



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 10:57 PM UTC

PDB ID : 8DVV / pdb_00008dvv
EMDB ID : EMD-27746
Title : Recombinant mouse RyR2 triple phosphomimetic mutant
S2807D/S2813D/S2030D in complex with FKBP12.6 and nanodisc under open-state conditions
Authors : Iyer, K.A.; Hu, Y.; Murayama, T.; Samso, M.
Deposited on : 2022-07-29
Resolution : 3.68 Å (reported)
Based on initial model : 6WOU

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:

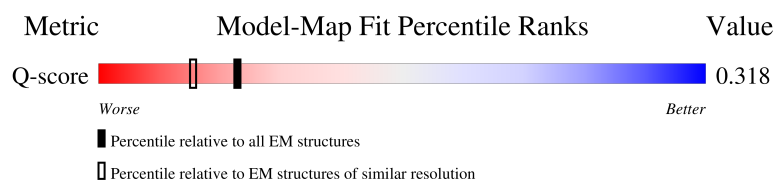
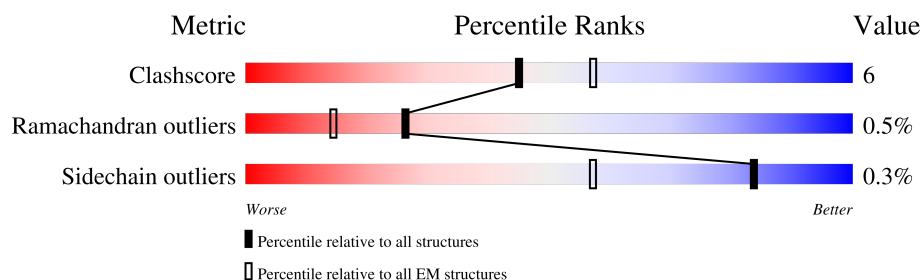
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.68 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	11376 (3.18 - 4.18)

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	4966	12% 66% 12% 22%
1	B	4966	12% 66% 12% 22%
1	C	4966	12% 66% 12% 22%
1	D	4966	12% 66% 12% 22%

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Mol	Chain	Length	Quality of chain	
2	E	107		
2	F	107		
2	G	107		.
2	H	107		

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 119280 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ryanodine receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3886	Total	C	N	O	S	0	0
			29055	18436	4944	5507	168		
1	B	3886	Total	C	N	O	S	0	0
			29055	18436	4944	5507	168		
1	C	3886	Total	C	N	O	S	0	0
			29055	18436	4944	5507	168		
1	D	3886	Total	C	N	O	S	0	0
			29055	18436	4944	5507	168		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2030	ASP	SER	engineered mutation	UNP E9Q401
A	2807	ASP	SER	engineered mutation	UNP E9Q401
A	2813	ASP	SER	engineered mutation	UNP E9Q401
B	2030	ASP	SER	engineered mutation	UNP E9Q401
B	2807	ASP	SER	engineered mutation	UNP E9Q401
B	2813	ASP	SER	engineered mutation	UNP E9Q401
C	2030	ASP	SER	engineered mutation	UNP E9Q401
C	2807	ASP	SER	engineered mutation	UNP E9Q401
C	2813	ASP	SER	engineered mutation	UNP E9Q401
D	2030	ASP	SER	engineered mutation	UNP E9Q401
D	2807	ASP	SER	engineered mutation	UNP E9Q401
D	2813	ASP	SER	engineered mutation	UNP E9Q401

- 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
			763	480	129	151	3		
2	F	107	Total	C	N	O	S	0	0
			763	480	129	151	3		
2	G	107	Total	C	N	O	S	0	0
			763	480	129	151	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	107	Total	C	N	O	S	0	0
			763	480	129	151	3		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

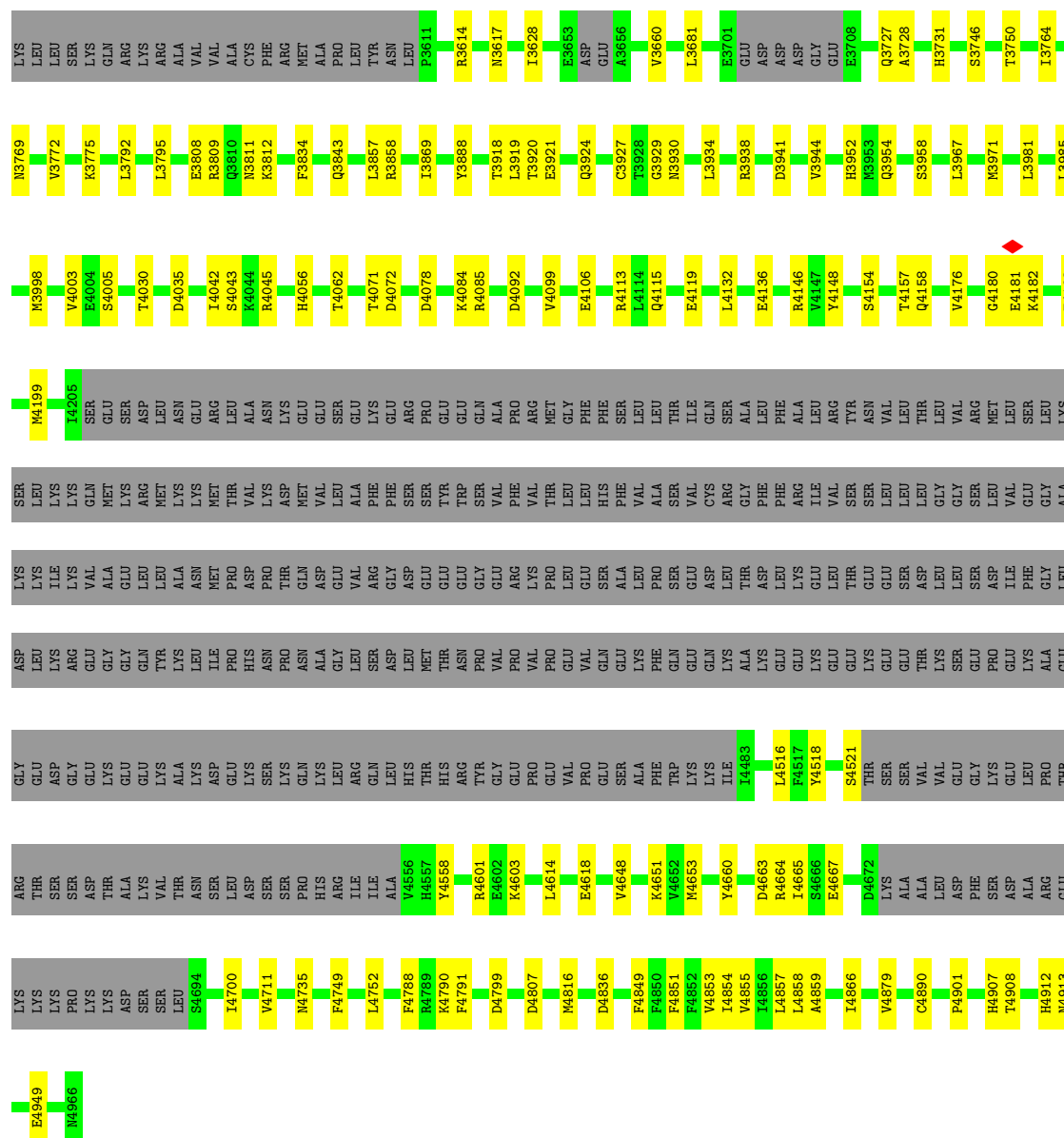
Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Ca	0
			1	1	
3	B	1	Total	Ca	0
			1	1	
3	C	1	Total	Ca	0
			1	1	
3	D	1	Total	Ca	0
			1	1	

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

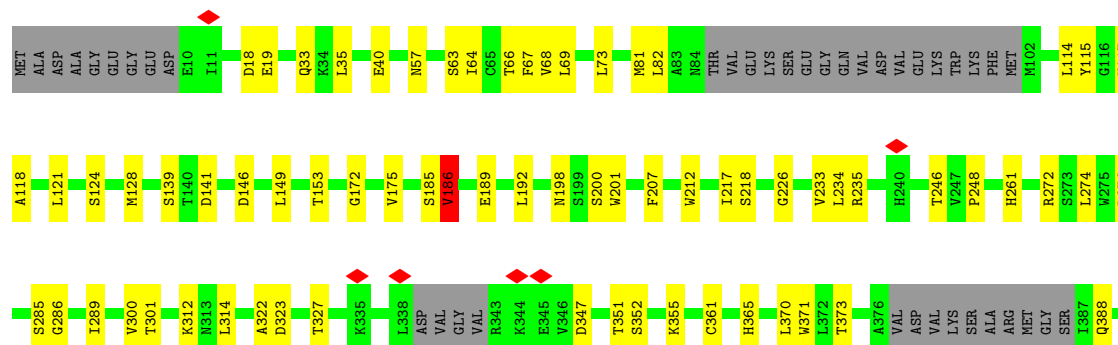
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Zn	0
			1	1	
4	B	1	Total	Zn	0
			1	1	
4	C	1	Total	Zn	0
			1	1	
4	D	1	Total	Zn	0
			1	1	

