1:D:4994:TYR:O	1:D:4998:LYS:N	2.48	0.42
1:B:4003:LEU:CD2	1:B:4012:LEU:HD23	2.50	0.42
1:B:4642:ALA:O	1:B:4646:LEU:HD23	2.20	0.42
1:D:1863:LEU:HD21	1:D:1870:VAL:HG12	2.01	0.42
1:A:4003:LEU:CD2	1:A:4012:LEU:HD23	2.50	0.42
1:B:3546:ASP:O	1:B:3597:GLN:NE2	2.49	0.42
1:C:35:LEU:HD22	1:C:49:LEU:HD21	2.02	0.42
1:C:4794:TRP:O	1:C:4798:MET:HE3	2.19	0.42
1:B:1220:GLN:OE1	1:B:1220:GLN:N	2.51	0.42
1:B:1515:VAL:HG22	1:B:1530:THR:HG23	2.02	0.42
1:B:1863:LEU:HD21	1:B:1870:VAL:HG12	2.01	0.42
1:C:2469:ILE:HG21	1:C:2502:MET:HE3	2.02	0.42
1:A:1690:ASP:OD1	1:A:1692:ALA:N	2.51	0.41
1:A:2440:MET:O	1:A:2441:HIS:ND1	2.53	0.41
1:D:1205:GLY:HA2	1:D:1211:LEU:HD21	2.01	0.41
1:D:2440:MET:O	1:D:2441:HIS:ND1	2.53	0.41
1:A:1515:VAL:HG22	1:A:1530:THR:HG23	2.02	0.41
1:A:2629:ASP:O	1:A:2633:LEU:N	2.51	0.41
1:B:3354:LEU:HD13	1:B:3415:TYR:HE2	1.86	0.41
1:D:4003:LEU:CD2	1:D:4012:LEU:HD23	2.50	0.41
1:C:1863:LEU:HD21	1:C:1870:VAL:HG12	2.01	0.41
1:C:2440:MET:O	1:C:2441:HIS:ND1	2.54	0.41
1:C:4218:ILE:O	1:C:4222:VAL:HG12	2.20	0.41
1:D:1042:ALA:O	1:D:1045:THR:OG1	2.30	0.41
1:D:4848:VAL:HG11	1:D:4887:MET:HE1	2.02	0.41
1:B:2650:ARG:O	1:B:2654:TYR:N	2.53	0.41
1:B:4215:ARG:NH2	3:B:5101:ATP:O2B	2.54	0.41
1:A:4215:ARG:NH2	3:A:5101:ATP:O2B	2.54	0.41
1:B:35:LEU:HD22	1:B:49:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:394:GLN:N	1:C:397:GLU:OE2	2.53	0.41
1:D:479:GLN:NE2	1:D:480:GLU:OE1	2.53	0.41
2:H:90:VAL:HG13	2:H:91:ILE:HG12	2.03	0.41
1:A:2650:ARG:O	1:A:2654:TYR:N	2.53	0.41
1:A:4848:VAL:HG11	1:A:4887:MET:HE1	2.02	0.41
1:B:2469:ILE:HG21	1:B:2502:MET:HE3	2.02	0.41
1:D:4215:ARG:NH2	3:D:5101:ATP:O2B	2.54	0.41
1:C:1220:GLN:OE1	1:C:1220:GLN:N	2.51	0.41
1:A:35:LEU:HD22	1:A:49:LEU:HD21	2.02	0.41
1:C:479:GLN:NE2	1:C:480:GLU:OE1	2.53	0.41
1:C:2973:PHE:CE1	1:C:2995:ILE:HD11	2.56	0.41
1:A:579:GLN:OE1	1:A:582:HIS:NE2	2.54	0.41
1:A:1220:GLN:OE1	1:A:1220:GLN:N	2.51	0.41
1:A:1863:LEU:HD21	1:A:1870:VAL:HG12	2.01	0.41
1:A:2929:PHE:O	1:A:2932:MET:HE3	2.21	0.41
1:A:3308:THR:OG1	1:A:3311:HIS:N	2.51	0.41
1:B:579:GLN:OE1	1:B:582:HIS:NE2	2.54	0.41
1:B:2954:ARG:HE	1:B:2955:PHE:H	1.69	0.41
1:B:4218:ILE:O	1:B:4222:VAL:HG12	2.20	0.41
1:C:579:GLN:OE1	1:C:582:HIS:NE2	2.54	0.41
1:C:1115:LEU:HD22	1:C:1193:SER:OG	2.21	0.41
1:C:2247:GLN:NE2	1:C:2279:SER:O	2.54	0.41
1:C:3576:TYR:HA	1:C:3579:LEU:HD13	2.03	0.41
1:C:4003:LEU:CD2	1:C:4012:LEU:HD23	2.50	0.41
1:D:2247:GLN:NE2	1:D:2279:SER:O	2.54	0.41
1:D:2469:ILE:HG21	1:D:2502:MET:HE3	2.02	0.41
1:D:3354:LEU:HD13	1:D:3415:TYR:HE2	1.86	0.41
1:A:2973:PHE:CE1	1:A:2995:ILE:HD11	2.56	0.41
1:B:3576:TYR:HA	1:B:3579:LEU:HD13	2.03	0.41
1:C:1639:LEU:HD11	1:C:1650:ILE:HA	2.03	0.41
1:C:3354:LEU:HD13	1:C:3415:TYR:HE2	1.86	0.41
1:C:4848:VAL:HG11	1:C:4887:MET:HE1	2.02	0.41
1:D:2973:PHE:CE1	1:D:2995:ILE:HD11	2.56	0.41
1:D:4144:ALA:O	1:D:4148:THR:OG1	2.24	0.41
2:G:90:VAL:HG13	2:G:91:ILE:HG12	2.03	0.41
1:A:2954:ARG:HE	1:A:2955:PHE:H	1.69	0.40
1:A:3891:LEU:HD22	1:A:3899:PHE:CZ	2.56	0.40
1:B:3808:GLY:O	1:B:3813:GLN:NE2	2.53	0.40
1:B:4848:VAL:HG11	1:B:4887:MET:HE1	2.02	0.40
1:A:1933:GLU:N	1:A:1933:GLU:OE1	2.55	0.40
1:A:4218:ILE:O	1:A:4222:VAL:HG12	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2929:PHE:O	1:B:2932:MET:HE3	2.21	0.40
1:C:4215:ARG:NH2	3:C:5101:ATP:O2B	2.54	0.40
1:D:1115:LEU:HD22	1:D:1193:SER:OG	2.21	0.40
1:D:4218:ILE:O	1:D:4222:VAL:HG12	2.20	0.40
1:A:2469:ILE:HG21	1:A:2502:MET:HE3	2.02	0.40
1:B:2247:GLN:NE2	1:B:2279:SER:O	2.54	0.40
1:B:2973:PHE:CE1	1:B:2995:ILE:HD11	2.56	0.40
1:C:2929:PHE:O	1:C:2932:MET:HE3	2.21	0.40
1:A:131:LEU:HD22	1:D:2456:ILE:HD13	2.04	0.40
1:A:3354:LEU:HD13	1:A:3415:TYR:HE2	1.85	0.40
1:A:3576:TYR:HA	1:A:3579:LEU:HD13	2.03	0.40
1:B:676:THR:OG1	1:B:677:ALA:N	2.55	0.40
1:D:2954:ARG:HE	1:D:2955:PHE:H	1.69	0.40
1:D:4794:TRP:CE2	1:D:4798:MET:HE1	2.56	0.40
1:B:1690:ASP:OD1	1:B:1692:ALA:N	2.51	0.40
1:B:2440:MET:O	1:B:2441:HIS:ND1	2.53	0.40
1:B:4794:TRP:CE2	1:B:4798:MET:HE1	2.56	0.40
1:D:579:GLN:OE1	1:D:582:HIS:NE2	2.54	0.40
1:D:3891:LEU:HD22	1:D:3899:PHE:CZ	2.56	0.40
2:F:90:VAL:HG13	2:F:91:ILE:HG12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	4188/5037 (83%)	3792 (90%)	385 (9%)	11 (0%)	36	70
1	B	4188/5037 (83%)	3794 (91%)	384 (9%)	10 (0%)	43	75
1	C	4188/5037 (83%)	3794 (91%)	384 (9%)	10 (0%)	43	75
1	D	4188/5037 (83%)	3795 (91%)	383 (9%)	10 (0%)	43	75

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	105/107 (98%)	95 (90%)	10 (10%)	0	100	100
2	F	105/107 (98%)	95 (90%)	10 (10%)	0	100	100
2	G	105/107 (98%)	95 (90%)	10 (10%)	0	100	100
2	H	105/107 (98%)	95 (90%)	10 (10%)	0	100	100
All	All	17172/20576 (84%)	15555 (91%)	1576 (9%)	41 (0%)	44	75