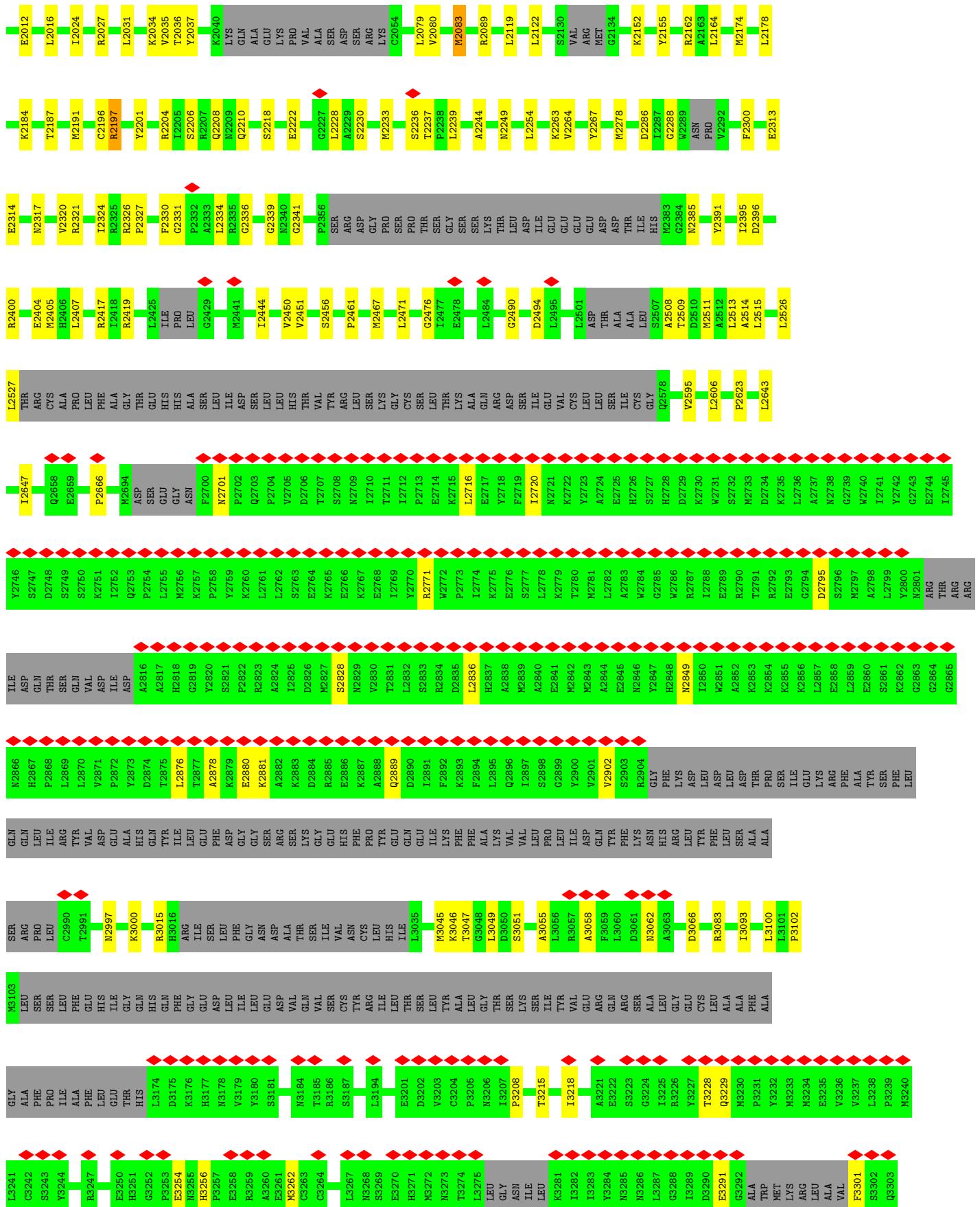


ALA	A3468	S3408	S3348	Y3284	A3221	LYS	PHE	M2846	W2786	H2726
LEU	L3469	H3409	E3349	N3285	S3222	SER	LYS	Y2847	R2787	S2727
TYR	K3470	N3410	A3350	N3286	S3223	ILE	ASP	L3056	R2787	S2727
ASP	R3471	F3411	A3351	L3287	G3224	VAL	ASP	R3057	L2788	D2728
PRO	K3472	K3412	L3352	G3288	I3225	GLU	LEU	W2849	E2789	D2729
ASN	L3473	R3413	L3353	I3289	R3226	ARG	ASP	L2850	R2790	K2730
THR	F3474	E3414	L3354	I3290	Y3227	GLN	THR	F3059	T2791	W2731
ARG	I3475	E3415	L3355	E3291	T3228	ARG	PRO	K2852	R2792	S2732
ASP	G3476	Q3416	D3356	G3292	Q3229	ALA	ILE	K2854	D2794	D2734
PRO	L3477	N3417	E3357	ALA	M3230	LEU	LYS	K2855	D2795	K2735
SER	N3478	F3418	F3358	TRP	P3231	GLY	LYS	K2856	S2796	L2736
ASP	I3479	V3419	T3359	MET	Y3232	CYS	ARG	L2857	R2797	L2737
PRO	C3480	V3420	T3360	LYS	N3233	LEU	PHE	E2858	A2798	K2738
ARG	A3481	Q3421	L3361	ARG	M3234	ALA	ALA	L2859	L2799	G2739
THR	F3482	N3422	A3362	LEU	E3235	PHE	SER	E2860	W2800	Y2800
VAL	G3483	E3423	R3363	VAL	V3236	ALA	PHE	S2861	N2801	ARG
GLU	Q3485	N3425	D3364	F3301	V3237	GLY	LEU	K2862	THR	THR
ARG	E3486	M3426	L3365	S3302	L3238	PHE	GLN	Q2863	ARG	G2743
VAL	L3487	K3427	Y3366	Q3303	P3239	ILE	ILE	G2864	ARG	G2744
L3551	G3552	D3432	A3367	Q3303	N3240	ALA	ARG	G2865	ILE	I2745
L3552	L3488	I3424	F3368	P3304	L3241	ALA	TYR	N2866	ASP	I2746
L3553	L3487	E3423	F3369	I3305	C3242	PHE	VAL	H2867	GLN	ASP
A3554	A3489	F3429	Y3370	N3307	S3243	GLU	ASP	P2868	SER	S2747
N3555	L3490	L3430	L3371	K3308	Y3244	THR	GLU	D2748	GLN	D2748
V3556	A3491	I3431	L3372	V3309	R3247	HIS	ALA	S2749	VAL	S2749
L3557	K3492	T3432	L3373	K3310	E3250	ILE	GLN	S2750	ASP	K2750
N3493	N3493	D3433	I3373	F3311	H3251	ARG	TYR	V2871	ILE	K2751
R3494	F3494	T3434	R3374	Q3312	E3250	ILE	GLU	P2872	ARG	L2752
L3560	F3495	K3435	F3375	L3313	H3251	PHE	LEU	Q2873	GLY	Q2753
E3561	S3496	S3436	V3376	L3314	G3252	GLY	PHE	D2874	ASP	P2754
K3562	L3497	K3437	D3377	K3315	P3253	ASP	GLY	T2875	GLY	L2755
K3563	L3498	M3438	Y3378	T3316	E3254	LEU	GLY	L2876	GLY	G2819
S3564	D3499	S3439	N3379	H3317	N3255	ASN	SER	T2877	ASP	Y2820
K3565	T3500	K3440	R3380	F3257	H3256	LEU	ARG	A2878	ASP	S2821
Y3566	E3501	A3441	A3381	F3257	R3256	GLU	ALA	K2879	ARG	P2758
THR	E3502	A3442	K3382	L3319	E3258	ASP	LYS	P2879	LYS	Y2759
GLY	E3503	I3443	W3383	R3320	R3186	GLN	GLY	E2880	GLY	R2823
ARG	V3504	S3444	L3384	L3321	E3261	VAL	HIS	K2881	GLU	A2824
TYR	R3505	D3445	K3385	M3322	K3262	SER	ASN	A2882	ASP	L2761
PHE	D3506	Q3446	K3386	E3323	C3263	CYS	PRO	K2883	THR	L2762
SER	I3507	E3447	P3387	K3324	C3264	TYR	TYR	D2884	TYR	S2763
LEU	I3508	R3448	N3388	L3325	C3264	ILE	GLU	R2885	GLU	E2764
VAL	R3509	K3449	P3389	K3326	L3267	LEU	GLN	R2885	GLU	K2765
GLU	S3510	K3450	GLU	ALA	N3268	THR	GLU	E2886	GLU	E2766
HIS	N3511	M3451	GLU	GLU	S3269	SER	ILE	K2887	ILE	V2830
ARG	I3512	K3452	GLU	K3327	H3271	SER	LYS	A2888	LYS	T2831
SER	H3513	R3453	LEU	K3328	K3270	THR	PHE	L2832	PHE	L2832
LYS	K3454	Q3455	PHE	E3334	N3272	TYR	GLY	Q2889	GLY	S2833
ALA	Q3515	G3455	ARG	S3334	N3273	ALA	ALA	D2890	ALA	R2834
VAL	G3516	D3456	VAL	E3335	N3274	LEU	LYS	I2891	LYS	D2835
TRP	L3517	R3457	ALA	E3336	L3275	GLY	VAL	F2892	VAL	L2836
HIS	E3519	Y3458	GLU	K3340	GLY	THR	THR	F2894	THR	H2837
ASP		S3459	VAL	L3339	LEU	GLY	VAL	K2895	GLY	A2838
PRO		M3460	ILE	K3340	ASN	THR	THR	Q2896	GLY	M2839
ALA		Q3461	GLU	L3339	ILE	GLY	THR	E2776	GLY	E2840
ILE		T3462	VAL	K3340	LEU	THR	THR	I2897	THR	E2841
ARG		S3463	ILE	A3343	K3281	LEU	THR	S2898	THR	L2778
TRP		L3464	ALA	R3344	I3282	GLY	THR	G2899	THR	K2779
GLN		V3465	ALA	D3346	I3283	THR	THR	Y2900	THR	M2843
MET		A3467	ALA	M3347		THR	THR	V2901	THR	L2781
			ALA			THR	THR	V2902	THR	L2782
			ALA			THR	THR	S2903	THR	A2783
			ALA			THR	THR	R2904	THR	K2784
			ALA			THR	THR	GLY	THR	G2785