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1548	LEU
1	A	2956	ALA
1	B	1548	LEU
1	B	2956	ALA
1	C	1548	LEU
1	C	2956	ALA
1	D	1548	LEU
1	D	2956	ALA
1	A	1277	TRP
1	A	2189	LYS
1	B	1277	TRP
1	B	2189	LYS
1	C	1277	TRP
1	C	2189	LYS
1	D	1277	TRP
1	D	2189	LYS
1	A	2953	LYS
1	B	2953	LYS
1	C	2953	LYS
1	D	2953	LYS
1	A	1561	VAL
1	A	1796	ALA
1	A	2620	GLN
1	A	2951	ILE
1	B	1561	VAL
1	B	1796	ALA
1	B	2620	GLN
1	B	2951	ILE
1	C	1561	VAL
1	C	1796	ALA
1	C	2620	GLN
1	C	2951	ILE

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Mol	Chain	Res	Type
1	D	1561	VAL
1	D	1796	ALA
1	D	2620	GLN
1	D	2951	ILE
1	A	1651	LEU
1	A	1469	VAL
1	B	1469	VAL
1	C	1469	VAL
1	D	1469	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	3479/4276 (81%)	3479 (100%)	0	100	100
1	B	3479/4276 (81%)	3479 (100%)	0	100	100
1	C	3479/4276 (81%)	3479 (100%)	0	100	100
1	D	3479/4276 (81%)	3479 (100%)	0	100	100
2	E	88/88 (100%)	88 (100%)	0	100	100
2	F	88/88 (100%)	88 (100%)	0	100	100
2	G	88/88 (100%)	88 (100%)	0	100	100
2	H	88/88 (100%)	88 (100%)	0	100	100
All	All	14268/17456 (82%)	14268 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	720	HIS
1	A	765	GLN
1	A	1484	HIS
1	A	1541	GLN

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Mol	Chain	Res	Type
1	A	2646	ASN
1	A	3466	ASN
1	A	3554	GLN
1	A	3766	GLN
1	A	3889	GLN
1	A	3960	GLN
1	A	3994	HIS
1	A	4102	GLN
1	B	765	GLN
1	B	1484	HIS
1	B	2646	ASN
1	B	3466	ASN
1	B	3766	GLN
1	B	3994	HIS
1	B	4037	ASN
1	B	4102	GLN
1	B	4124	ASN
1	B	4857	ASN
1	C	475	GLN
1	C	765	GLN
1	C	1484	HIS
1	C	2646	ASN
1	C	3466	ASN
1	C	3766	GLN
1	C	3889	GLN
1	C	3960	GLN
1	C	3994	HIS
1	C	4102	GLN
1	C	4124	ASN
1	C	4857	ASN
1	D	765	GLN
1	D	1484	HIS
1	D	1541	GLN
1	D	2646	ASN
1	D	3466	ASN
1	D	3766	GLN
1	D	3889	GLN
1	D	3960	GLN
1	D	3994	HIS
1	D	4037	ASN
1	D	4102	GLN
1	D	4857	ASN

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Mol	Chain	Res	Type
2	E	25	HIS
2	F	25	HIS
2	G	25	HIS
2	H	25	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 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	$\# Z > 2$
3	ATP	D	5101	-	32,33,33	0.30	0	48,52,52	0.69	0
3	ATP	A	5101	-	32,33,33	0.31	0	48,52,52	0.69	0
3	ATP	B	5101	-	32,33,33	0.31	0	48,52,52	0.69	0
3	ATP	C	5101	-	32,33,33	0.32	0	48,52,52	0.69	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
3	ATP	D	5101	-	-	6/22/38/38	0/3/3/3
3	ATP	A	5101	-	-	6/22/38/38	0/3/3/3
3	ATP	B	5101	-	-	6/22/38/38	0/3/3/3
3	ATP	C	5101	-	-	6/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (24) torsion outliers are listed below:

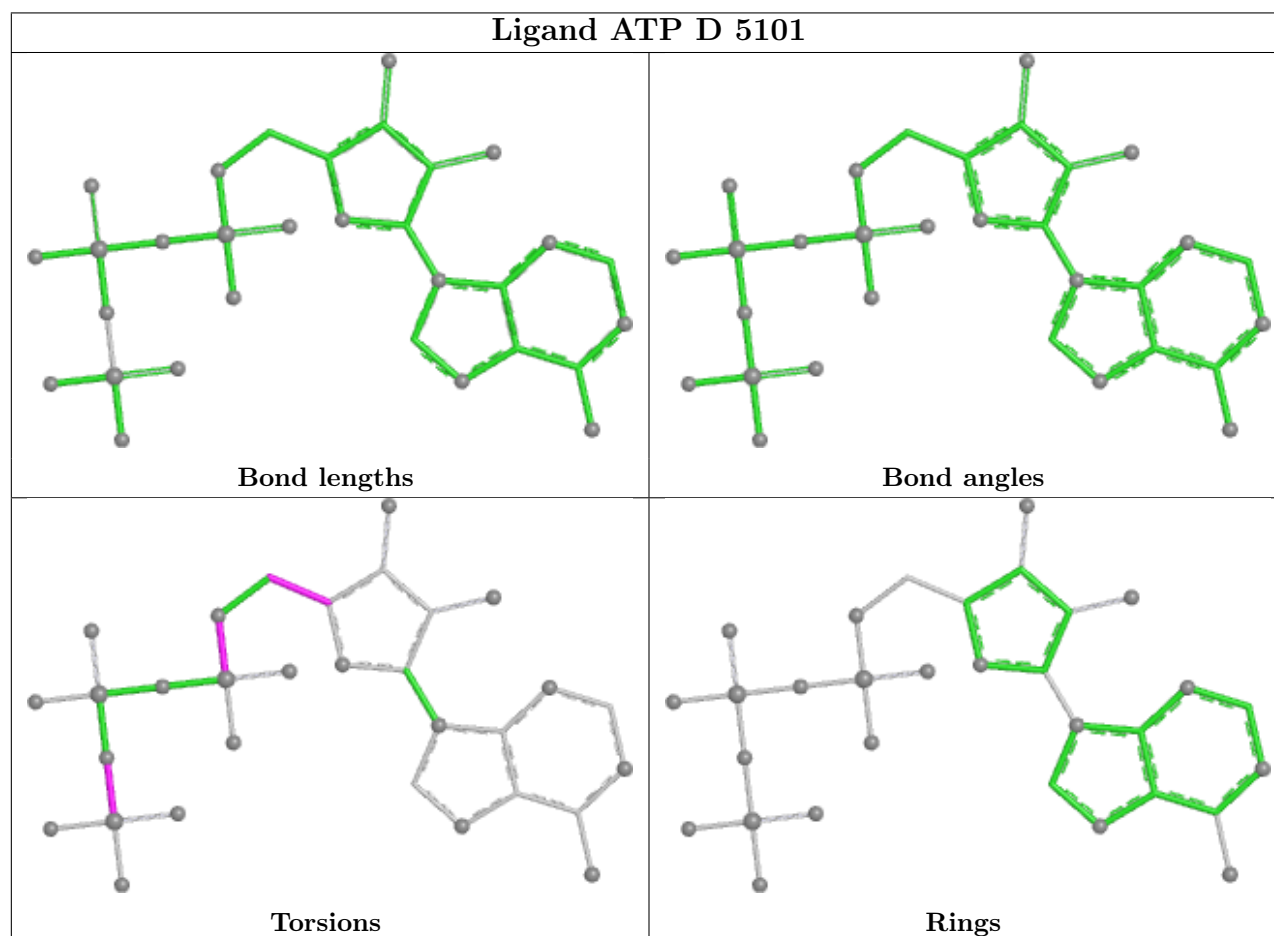
Mol	Chain	Res	Type	Atoms
3	A	5101	ATP	C5'-O5'-PA-O1A
3	A	5101	ATP	C5'-O5'-PA-O2A
3	A	5101	ATP	C5'-O5'-PA-O3A
3	A	5101	ATP	O4'-C4'-C5'-O5'
3	A	5101	ATP	C3'-C4'-C5'-O5'
3	B	5101	ATP	C5'-O5'-PA-O1A
3	B	5101	ATP	C5'-O5'-PA-O2A
3	B	5101	ATP	C5'-O5'-PA-O3A
3	B	5101	ATP	O4'-C4'-C5'-O5'
3	B	5101	ATP	C3'-C4'-C5'-O5'
3	C	5101	ATP	C5'-O5'-PA-O1A
3	C	5101	ATP	C5'-O5'-PA-O2A
3	C	5101	ATP	C5'-O5'-PA-O3A
3	C	5101	ATP	O4'-C4'-C5'-O5'
3	C	5101	ATP	C3'-C4'-C5'-O5'
3	D	5101	ATP	C5'-O5'-PA-O1A
3	D	5101	ATP	C5'-O5'-PA-O2A
3	D	5101	ATP	C5'-O5'-PA-O3A
3	D	5101	ATP	O4'-C4'-C5'-O5'
3	D	5101	ATP	C3'-C4'-C5'-O5'
3	A	5101	ATP	PB-O3B-PG-O2G
3	B	5101	ATP	PB-O3B-PG-O2G
3	C	5101	ATP	PB-O3B-PG-O2G
3	D	5101	ATP	PB-O3B-PG-O2G