• Molecule 1: Ryanodine receptor 2



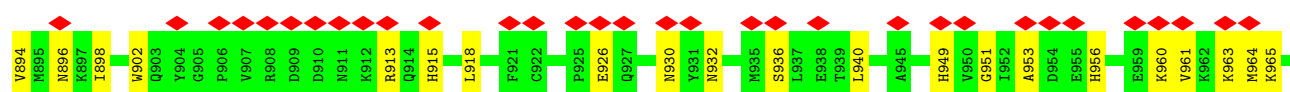


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- Molecule 1: Ryanodine receptor 2

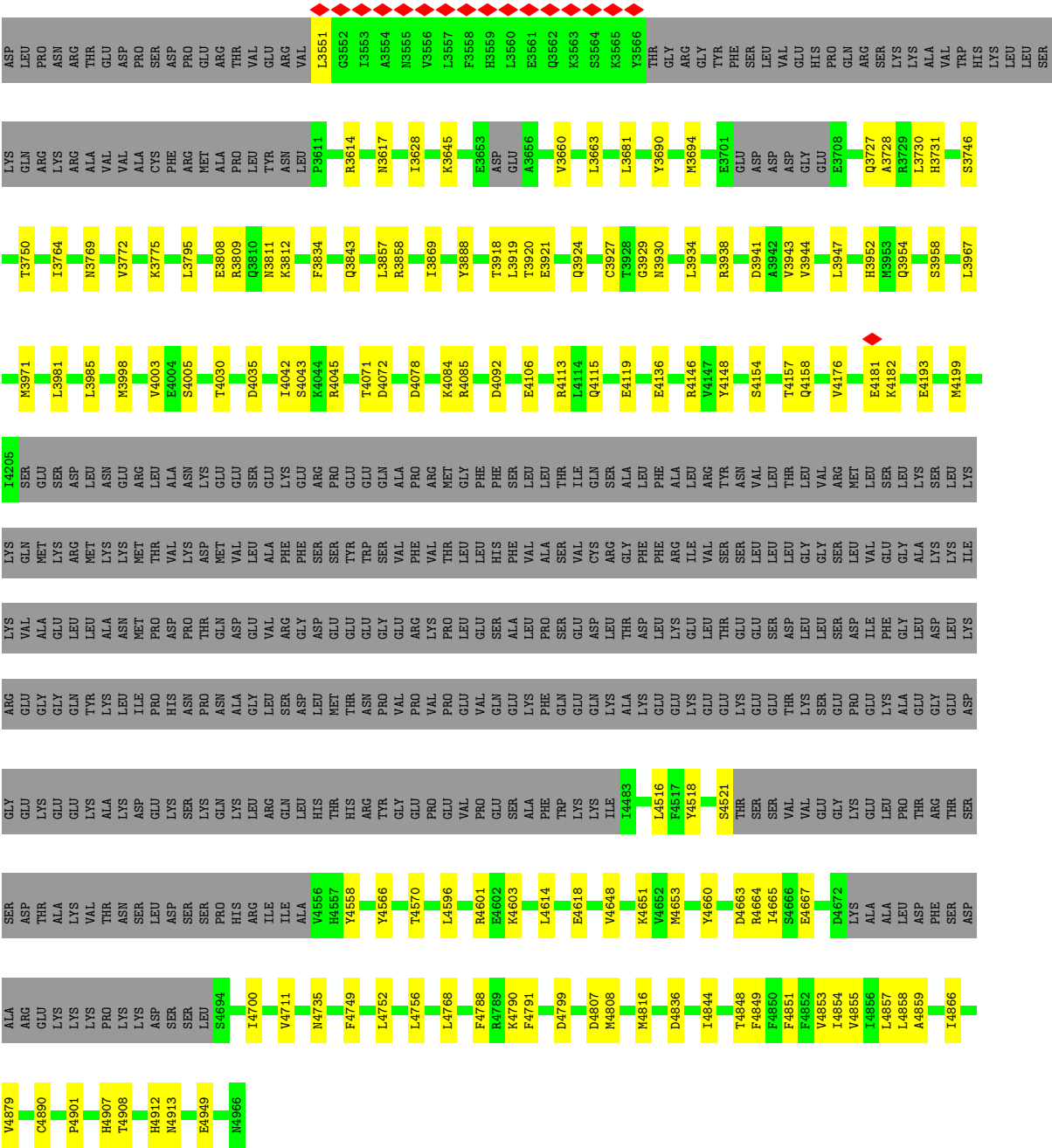




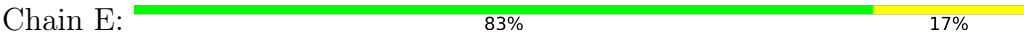


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Y1060	G1061	HIS	LEU	GLU	ALA	PRO	ASP	ARG	ALA	GLU	CYS	SER	GLY	THR	R1089	R1100	F1103	V1108	D1112	W1117	P1124	G1129	F1135	A1136	F1137	Q1143	R1144	W1145	Y1152	D1160	C1164	M1165	V1166	D1167	E1170	H1171	T1172												
M1173	T1176	N1178	G1179	E1180	L1190	K1193	D1194	F1195	D1199	C1205	S1206	Q1211	R1214	M1215	N1216	F1217	T1223	L1224	K1225	F1239	T1243	N1244	R1245	W1250	L1251	P1262	I1268	E1269	I1273	P1281	Q1287	F1290	N1294	M1295	N1296	I1299	Y1302												
P1307	I1308	CYS	ALA	VAL	PHE	SER	LYS	GLY	GLY	PRO	GLY	ALA	PHE	TYR	PRO	LYS	LEU	GLU	ASP	PHE	VAL	ASP	PHE	GLU	VAL	MET	LYS	THR	ALA	HIS	ASP	VAL	PRO	ASP	TYR	ARG	ILE	ASP	LYS	GLU	THR	PRO							
LYS	PRO	ASN	HIS	VAL	ASN	LYS	ASP	PRO	GLN	ARG	LEU	GLN	ARG	GLY	ARG	ASN	LYS	PRO	THR	HIS	SER	ALA	ARG	LEU	THR	MET	ASP	VAL	ALA	ASP	ARG	ASP	ASP	GLY	TYR	THR	GLU	ASP	GLY	ASN	ASN	VAL							
P1434	G1444	W1445	I1446	F1450	V1462	R1463	T1464	T1465	T1466	V1467	G1474	E1478	S1479	I1480	C1485	V1488	G1499	N1502	G1505	V1511	L1519	I1522	A1523	N1524	Y1532	T1538	V1544	P1551	ASN	VAL	PHE	GLN	PHE	GLU	LEU	GLY	ARG	ILE	LYS	ASN	VAL								
MET	PRO	ALA	GLY	PHE	SER	LYS	LYS	PRO	VAL	GLN	CYS	PRO	ARG	PRO	VAL	GLN	PHE	SER	HIS	V1595	P1601	N1602	L1619	A1674	P1684	Q1685	E1691	M1695	P1696	L1712	M1722	N1723	I1737	F1740	P1741	L1754	P1767												
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GLU	GLU	ALA	GLY	LYS	ARG	PRO	GLU	G1891	V1901	M1905	D1914	R1918	I1924	F1927	L1935	E1945	VAL	MET	GLN	ALA	ASN	GLU	MET	SER	ALA	ALA	VAL	THR	ALA	ARG	LYS	THR	ARG	PHE	GLN	GLU	ILE	ASN	MET	LEU									
ASN	PHE	LYS	ASP	LYS	SER	CYS	PRO	GLU	ILE	ARG	GLN	L1995	L2002	C2006	E2012	L2016	I2024	R2027	L2031	K2034	V2035	T2036	Y2037	K2040	LYS	GLN	ALA	GLU	LYS	ASP	PRO	VAL	SER	ASP	ARG	LYS	C2054	M2065	L2079	V2080									
M2083	R2089	L2101	K2263	L2119	L2122	S2130	VAL	ARG	G2134	K2152	Y2155	R2162	A2163	L2164	M2174	L2178	K2184	T2187	M2191	C2196	R2197	Y2201	Q2208	N2209	Q2210	S2218	E2222	L2228	A2229	S2230	M2233	S2236	T2237	P2238	L2239	A2244													
N2249	L2254	K2263	V2264	Y2267	M2278	G2288	V2289	ASN	P2290	V2292	F2300	E2314	V2320	R2321	L2324	R2325	P2327	F2330	G2331	P2332	A2333	R2335	G2336	G2339	N2340	G2341	P2356	SER	ARG	ASP	GLY	PRO	SER	PRO	SER	GLY	SER	SER	LYS	THR	ILE	GLU							
GLU	GLU	ASP	THR	ILE	HIS	M2383	G2384	N2385	Y2391	I2395	D2396	R2400	E2404	M2405	H2406	L2407	R2417	L2418	R2419	L2425	PRO	LEU	G2429	M2441	I2444	V2450	V2451	S2456	P2461	M2467	L2471	G2476	I2477	L2484	G2490	D2494	L2495	L2501											
ASP	THR	ALA	ALA	S2507	A2508	T2509	M2511	A2512	L2513	A2514	L2515	L2526	L2527	THR	ARG	CYS	ALA	GLY	THR	GLU	HIS	ALA	SER	LEU	ILE	ASP	SER	LEU	LEU	HIS	THR	VAL	TYR	ARG	LEU	SER	GLY	CYS	SER	THR	LYS	ALA	GLN	ARG	ASP	SER	ILE	GLU	VAL