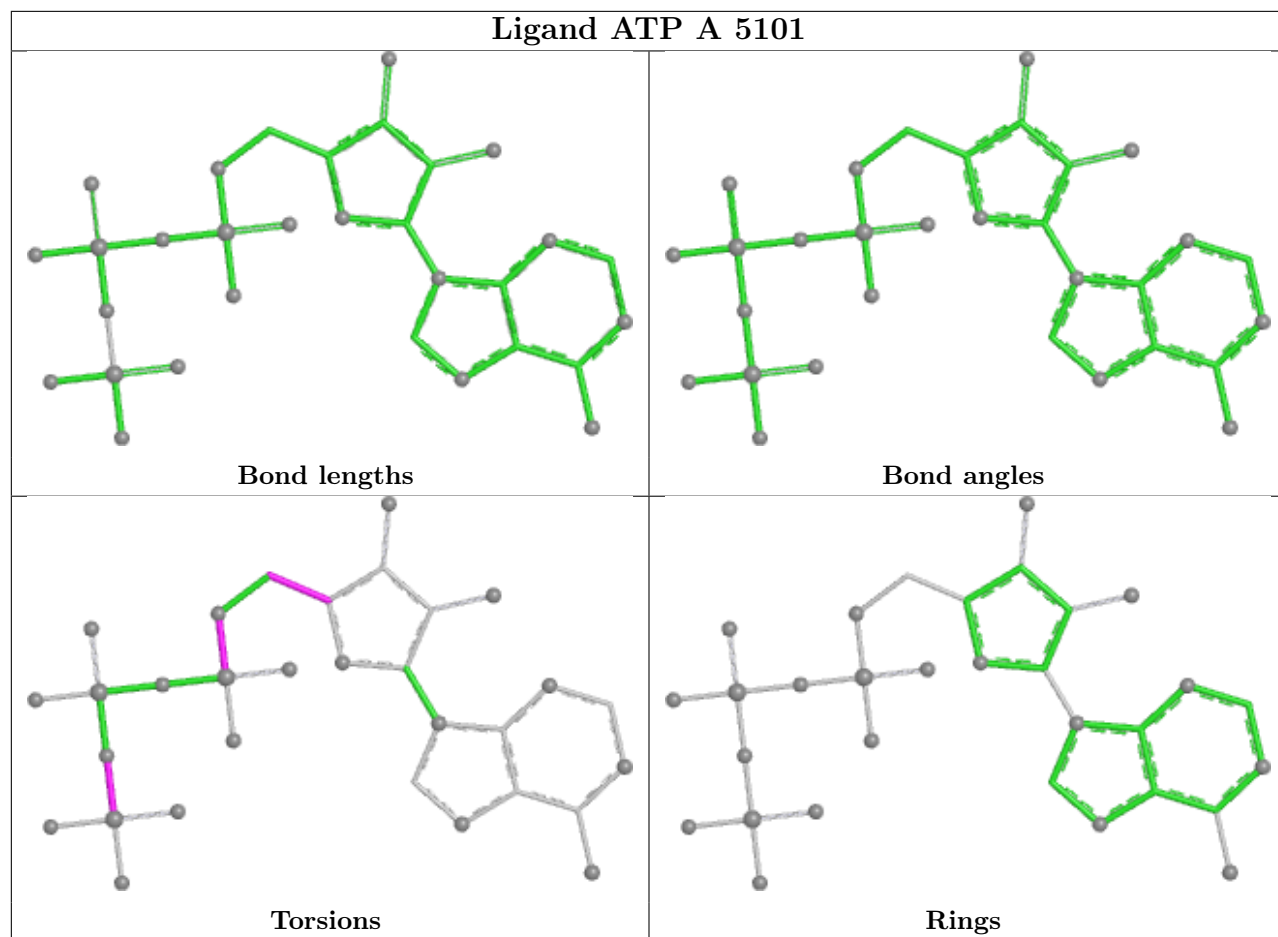
There are no ring outliers.

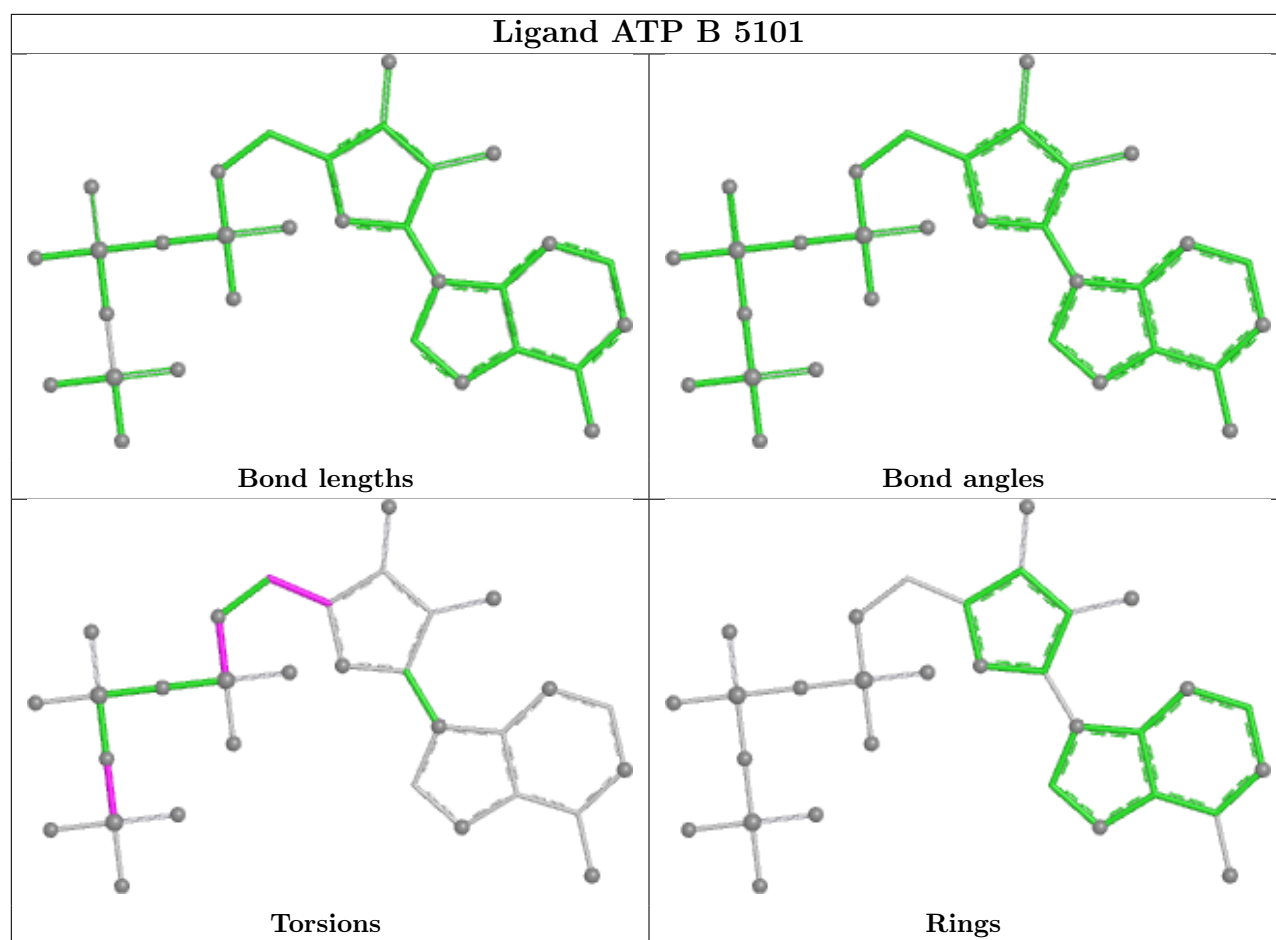
4 monomers are involved in 4 short contacts:

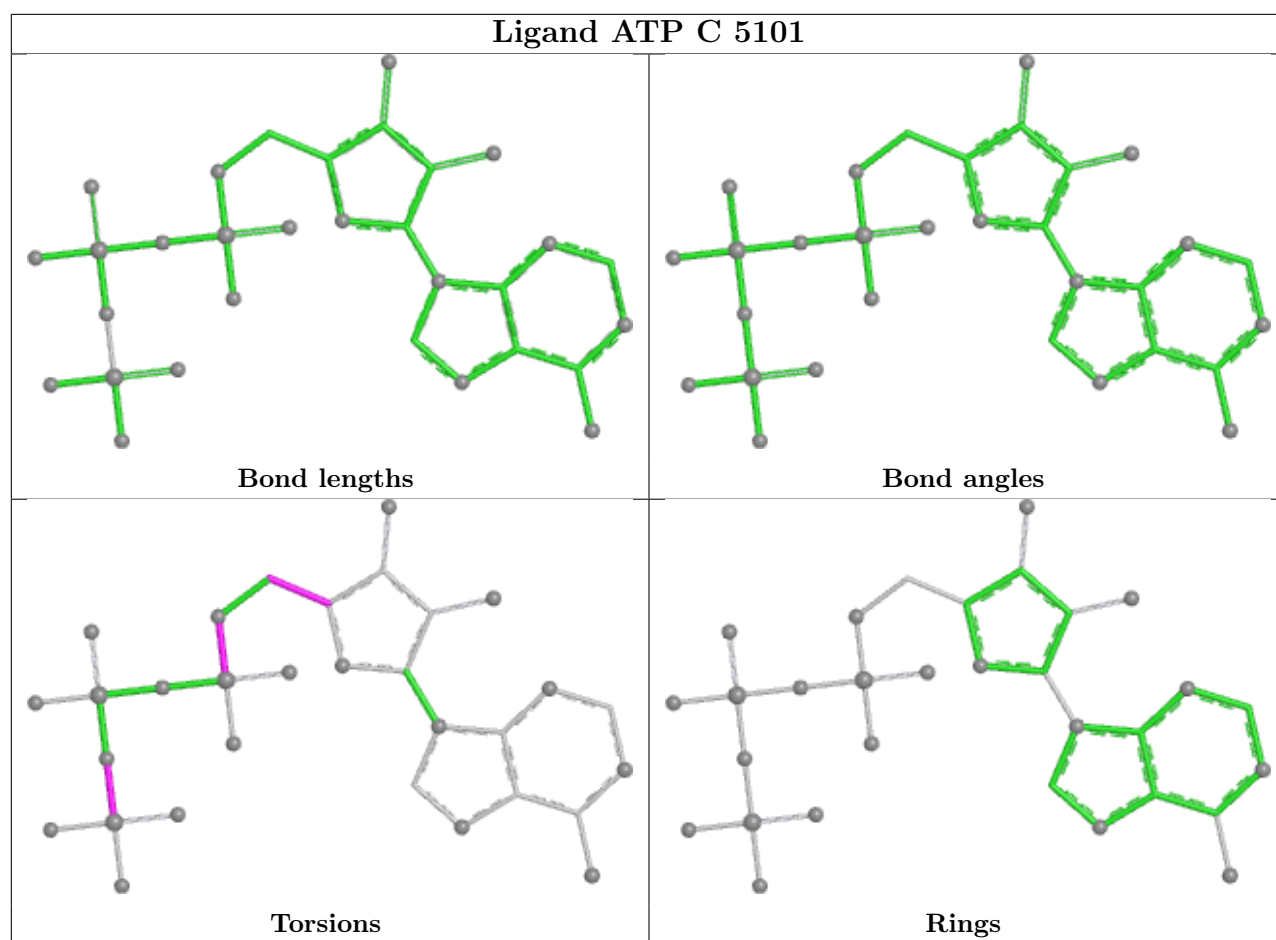
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	5101	ATP	1	0
3	A	5101	ATP	1	0
3	B	5101	ATP	1	0
3	C	5101	ATP	1	0

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.

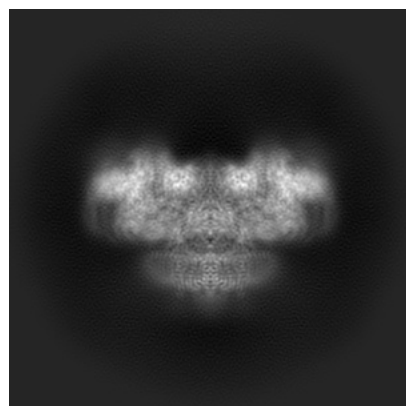
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25710. These allow visual inspection of the internal detail of the map and identification of artifacts.

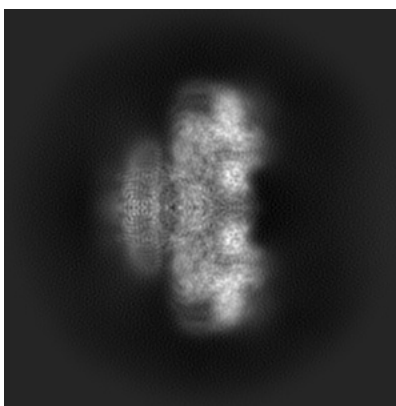
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

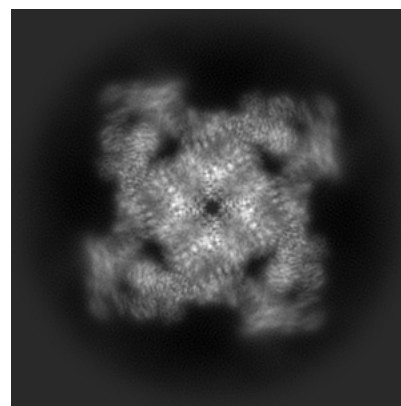
6.1.1 Primary map



X

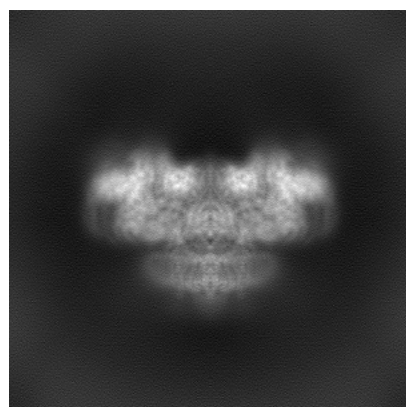


Y

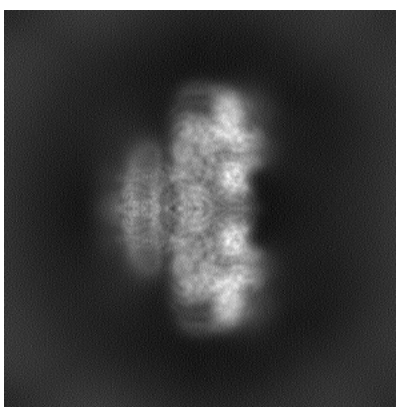


Z

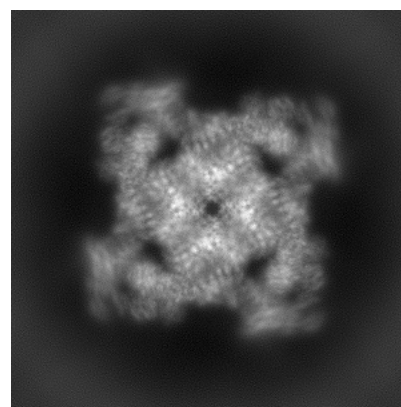
6.1.2 Raw map



X



Y

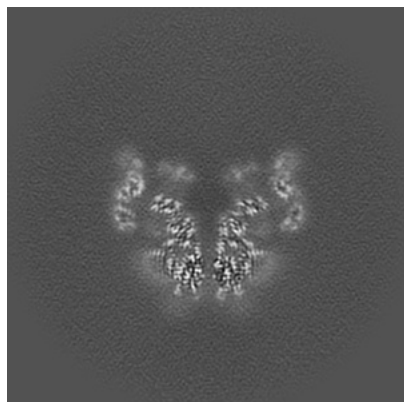


Z

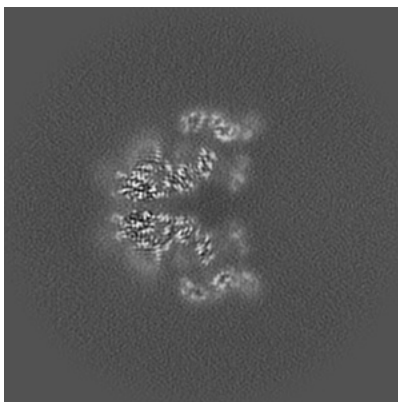
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