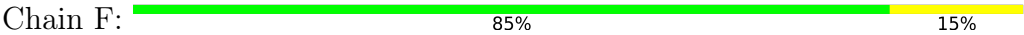
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K3412	R3413	E3414	E3415	K3416	N3417	F3418	V3419	F3420	Q3421	Q3422	E3423	I3424	N3425	N3426	M3427	S3428	F3429	L3430	I3431	F3432	D3433	F3434	K3435	S3436	F3437	M3438	S3439	K3440	A3441	A3442	I3443	S3444	D3445	Q3446	E3447	R3448	K3449	K3450	N3451	K3452	R3453	K3454	G3455	D3456	R3457	Y3458	S3459	K3460	Q3461	T3462	S3463	ARG	TRP	L3464	I3465	V3466	A3467	A3468	L3469	K3470	R3471			
G3288	I3289	D3290	E3291	G3292	ALA	TRP	MET	LYS	ARG	LEU	ALA	VAL	F3301	S3302	Q3303	P3304	I3305	H3306	N3307	K3308	V3309	K3310	Q3311	Q3312	L3313	L3314	K3315	T3316	H3317	F3318	L3319	P3320	L3321	M3322	E3323	K3324	L3325	N3326	K3327	K3328	A3329	V3333	S3334	E3335	E3336	L3339	K3340	A3343	R3344	G3345	D3346	N3347	S3348	E3349	A3350	E3351								
L3352	L3353	I3354	L3355	D3356	E3357	F3358	T3359	T3360	L3361	A3362	R3363	D3364	L3365	Y3366	A3367	F3368	Y3369	P3370	L3371	L3372	I3373	R3374	F3375	V3376	D3377	Y3378	N3379	K3380	A3381	K3382	V3383	L3384	K3385	E3386	P3387	N3388	F3389	GLU	ALA	GLU	LEU	PHE	ARG	MET	VAL	ALA	GLU	VAL	PHE	ILE	Y3404	V3405	S3406	K3407	S3408	H3409	N3410	F3411						
I3225	R3226	Y3227	Q3228	Q3229	M3230	P3231	Y3232	M3233	M3234	E3235	V3236	V3237	L3238	P3239	M3240	L3241	C3242	S3243	Y3244	R3247	E3250	H3251	G3252	P3253	E3254	N3255	K3256	P3257	E3258	R3259	A3260	E3261	K3262	C3263	C3264	L3267	N3268	S3269	E3270	H3271	M3272	N3273	P3274	L3275	LEU	GLY	ASN	ILE	LEU	K3281	I3282	I3283	Y3284	N3285	N3286	L3287								
A3058	F3059	L3060	N3062	A3063	D3066	R3083	I3093	L3100	I3101	P3102	M3103	LEU	SER	SER	LEU	PHE	GLU	HIS	ILE	K3000	R3015	H3016	ARG	ILE	SER	LEU	PHE	GLY	ASN	ALA	THR	SER	VAL	GLN	VAL	C3263	E3201	D3202	V3203	C3204	P3205	N3206	T3207	P3208	T3215	L3218	A3221	E3222	S3223	G3224														
ASP	LEU	THR	PRO	SER	ILE	GLU	LYS	ARG	ALA	PHE	GLN	LEU	THR	ASP	GLN	VAL	TYR	ASP	GLU	ALA	HIS	TYR	ILE	GLU	PHE	GLY	ASP	ARG	LYS	THR	LEU	GLY	ASN	ALA	THR	SER	VAL	GLN	GLU	ILE	ILE	LYS	PHE	ALA	LYS	VAL	VAL	LEU	PRO	LEU	Q2896	T2897	E2898	G2899	Y2900	V2901	V2902	S2903	R2904	GLY	PHE	LYS	ASP	LEU
CYS	LEU	SER	ILE	CYS	GLY	V2595	L2606	P2623	L2643	I2647	Q2658	E2659	P2666	W2694	ASP	SER	GLY	GLY	ASN	F2700	N2701	P2702	Q2703	P2704	V2705	D2706	T2707	S2708	N2709	I2710	T2711	I2712	P2713	E2714	K2715	L2716	E2717	V2718	F2719	T2720	N2721	K2722	V2723	A2724	E2725	H2726	S2727	H2728	D2729															
K2730	W2731	S2732	M2733	D2734	K2735	L2736	A2737	N2738	G2739	W2740	I2741	Y2742	G2743	E2744	I2745	Y2746	S2747	D2748	S2749	K2750	I2752	Q2753	P2754	L2755	M2756	K2757	P2758	Y2759	K2760	L2761	L2762	S2763	E2764	K2765	E2766	I2769	Y2770	R2771	W2772	P2773	I2774	K2775	E2776	S2777	L2778	K2779	T2780	M2781	L2782	A2783	W2784	G2785	W2786	R2787	I2788	E2789								



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

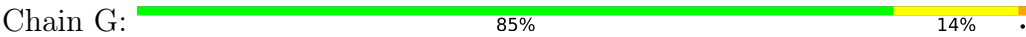


● Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

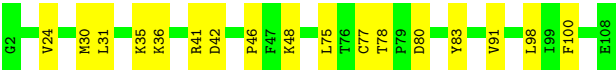
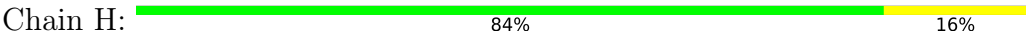




- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	73782	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.311	Depositor
Minimum map value	-0.628	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.12	Depositor
Map size ($\text{\AA}$)	496.80002, 496.80002, 496.80002	wwPDB
Map dimensions	460, 460, 460	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.13	0/29611	0.37	3/40214 (0.0%)
1	B	0.13	0/29611	0.37	3/40214 (0.0%)
1	C	0.13	0/29611	0.37	3/40214 (0.0%)
1	D	0.13	0/29611	0.37	3/40214 (0.0%)
2	E	0.09	0/778	0.31	0/1060
2	F	0.10	0/778	0.31	0/1060
2	G	0.09	0/778	0.31	0/1060
2	H	0.10	0/778	0.31	0/1060
All	All	0.13	0/121556	0.37	12/165096 (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

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1124	PRO	N-CA-CB	7.41	110.24	103.20
1	D	1124	PRO	N-CA-CB	7.41	110.24	103.20
1	C	1124	PRO	N-CA-CB	7.39	110.22	103.20
1	B	1124	PRO	N-CA-CB	7.36	110.19	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	413	SER	CB-CA-C	-6.74	108.79	116.54
1	C	413	SER	CB-CA-C	-6.71	108.83	116.54
1	D	413	SER	CB-CA-C	-6.69	108.85	116.54
1	B	413	SER	CB-CA-C	-6.68	108.85	116.54
1	A	2197	ARG	CB-CA-C	-5.95	109.70	116.54
1	B	2197	ARG	CB-CA-C	-5.93	109.72	116.54
1	D	2197	ARG	CB-CA-C	-5.93	109.72	116.54
1	C	2197	ARG	CB-CA-C	-5.91	109.74	116.54

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	4181	GLU	Peptide
1	B	4181	GLU	Peptide
1	C	4181	GLU	Peptide
1	D	4181	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	29055	0	27182	364	0
1	B	29055	0	27182	358	0
1	C	29055	0	27182	364	0
1	D	29055	0	27182	375	0
2	E	763	0	709	12	0
2	F	763	0	709	11	0
2	G	763	0	709	11	0
2	H	763	0	709	11	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1	0	0	0	0
All	All	119280	0	111564	1458	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 6.

All (1458) 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:189:GLU:OE1	1:B:2417:ARG:NH1	2.24	0.71
1:D:1205:CYS:SG	1:D:1206:SER:N	2.64	0.71
1:A:1205:CYS:SG	1:A:1206:SER:N	2.64	0.71
1:C:1205:CYS:SG	1:C:1206:SER:N	2.64	0.71
1:B:1205:CYS:SG	1:B:1206:SER:N	2.64	0.70
1:C:695:VAL:HB	1:C:727:PHE:HB3	1.76	0.67
1:B:695:VAL:HB	1:B:727:PHE:HB3	1.76	0.67
1:A:695:VAL:HB	1:A:727:PHE:HB3	1.76	0.67
1:C:189:GLU:OE1	1:D:2417:ARG:NH1	2.28	0.67
1:D:695:VAL:HB	1:D:727:PHE:HB3	1.76	0.66
1:B:189:GLU:OE1	1:C:2417:ARG:NH1	2.28	0.66
1:A:1450:PHE:HA	1:A:1485:CYS:HB3	1.78	0.66
1:A:2417:ARG:NH1	1:D:189:GLU:OE1	2.29	0.65
1:A:234:LEU:HD12	1:A:408:SER:HB3	1.79	0.65
1:A:3469:LEU:HD11	1:A:3476:GLY:HA3	1.79	0.65
1:D:3469:LEU:HD11	1:D:3476:GLY:HA3	1.79	0.65
1:B:234:LEU:HD12	1:B:408:SER:HB3	1.79	0.65
1:C:234:LEU:HD12	1:C:408:SER:HB3	1.79	0.65
1:C:1450:PHE:HA	1:C:1485:CYS:HB3	1.78	0.65
1:C:1684:PRO:HG3	2:G:42:ASP:HB2	1.78	0.64
1:B:1684:PRO:HG3	2:F:42:ASP:HB2	1.78	0.64
1:D:234:LEU:HD12	1:D:408:SER:HB3	1.79	0.64
1:C:3469:LEU:HD11	1:C:3476:GLY:HA3	1.79	0.64
1:B:1450:PHE:HA	1:B:1485:CYS:HB3	1.77	0.64
1:B:3469:LEU:HD11	1:B:3476:GLY:HA3	1.79	0.64
1:D:1450:PHE:HA	1:D:1485:CYS:HB3	1.78	0.64
1:A:1684:PRO:HG3	2:E:42:ASP:HB2	1.78	0.64
1:A:312:LYS:HG3	1:A:394:HIS:HA	1.80	0.64
1:B:2196:CYS:SG	1:B:2197:ARG:N	2.71	0.64
1:D:312:LYS:HG3	1:D:394:HIS:HA	1.80	0.64
1:D:1684:PRO:HG3	2:H:42:ASP:HB2	1.78	0.63
1:B:186:VAL:O	1:C:2417:ARG:NH2	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:LYS:HG3	1:B:394:HIS:HA	1.79	0.63
1:C:312:LYS:HG3	1:C:394:HIS:HA	1.80	0.63
1:C:732:LEU:HB2	1:C:740:THR:HA	1.81	0.63
1:C:3769:ASN:HB2	1:C:3772:VAL:HG22	1.81	0.63
1:A:2196:CYS:SG	1:A:2197:ARG:N	2.71	0.63
1:B:732:LEU:HB2	1:B:740:THR:HA	1.81	0.63
1:A:3769:ASN:HB2	1:A:3772:VAL:HG22	1.81	0.62
1:D:732:LEU:HB2	1:D:740:THR:HA	1.81	0.62
1:D:3769:ASN:HB2	1:D:3772:VAL:HG22	1.81	0.62
1:A:732:LEU:HB2	1:A:740:THR:HA	1.81	0.62
1:B:1268:ILE:HD12	1:B:1290:PHE:HZ	1.65	0.62
1:C:1268:ILE:HD12	1:C:1290:PHE:HZ	1.65	0.62
1:D:3451:MET:SD	1:D:3454:LYS:NZ	2.73	0.62
1:B:3769:ASN:HB2	1:B:3772:VAL:HG22	1.81	0.62
1:C:4859:ALA:HB1	1:D:4866:ILE:HD11	1.81	0.62
1:B:189:GLU:OE2	1:C:2321:ARG:NH2	2.32	0.62
1:C:66:THR:HG22	1:C:217:ILE:HG12	1.82	0.62
1:D:66:THR:HG22	1:D:217:ILE:HG12	1.81	0.62
1:A:1268:ILE:HD12	1:A:1290:PHE:HZ	1.65	0.62
1:A:4859:ALA:HB1	1:B:4866:ILE:HD11	1.81	0.62
1:B:3843:GLN:HG3	1:B:3921:GLU:HG3	1.82	0.62
1:C:1167:ASP:H	1:C:1173:MET:HE1	1.65	0.62
1:D:1268:ILE:HD12	1:D:1290:PHE:HZ	1.64	0.62
1:A:4866:ILE:HD11	1:D:4859:ALA:HB1	1.81	0.62
1:D:1167:ASP:H	1:D:1173:MET:HE1	1.65	0.62
1:A:1167:ASP:H	1:A:1173:MET:HE1	1.65	0.61
1:C:3451:MET:SD	1:C:3454:LYS:NZ	2.73	0.61
1:A:3843:GLN:HG3	1:A:3921:GLU:HG3	1.82	0.61
1:C:539:ALA:HA	1:C:542:ARG:HD2	1.82	0.61
1:A:3451:MET:SD	1:A:3454:LYS:NZ	2.73	0.61
1:D:539:ALA:HA	1:D:542:ARG:HD2	1.82	0.61
1:A:186:VAL:O	1:B:2417:ARG:NH2	2.34	0.61
1:A:1914:ASP:OD1	1:A:2089:ARG:NH2	2.34	0.61
1:A:2417:ARG:NH2	1:D:186:VAL:O	2.34	0.61
1:B:3451:MET:SD	1:B:3454:LYS:NZ	2.73	0.61
1:C:1914:ASP:OD1	1:C:2089:ARG:NH2	2.34	0.61
1:C:3049:LEU:HB2	1:C:3093:ILE:HD11	1.83	0.61
1:A:758:CYS:HB3	1:A:766:ILE:HD12	1.82	0.61
1:B:66:THR:HG22	1:B:217:ILE:HG12	1.81	0.61
1:B:758:CYS:HB3	1:B:766:ILE:HD12	1.83	0.60
1:B:539:ALA:HA	1:B:542:ARG:HD2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3049:LEU:HB2	1:B:3093:ILE:HD11	1.83	0.60
1:A:701:GLU:HG2	1:A:1462:VAL:HG13	1.83	0.60
1:A:1160:ASP:OD1	1:A:1178:ASN:ND2	2.34	0.60
1:C:758:CYS:HB3	1:C:766:ILE:HD12	1.83	0.60
1:D:1160:ASP:OD1	1:D:1178:ASN:ND2	2.34	0.60
1:A:66:THR:HG22	1:A:217:ILE:HG12	1.82	0.60
1:B:1914:ASP:OD1	1:B:2089:ARG:NH2	2.34	0.60
1:D:1914:ASP:OD1	1:D:2089:ARG:NH2	2.34	0.60
1:C:186:VAL:O	1:D:2417:ARG:NH2	2.34	0.60
1:C:701:GLU:HG2	1:C:1462:VAL:HG13	1.83	0.60
1:C:1160:ASP:OD1	1:C:1178:ASN:ND2	2.34	0.60
1:C:1190:LEU:HD21	1:C:1193:LYS:HG3	1.83	0.60
1:A:539:ALA:HA	1:A:542:ARG:HD2	1.82	0.60
1:B:1160:ASP:OD1	1:B:1178:ASN:ND2	2.34	0.60
1:B:1167:ASP:H	1:B:1173:MET:HE1	1.65	0.60
1:D:758:CYS:HB3	1:D:766:ILE:HD12	1.83	0.60
1:A:1190:LEU:HD21	1:A:1193:LYS:HG3	1.83	0.60
1:D:3843:GLN:HG3	1:D:3921:GLU:HG3	1.82	0.60
1:C:3843:GLN:HG3	1:C:3921:GLU:HG3	1.82	0.59
1:B:701:GLU:HG2	1:B:1462:VAL:HG13	1.83	0.59
1:C:2196:CYS:SG	1:C:2197:ARG:N	2.71	0.59
1:A:189:GLU:OE2	1:B:2321:ARG:NH2	2.35	0.59
1:A:725:TYR:HD2	1:A:732:LEU:HA	1.68	0.59
1:A:2254:LEU:O	1:A:3809:ARG:NH1	2.36	0.59