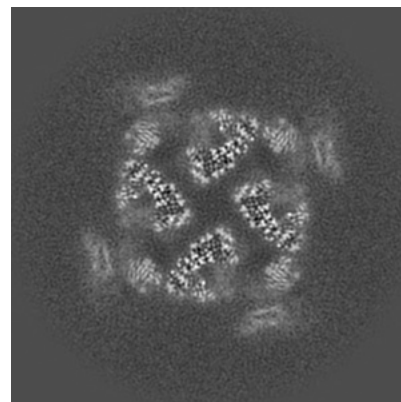
6.2.1 Primary map



X Index: 215

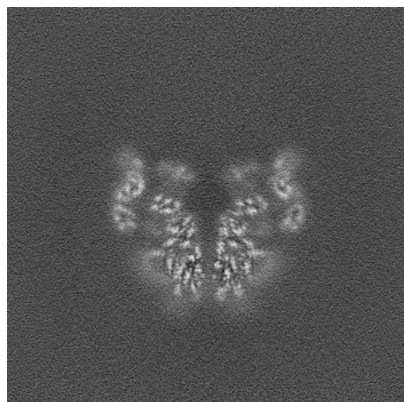


Y Index: 215

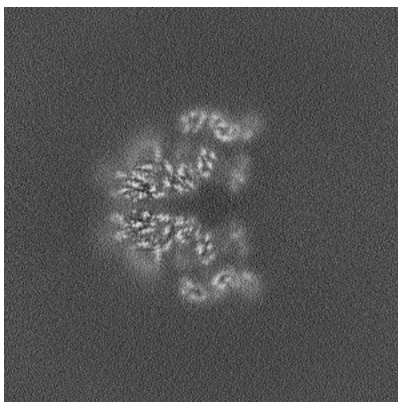


Z Index: 215

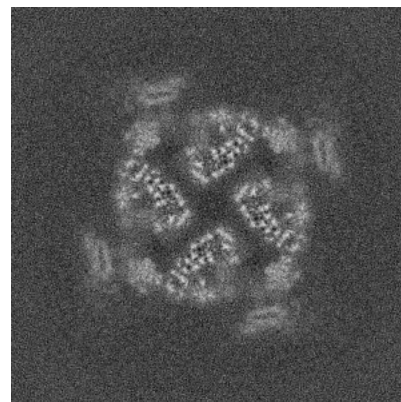
6.2.2 Raw map



X Index: 215



Y Index: 215

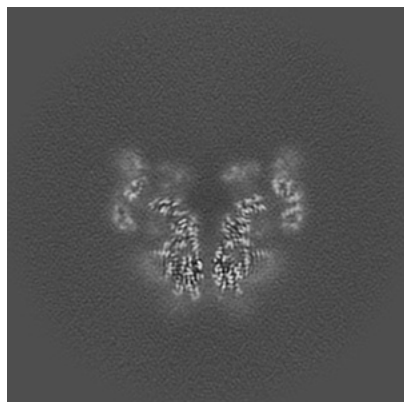


Z Index: 215

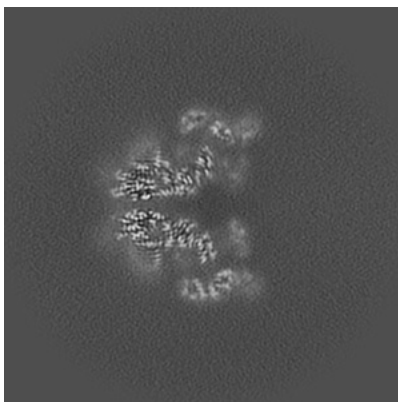
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

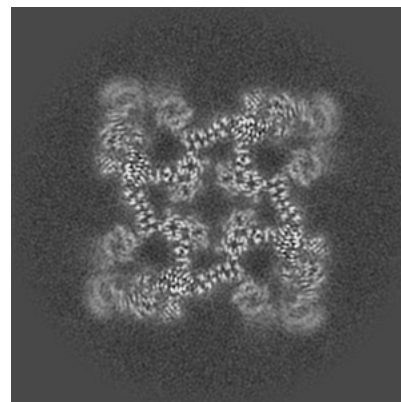
6.3.1 Primary map



X Index: 218

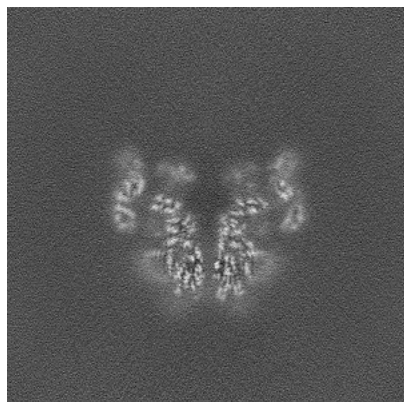


Y Index: 218

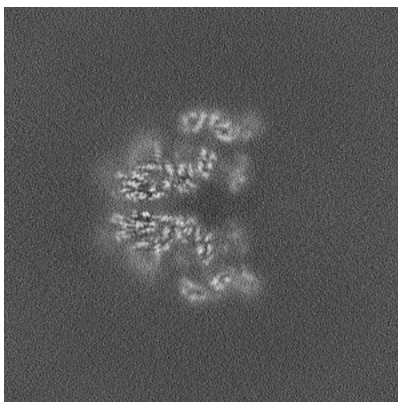


Z Index: 240

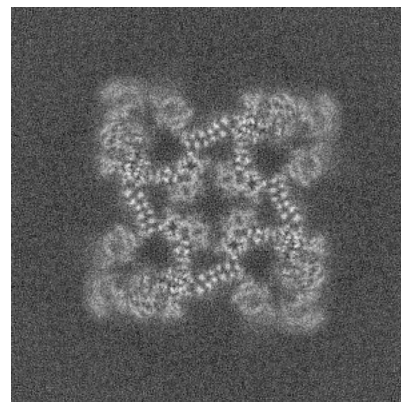
6.3.2 Raw map



X Index: 214



Y Index: 214

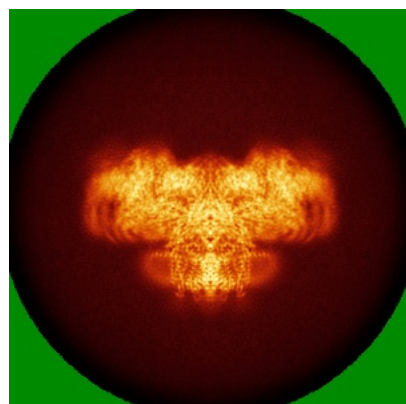


Z Index: 240

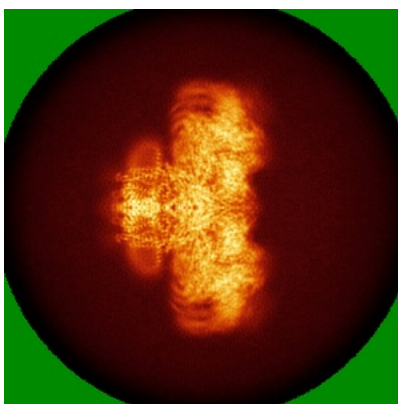
The images above show the largest variance slices of the map in three orthogonal directions.

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

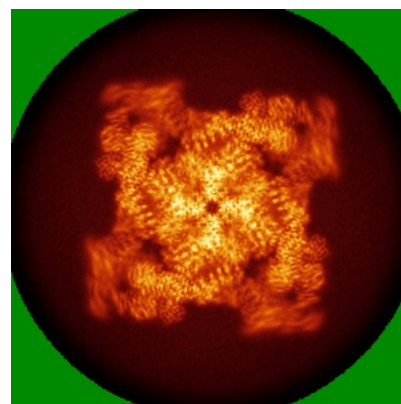
6.4.1 Primary map



X

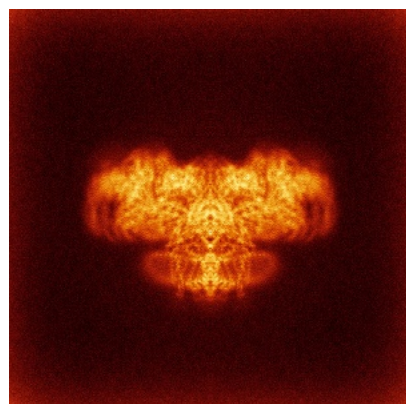


Y

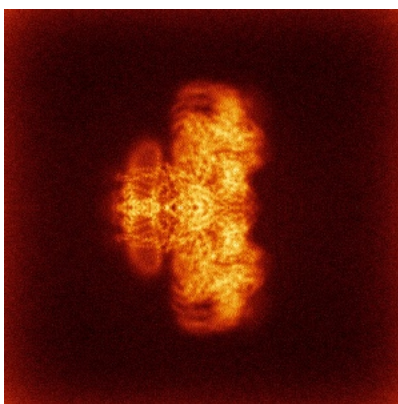


Z

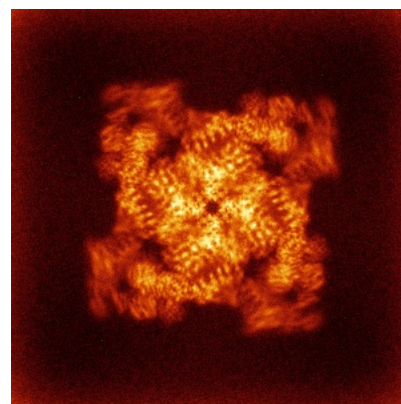
6.4.2 Raw map



X



Y

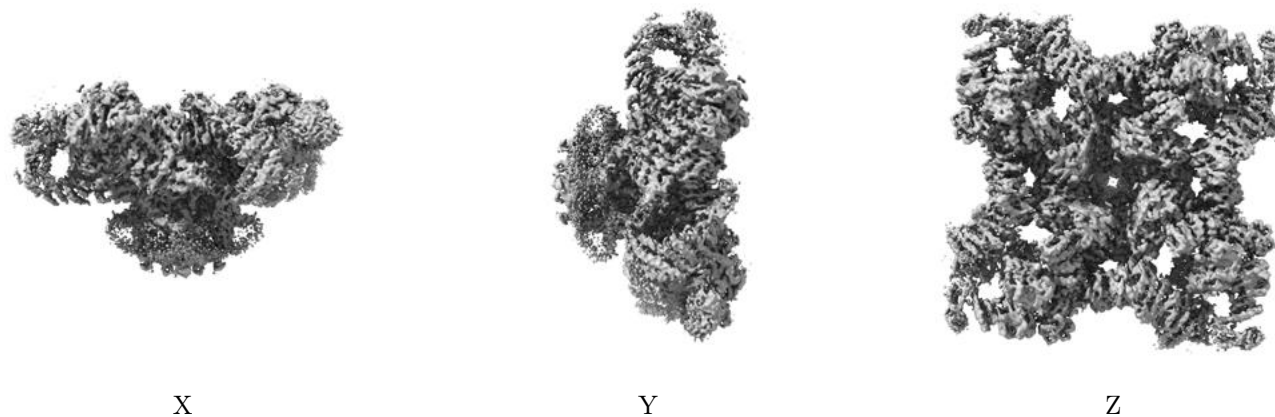


Z

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 0.176. 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.

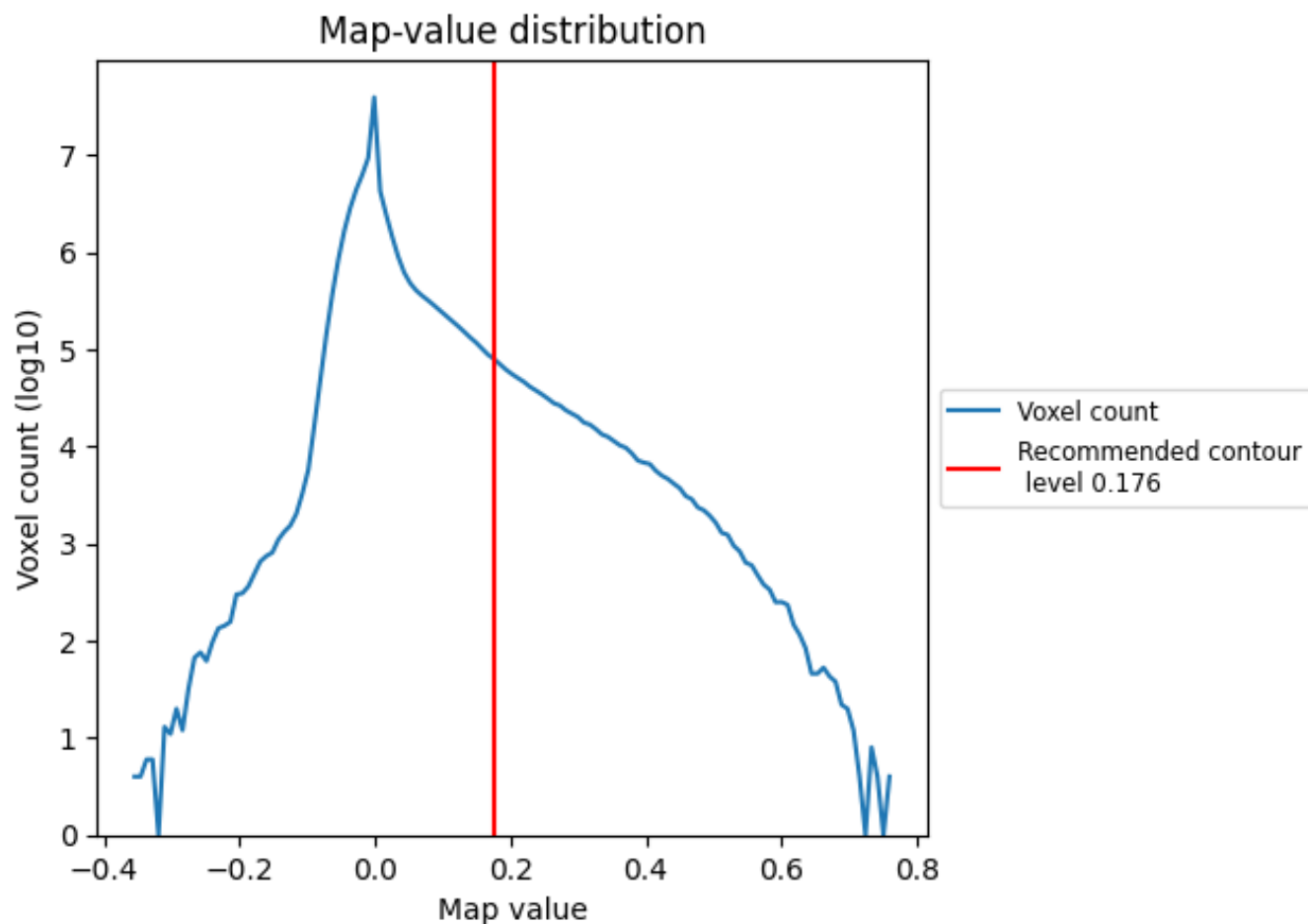
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

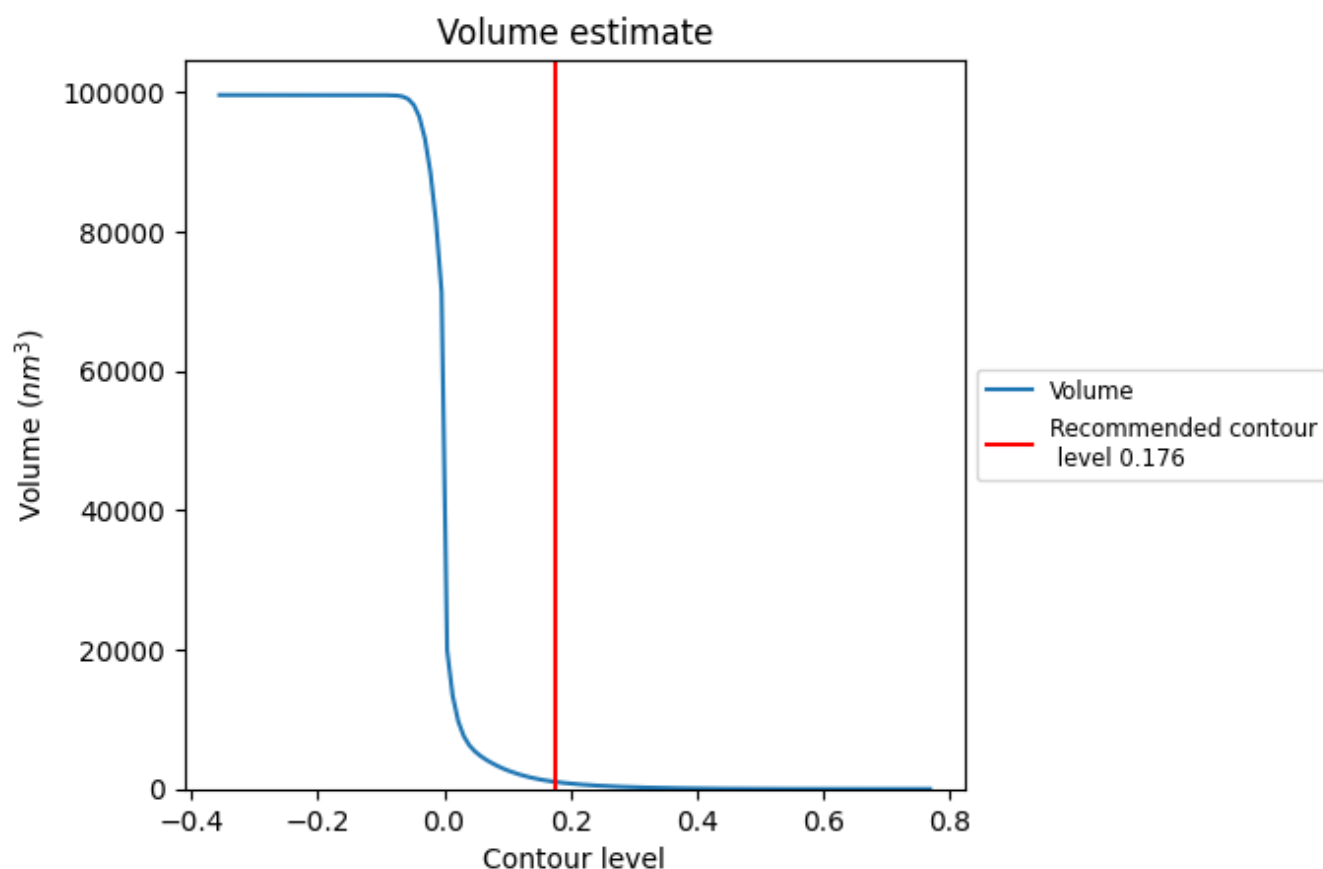
This section contains the results of statistical analysis of the map.