1:D:725:TYR:HD2	1:D:732:LEU:HA	1.68	0.59
1:A:2526:LEU:HD22	1:A:2606:LEU:HD22	1.85	0.59
1:A:3049:LEU:HB2	1:A:3093:ILE:HD11	1.82	0.59
1:B:725:TYR:HD2	1:B:732:LEU:HA	1.68	0.59
1:C:725:TYR:HD2	1:C:732:LEU:HA	1.68	0.59
1:D:1190:LEU:HD21	1:D:1193:LYS:HG3	1.83	0.59
1:D:3049:LEU:HB2	1:D:3093:ILE:HD11	1.83	0.59
1:B:81:MET:SD	1:B:81:MET:N	2.76	0.59
1:B:1190:LEU:HD21	1:B:1193:LYS:HG3	1.83	0.59
1:B:2526:LEU:HD22	1:B:2606:LEU:HD22	1.85	0.59
1:D:701:GLU:HG2	1:D:1462:VAL:HG13	1.83	0.59
1:A:81:MET:SD	1:A:81:MET:N	2.76	0.59
1:D:3944:VAL:HG13	1:D:4005:SER:HB3	1.85	0.59
1:B:2254:LEU:O	1:B:3809:ARG:NH1	2.36	0.58
1:B:3215:THR:HA	1:B:3218:ILE:HD12	1.85	0.58
1:C:3215:THR:HA	1:C:3218:ILE:HD12	1.86	0.58
1:C:3944:VAL:HG13	1:C:4005:SER:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2254:LEU:O	1:D:3809:ARG:NH1	2.36	0.58
1:D:2526:LEU:HD22	1:D:2606:LEU:HD22	1.85	0.58
1:B:2184:LYS:O	1:B:2187:THR:OG1	2.20	0.58
1:C:2526:LEU:HD22	1:C:2606:LEU:HD22	1.85	0.58
1:D:81:MET:SD	1:D:81:MET:N	2.76	0.58
1:A:2321:ARG:NH2	1:D:189:GLU:OE2	2.37	0.58
1:A:3215:THR:HA	1:A:3218:ILE:HD12	1.86	0.58
1:C:2254:LEU:O	1:C:3809:ARG:NH1	2.36	0.58
1:D:1294:ASN:O	1:D:1296:ASN:ND2	2.37	0.58
2:G:46:PRO:HG2	2:G:48:LYS:HZ1	1.69	0.58
1:A:1294:ASN:O	1:A:1296:ASN:ND2	2.37	0.57
1:B:3944:VAL:HG13	1:B:4005:SER:HB3	1.85	0.57
1:C:81:MET:SD	1:C:81:MET:N	2.76	0.57
1:C:189:GLU:OE2	1:D:2321:ARG:NH2	2.37	0.57
1:D:2184:LYS:O	1:D:2187:THR:OG1	2.20	0.57
2:F:46:PRO:HG2	2:F:48:LYS:HZ1	1.69	0.57
1:C:965:LYS:HE2	1:C:983:LEU:HD13	1.86	0.57
1:C:1794:GLN:O	1:C:1797:THR:OG1	2.21	0.57
1:D:3215:THR:HA	1:D:3218:ILE:HD12	1.86	0.57
1:C:4907:HIS:HE1	1:C:4912:HIS:ND1	2.03	0.57
1:B:2326:ARG:NH1	1:B:2327:PRO:O	2.38	0.57
1:D:2196:CYS:SG	1:D:2197:ARG:N	2.71	0.57
1:A:3944:VAL:HG13	1:A:4005:SER:HB3	1.85	0.57
1:D:4907:HIS:HE1	1:D:4912:HIS:ND1	2.03	0.57
1:A:1848:GLU:H	1:A:1849:PRO:HD2	1.70	0.57
1:C:2326:ARG:NH1	1:C:2327:PRO:O	2.38	0.57
1:B:1848:GLU:H	1:B:1849:PRO:HD2	1.70	0.57
1:B:4907:HIS:HE1	1:B:4912:HIS:ND1	2.03	0.57
1:B:4859:ALA:HB1	1:C:4866:ILE:HD11	1.86	0.57
1:C:33:GLN:N	1:C:33:GLN:OE1	2.38	0.57
1:D:1848:GLU:H	1:D:1849:PRO:HD2	1.70	0.57
1:A:3981:LEU:HB3	1:A:3998:MET:HE1	1.87	0.56
1:C:1294:ASN:O	1:C:1296:ASN:ND2	2.37	0.56
1:D:33:GLN:N	1:D:33:GLN:OE1	2.38	0.56
1:D:965:LYS:HE2	1:D:983:LEU:HD13	1.86	0.56
1:B:965:LYS:HE2	1:B:983:LEU:HD13	1.86	0.56
1:B:3344:ARG:O	1:B:3366:TYR:OH	2.23	0.56
1:D:2326:ARG:NH1	1:D:2327:PRO:O	2.38	0.56
1:A:965:LYS:HE2	1:A:983:LEU:HD13	1.86	0.56
1:A:3344:ARG:O	1:A:3366:TYR:OH	2.23	0.56
1:B:1794:GLN:O	1:B:1797:THR:OG1	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3981:LEU:HB3	1:B:3998:MET:HE1	1.87	0.56
1:C:2236:SER:HB2	1:C:2239:LEU:HB2	1.88	0.56
1:A:4790:LYS:NZ	1:A:4836:ASP:OD2	2.37	0.56
1:B:1294:ASN:O	1:B:1296:ASN:ND2	2.37	0.56
1:D:2236:SER:HB2	1:D:2239:LEU:HB2	1.88	0.56
2:E:46:PRO:HG2	2:E:48:LYS:HZ1	1.70	0.56
2:H:46:PRO:HG2	2:H:48:LYS:HZ1	1.70	0.56
1:C:2002:LEU:HB3	1:C:2006:CYS:HB2	1.88	0.56
1:D:1777:TYR:HD1	1:D:1778:GLN:HG2	1.71	0.56
1:D:2836:LEU:HD21	1:D:2902:VAL:H	1.71	0.56
1:D:3344:ARG:O	1:D:3366:TYR:OH	2.23	0.56
1:A:33:GLN:OE1	1:A:33:GLN:N	2.38	0.56
1:A:2326:ARG:NH1	1:A:2327:PRO:O	2.38	0.56
1:A:4907:HIS:HE1	1:A:4912:HIS:ND1	2.03	0.56
1:B:1674:ALA:HB1	1:B:1780:SER:HB2	1.88	0.56
1:C:3344:ARG:O	1:C:3366:TYR:OH	2.23	0.56
1:B:235:ARG:HB2	1:B:406:SER:HB3	1.88	0.56
1:C:1173:MET:HE3	1:C:1195:PHE:HZ	1.71	0.56
1:C:235:ARG:HB2	1:C:406:SER:HB3	1.88	0.56
1:C:1777:TYR:HD1	1:C:1778:GLN:HG2	1.71	0.56
1:A:1674:ALA:HB1	1:A:1780:SER:HB2	1.88	0.55
1:A:2836:LEU:HD21	1:A:2902:VAL:H	1.71	0.55
1:B:33:GLN:N	1:B:33:GLN:OE1	2.38	0.55
1:B:2236:SER:HB2	1:B:2239:LEU:HB2	1.88	0.55
1:D:1740:PHE:HD1	1:D:1741:PRO:HD2	1.72	0.55
1:D:4003:VAL:HG11	1:D:4113:ARG:HD2	1.88	0.55
1:A:1112:ASP:O	1:A:1211:GLN:NE2	2.40	0.55
1:C:2184:LYS:O	1:C:2187:THR:OG1	2.20	0.55
1:C:3083:ARG:HH12	1:C:3208:PRO:HG3	1.72	0.55
1:D:2002:LEU:HB3	1:D:2006:CYS:HB2	1.88	0.55
1:A:1243:THR:HG22	1:A:1245:ARG:H	1.71	0.55
1:A:3083:ARG:HH12	1:A:3208:PRO:HG3	1.72	0.55
1:B:697:TRP:H	1:B:724:SER:HB2	1.72	0.55
1:C:3981:LEU:HB3	1:C:3998:MET:HE1	1.87	0.55
1:C:4003:VAL:HG11	1:C:4113:ARG:HD2	1.89	0.55
1:D:624:ALA:HB1	1:D:629:GLN:HB3	1.89	0.55
1:D:3083:ARG:HH12	1:D:3208:PRO:HG3	1.72	0.55
1:D:3981:LEU:HB3	1:D:3998:MET:HE1	1.87	0.55
1:A:1777:TYR:HD1	1:A:1778:GLN:HG2	1.71	0.55
1:B:2002:LEU:HB3	1:B:2006:CYS:HB2	1.88	0.55