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.

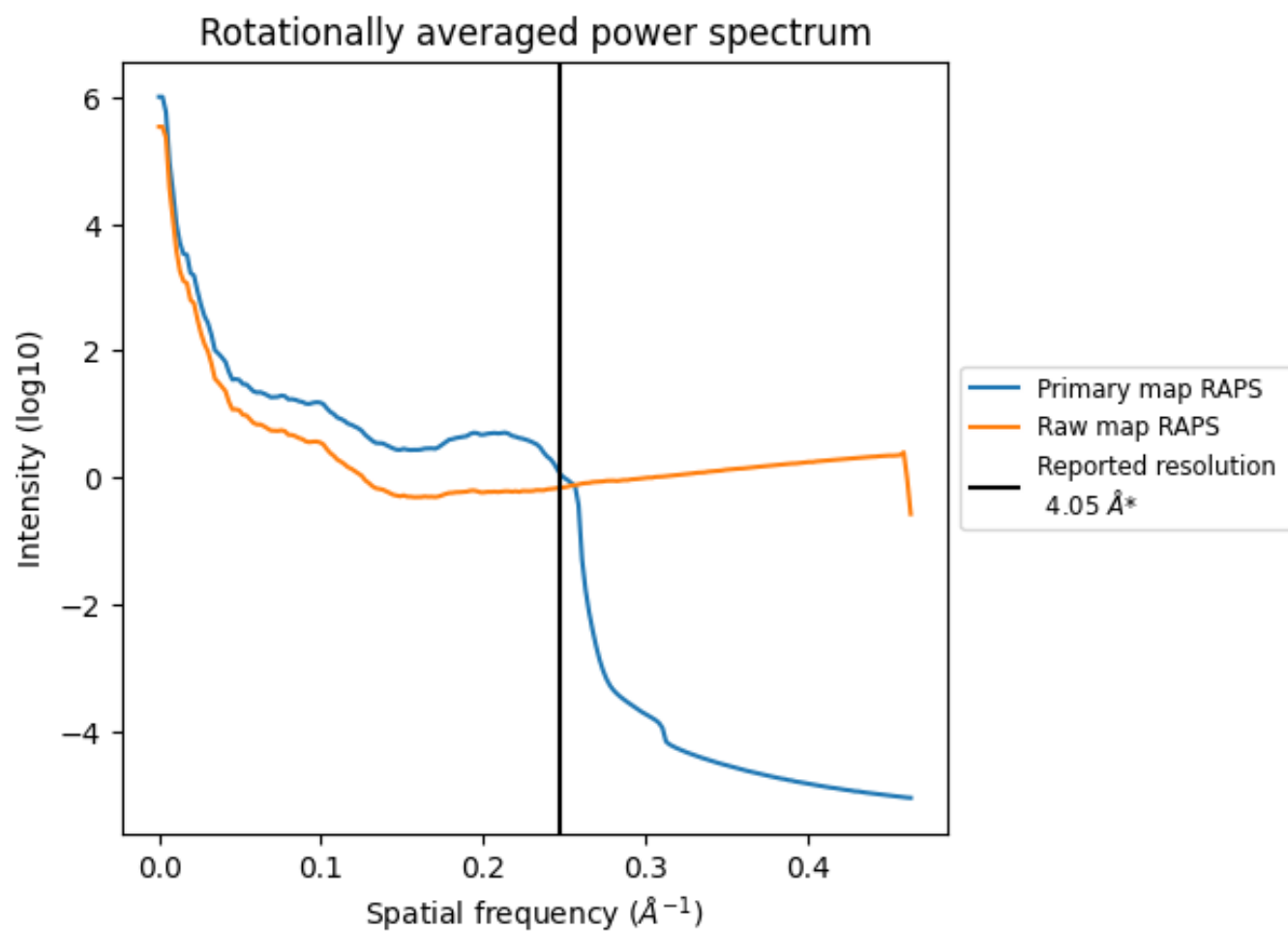
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1017 nm³; this corresponds to an approximate mass of 918 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 ⓘ

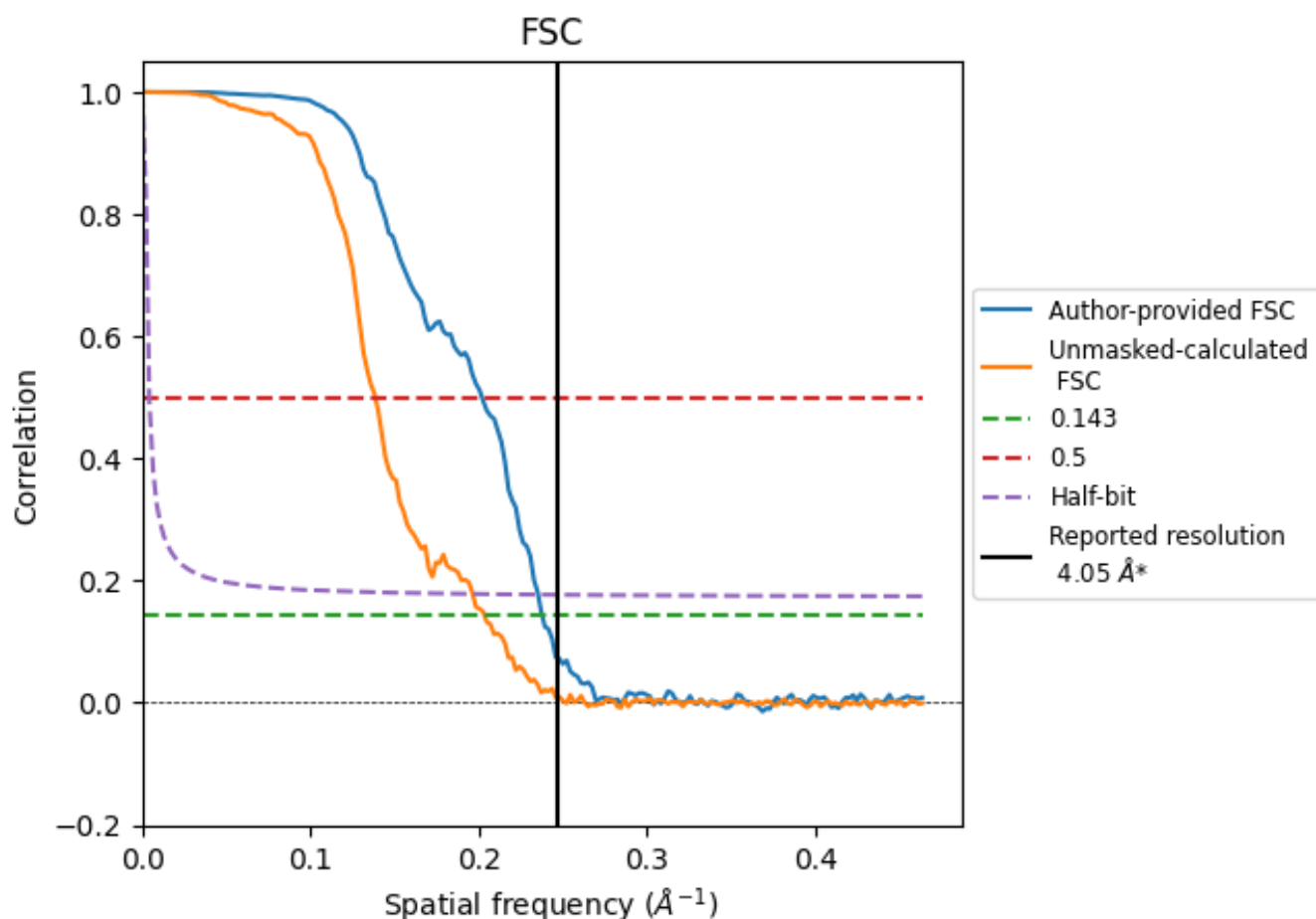


*Reported resolution corresponds to spatial frequency of 0.247 $\text{\AA}^{-1}$

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 0.247 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

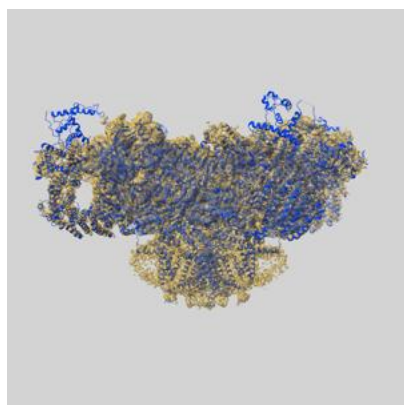
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.05	-	-
Author-provided FSC curve	4.21	4.95	4.25
Unmasked-calculated*	4.91	7.22	5.09

*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 4.91 differs from the reported value 4.05 by more than 10 %

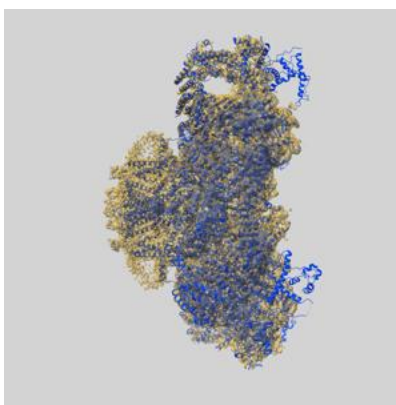
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-25710 and PDB model 7T65. Per-residue inclusion information can be found in section [3](#) on page [7](#).