1:C:514:PHE:HA	1:C:517:VAL:HG12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2836:LEU:HD21	1:C:2902:VAL:H	1.71	0.55
1:D:1173:MET:HE3	1:D:1195:PHE:HZ	1.71	0.55
1:A:3045:MET:HG2	1:A:3093:ILE:HG12	1.89	0.55
1:C:697:TRP:H	1:C:724:SER:HB2	1.72	0.55
1:A:697:TRP:H	1:A:724:SER:HB2	1.72	0.55
1:A:2236:SER:HB2	1:A:2239:LEU:HB2	1.88	0.55
1:A:4003:VAL:HG11	1:A:4113:ARG:HD2	1.88	0.55
1:B:1777:TYR:HD1	1:B:1778:GLN:HG2	1.71	0.55
1:B:2836:LEU:HD21	1:B:2902:VAL:H	1.71	0.55
1:D:235:ARG:HB2	1:D:406:SER:HB3	1.88	0.55
1:A:217:ILE:O	1:A:285:SER:N	2.40	0.55
1:A:235:ARG:HB2	1:A:406:SER:HB3	1.88	0.55
1:A:272:ARG:HB2	1:A:492:GLU:HG2	1.89	0.55
1:A:514:PHE:HA	1:A:517:VAL:HG12	1.88	0.55
1:B:2716:LEU:HD13	1:B:2720:ILE:HG21	1.89	0.55
1:B:3083:ARG:HH12	1:B:3208:PRO:HG3	1.72	0.55
1:D:755:ILE:HG22	1:D:770:ILE:HG12	1.89	0.55
1:C:217:ILE:O	1:C:285:SER:N	2.40	0.55
1:C:624:ALA:HB1	1:C:629:GLN:HB3	1.89	0.55
1:D:896:ASN:ND2	1:D:1052:GLU:OE1	2.40	0.55
1:D:1112:ASP:O	1:D:1211:GLN:NE2	2.40	0.55
1:D:3920:THR:O	1:D:3924:GLN:N	2.40	0.55
1:B:272:ARG:HB2	1:B:492:GLU:HG2	1.89	0.55
1:B:3045:MET:HG2	1:B:3093:ILE:HG12	1.89	0.55
1:C:1243:THR:HG22	1:C:1245:ARG:H	1.71	0.55
1:D:1674:ALA:HB1	1:D:1780:SER:HB2	1.88	0.55
1:A:1740:PHE:HD1	1:A:1741:PRO:HD2	1.72	0.55
1:B:1243:THR:HG22	1:B:1245:ARG:H	1.71	0.55
1:C:1112:ASP:O	1:C:1211:GLN:NE2	2.40	0.55
1:C:1740:PHE:HD1	1:C:1741:PRO:HD2	1.72	0.55
1:C:2036:THR:HG21	1:C:3628:ILE:HG21	1.89	0.55
1:D:3045:MET:HG2	1:D:3093:ILE:HG12	1.89	0.55
1:A:1173:MET:HE3	1:A:1195:PHE:HZ	1.71	0.54
1:B:3731:HIS:O	1:B:3775:LYS:NZ	2.41	0.54
1:D:697:TRP:H	1:D:724:SER:HB2	1.72	0.54
1:D:1243:THR:HG22	1:D:1245:ARG:H	1.71	0.54
1:D:2331:GLY:HA3	1:D:2341:GLY:H	1.72	0.54
1:A:589:ILE:HG21	1:A:617:LEU:HD21	1.89	0.54
1:A:2331:GLY:HA3	1:A:2341:GLY:H	1.72	0.54
1:A:2716:LEU:HD13	1:A:2720:ILE:HG21	1.89	0.54
1:A:4849:PHE:O	1:A:4853:VAL:HG12	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:896:ASN:ND2	1:C:1052:GLU:OE1	2.40	0.54
1:C:1674:ALA:HB1	1:C:1780:SER:HB2	1.88	0.54
1:C:1848:GLU:H	1:C:1849:PRO:HD2	1.70	0.54
1:C:3920:THR:O	1:C:3924:GLN:N	2.40	0.54
1:A:547:ASN:HB2	1:A:550:GLN:HB2	1.89	0.54
1:A:2002:LEU:HB3	1:A:2006:CYS:HB2	1.88	0.54
1:A:3015:ARG:NH1	1:A:3083:ARG:O	2.40	0.54
1:B:1173:MET:HE3	1:B:1195:PHE:HZ	1.71	0.54
1:D:272:ARG:HB2	1:D:492:GLU:HG2	1.89	0.54
1:D:514:PHE:HA	1:D:517:VAL:HG12	1.89	0.54
1:B:4849:PHE:O	1:B:4853:VAL:HG12	2.07	0.54
1:C:3015:ARG:NH1	1:C:3083:ARG:O	2.40	0.54
1:D:3731:HIS:O	1:D:3775:LYS:NZ	2.41	0.54
1:A:4648:VAL:HA	1:A:4651:LYS:HD2	1.89	0.54
1:B:217:ILE:O	1:B:285:SER:N	2.40	0.54
1:B:1112:ASP:O	1:B:1211:GLN:NE2	2.40	0.54
1:B:4003:VAL:HG11	1:B:4113:ARG:HD2	1.88	0.54
1:C:547:ASN:HB2	1:C:550:GLN:HB2	1.89	0.54
1:C:3614:ARG:O	1:C:3617:ASN:ND2	2.41	0.54
1:D:217:ILE:O	1:D:285:SER:N	2.40	0.54
1:D:547:ASN:HB2	1:D:550:GLN:HB2	1.90	0.54
1:D:1794:GLN:O	1:D:1797:THR:OG1	2.21	0.54
1:A:679:VAL:HA	1:A:800:VAL:HG12	1.90	0.54
1:A:3731:HIS:O	1:A:3775:LYS:NZ	2.41	0.54
1:B:172:GLY:O	1:C:3938:ARG:NH1	2.41	0.54
1:B:2331:GLY:HA3	1:B:2341:GLY:H	1.72	0.54
1:C:4849:PHE:O	1:C:4853:VAL:HG12	2.07	0.54
1:D:322:ALA:HB1	1:D:327:THR:HG21	1.90	0.54
1:D:3015:ARG:NH1	1:D:3083:ARG:O	2.40	0.54
1:D:3614:ARG:O	1:D:3617:ASN:ND2	2.41	0.54
1:A:755:ILE:HG22	1:A:770:ILE:HG12	1.89	0.54
1:A:896:ASN:ND2	1:A:1052:GLU:OE1	2.40	0.54
1:A:1795:MET:HE2	1:A:1822:LEU:HD21	1.89	0.54
1:B:3614:ARG:O	1:B:3617:ASN:ND2	2.41	0.54
1:C:4648:VAL:HA	1:C:4651:LYS:HD2	1.89	0.54
1:B:413:SER:OG	1:B:414:ARG:N	2.41	0.54
1:B:624:ALA:HB1	1:B:629:GLN:HB3	1.89	0.54
1:B:896:ASN:ND2	1:B:1052:GLU:OE1	2.40	0.54
1:C:272:ARG:HB2	1:C:492:GLU:HG2	1.89	0.54
1:C:755:ILE:HG22	1:C:770:ILE:HG12	1.89	0.54
1:C:2024:ILE:HA	1:C:2027:ARG:HH12	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4849:PHE:O	1:D:4853:VAL:HG12	2.07	0.54
1:A:3920:THR:O	1:A:3924:GLN:N	2.40	0.54
1:B:370:LEU:HD12	1:B:396:GLU:HA	1.90	0.54
1:B:547:ASN:HB2	1:B:550:GLN:HB2	1.89	0.54
1:B:679:VAL:HA	1:B:800:VAL:HG12	1.90	0.54
1:B:1137:PHE:HA	1:B:1144:ARG:HA	1.90	0.54
1:B:3920:THR:O	1:B:3924:GLN:N	2.40	0.54
1:C:322:ALA:HB1	1:C:327:THR:HG21	1.90	0.54
1:C:679:VAL:HA	1:C:800:VAL:HG12	1.90	0.54
1:C:3045:MET:HG2	1:C:3093:ILE:HG12	1.89	0.54
1:A:1137:PHE:HA	1:A:1144:ARG:HA	1.90	0.54
1:B:322:ALA:HB1	1:B:327:THR:HG21	1.90	0.54
1:B:983:LEU:HD21	1:B:1059:GLY:HA3	1.90	0.54
1:C:192:LEU:O	1:C:212:TRP:NE1	2.39	0.54
1:C:3731:HIS:O	1:C:3775:LYS:NZ	2.40	0.54
1:D:2024:ILE:HA	1:D:2027:ARG:HH12	1.73	0.54
1:D:2036:THR:HG21	1:D:3628:ILE:HG21	1.89	0.54