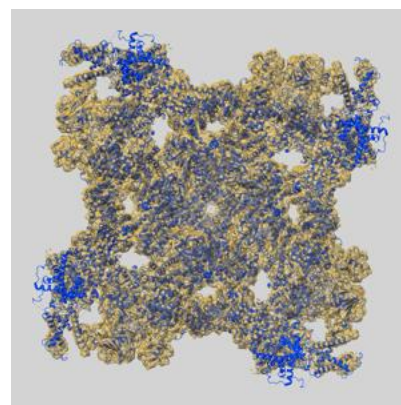
9.1 Map-model overlay [i](#)



X



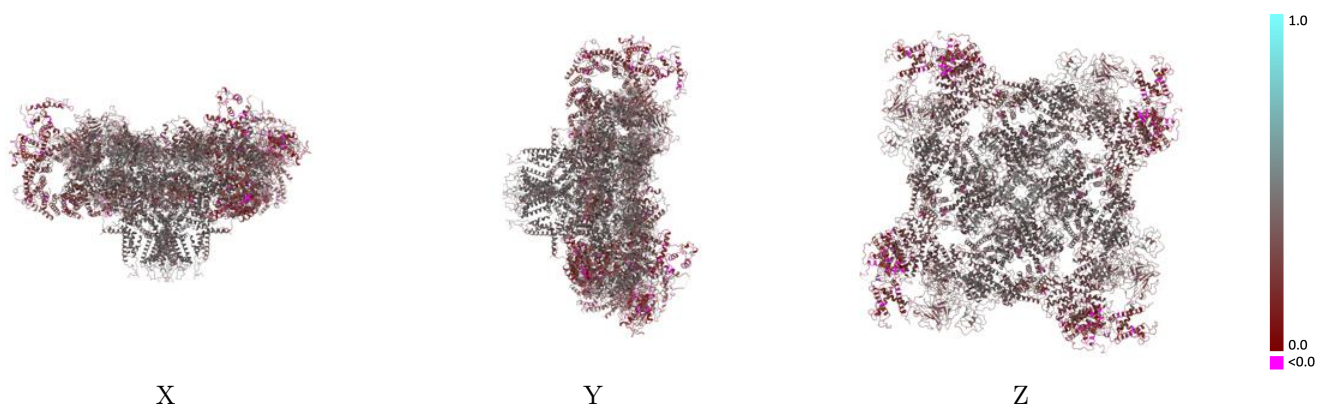
Y



Z

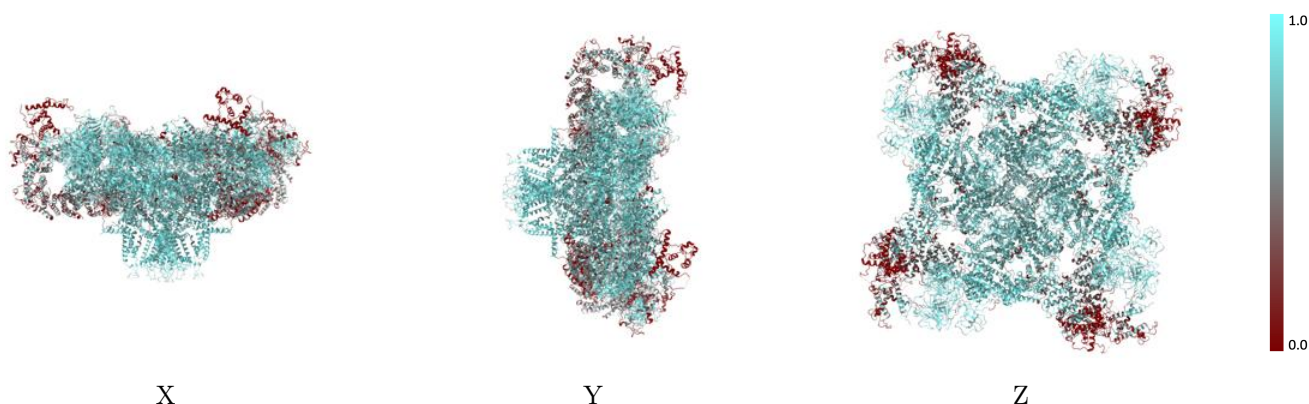
The images above show the 3D surface view of the map at the recommended contour level 0.176 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



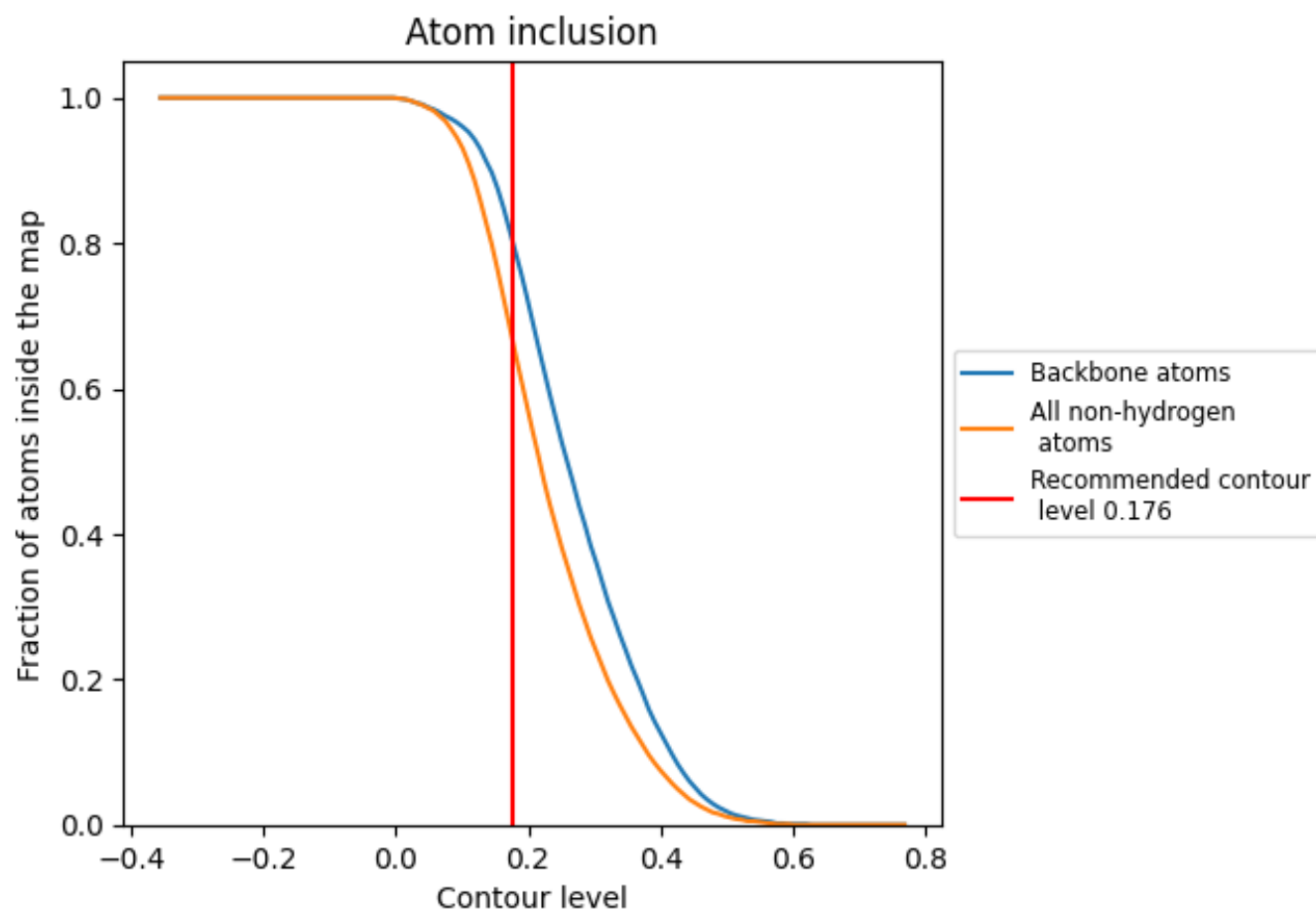
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.176).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 67% 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 (0.176) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6680	0.3480
A	0.6650	0.3460
B	0.6650	0.3470
C	0.6650	0.3460
D	0.6650	0.3460
E	0.7840	0.3990
F	0.7840	0.4000
G	0.7870	0.3980
H	0.7850	0.3970

1.0

0.0

<0.0