1:A:3614:ARG:O	1:A:3617:ASN:ND2	2.41	0.53
1:B:4648:VAL:HA	1:B:4651:LYS:HD2	1.89	0.53
1:C:2716:LEU:HD13	1:C:2720:ILE:HG21	1.89	0.53
1:D:361:CYS:O	1:D:403:LEU:N	2.38	0.53
1:D:1712:LEU:HB3	1:D:1832:MET:HE1	1.91	0.53
1:D:2716:LEU:HD13	1:D:2720:ILE:HG21	1.89	0.53
1:A:983:LEU:HD21	1:A:1059:GLY:HA3	1.90	0.53
1:A:3102:PRO:HB2	1:A:3229:GLN:HB3	1.90	0.53
1:A:3938:ARG:NH1	1:D:172:GLY:O	2.41	0.53
1:B:1795:MET:HE2	1:B:1822:LEU:HD21	1.89	0.53
1:B:3015:ARG:NH1	1:B:3083:ARG:O	2.40	0.53
1:C:1137:PHE:HA	1:C:1144:ARG:HA	1.90	0.53
1:C:1723:ASN:O	1:C:1918:ARG:NH2	2.42	0.53
1:C:4790:LYS:NZ	1:C:4836:ASP:OD2	2.37	0.53
1:D:370:LEU:HD12	1:D:396:GLU:HA	1.90	0.53
1:D:2210:GLN:NE2	1:D:2244:ALA:O	2.41	0.53
1:A:322:ALA:HB1	1:A:327:THR:HG21	1.90	0.53
1:A:1723:ASN:O	1:A:1918:ARG:NH2	2.42	0.53
1:B:1740:PHE:HD1	1:B:1741:PRO:HD2	1.71	0.53
1:C:983:LEU:HD21	1:C:1059:GLY:HA3	1.90	0.53
1:C:2210:GLN:NE2	1:C:2244:ALA:O	2.41	0.53
1:C:2331:GLY:HA3	1:C:2341:GLY:H	1.72	0.53
1:D:589:ILE:HG21	1:D:617:LEU:HD21	1.89	0.53
1:D:1723:ASN:O	1:D:1918:ARG:NH2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4648:VAL:HA	1:D:4651:LYS:HD2	1.89	0.53
1:B:514:PHE:HA	1:B:517:VAL:HG12	1.89	0.53
1:C:986:ILE:HG12	1:C:1058:LEU:HB3	1.90	0.53
1:C:1712:LEU:HB3	1:C:1832:MET:HE1	1.91	0.53
1:D:679:VAL:HA	1:D:800:VAL:HG12	1.90	0.53
1:A:3055:ALA:HB3	1:A:3100:LEU:HD13	1.90	0.53
1:B:2036:THR:HG21	1:B:3628:ILE:HG21	1.89	0.53
1:D:3102:PRO:HB2	1:D:3229:GLN:HB3	1.90	0.53
1:D:4790:LYS:NZ	1:D:4836:ASP:OD2	2.37	0.53
1:A:624:ALA:HB1	1:A:629:GLN:HB3	1.89	0.53
1:B:589:ILE:HG21	1:B:617:LEU:HD21	1.89	0.53
1:B:986:ILE:HG12	1:B:1058:LEU:HB3	1.90	0.53
1:C:3055:ALA:HB3	1:C:3100:LEU:HD13	1.90	0.53
1:D:1795:MET:HE2	1:D:1822:LEU:HD21	1.89	0.53
2:E:75:LEU:N	2:E:100:PHE:O	2.42	0.53
1:A:2036:THR:HG21	1:A:3628:ILE:HG21	1.89	0.53
1:B:755:ILE:HG22	1:B:770:ILE:HG12	1.89	0.53
1:B:3055:ALA:HB3	1:B:3100:LEU:HD13	1.90	0.53
1:C:3291:GLU:OE1	1:C:3301:PHE:N	2.42	0.53
1:A:1794:GLN:O	1:A:1797:THR:OG1	2.21	0.53
1:A:2490:GLY:O	1:A:2494:ASP:N	2.39	0.53
1:C:3102:PRO:HB2	1:C:3229:GLN:HB3	1.90	0.53
2:E:24:VAL:HG13	2:E:48:LYS:HE3	1.91	0.53
2:F:75:LEU:N	2:F:100:PHE:O	2.42	0.53
1:C:370:LEU:HD12	1:C:396:GLU:HA	1.90	0.53
1:C:1434:PRO:HB2	1:C:1502:ASN:HB3	1.91	0.53
2:G:24:VAL:HG13	2:G:48:LYS:HE3	1.91	0.53
1:A:1712:LEU:HB3	1:A:1832:MET:HE1	1.91	0.53
1:A:2184:LYS:O	1:A:2187:THR:OG1	2.20	0.53
1:B:2024:ILE:HA	1:B:2027:ARG:HH12	1.73	0.53
1:B:2396:ASP:OD1	1:B:2400:ARG:NH1	2.42	0.53
1:B:3291:GLU:OE1	1:B:3301:PHE:N	2.42	0.53
1:C:172:GLY:O	1:D:3938:ARG:NH1	2.42	0.53
1:A:3291:GLU:OE1	1:A:3301:PHE:N	2.42	0.52
1:A:4853:VAL:HA	1:A:4857:LEU:HD12	1.91	0.52
1:B:1712:LEU:HB3	1:B:1832:MET:HE1	1.91	0.52
1:B:1723:ASN:O	1:B:1918:ARG:NH2	2.42	0.52
1:D:3954:GLN:O	1:D:3958:SER:OG	2.28	0.52
1:C:2396:ASP:OD1	1:C:2400:ARG:NH1	2.42	0.52
1:A:2210:GLN:NE2	1:A:2244:ALA:O	2.41	0.52
1:A:3681:LEU:HD22	1:A:3746:SER:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3954:GLN:O	1:A:3958:SER:OG	2.27	0.52
1:B:4790:LYS:NZ	1:B:4836:ASP:OD2	2.37	0.52
1:C:1795:MET:HE2	1:C:1822:LEU:HD21	1.89	0.52
1:C:3681:LEU:HD22	1:C:3746:SER:HB2	1.91	0.52
1:D:2396:ASP:OD1	1:D:2400:ARG:NH1	2.42	0.52
1:C:504:ARG:HD2	1:C:505:LEU:HD13	1.92	0.52
1:D:986:ILE:HG12	1:D:1058:LEU:HB3	1.90	0.52
1:D:3681:LEU:HD22	1:D:3746:SER:HB2	1.91	0.52
1:B:3102:PRO:HB2	1:B:3229:GLN:HB3	1.90	0.52
1:C:1444:GLY:HA3	1:C:1488:VAL:HA	1.92	0.52
1:C:1691:GLU:OE1	1:C:1791:LYS:NZ	2.36	0.52
1:D:1137:PHE:HA	1:D:1144:ARG:HA	1.90	0.52
1:D:1434:PRO:HB2	1:D:1502:ASN:HB3	1.91	0.52
1:D:3291:GLU:OE1	1:D:3301:PHE:N	2.42	0.52
2:H:75:LEU:N	2:H:100:PHE:O	2.42	0.52
1:A:504:ARG:HD2	1:A:505:LEU:HD13	1.92	0.52
1:B:504:ARG:HD2	1:B:505:LEU:HD13	1.92	0.52
1:B:2210:GLN:NE2	1:B:2244:ALA:O	2.41	0.52
1:C:413:SER:OG	1:C:414:ARG:N	2.41	0.52
1:D:504:ARG:HD2	1:D:505:LEU:HD13	1.92	0.52
2:F:24:VAL:HG13	2:F:48:LYS:HE3	1.90	0.52
2:H:24:VAL:HG13	2:H:48:LYS:HE3	1.90	0.52
1:A:370:LEU:HD12	1:A:396:GLU:HA	1.90	0.52
1:A:2024:ILE:HA	1:A:2027:ARG:HH12	1.73	0.52
1:D:778:MET:SD	1:D:778:MET:N	2.83	0.52
1:D:1444:GLY:HA3	1:D:1488:VAL:HA	1.92	0.52
1:A:218:SER:HA	1:A:286:GLY:H	1.75	0.52
1:B:1723:ASN:ND2	1:B:1914:ASP:OD2	2.41	0.52
1:C:589:ILE:HG21	1:C:617:LEU:HD21	1.89	0.52
1:C:3919:LEU:HD22	1:C:3934:LEU:HD21	1.92	0.52
1:D:983:LEU:HD21	1:D:1059:GLY:HA3	1.90	0.52
1:A:413:SER:OG	1:A:414:ARG:N	2.41	0.52
1:A:2396:ASP:OD1	1:A:2400:ARG:NH1	2.42	0.52
1:C:1100:ARG:HA	1:C:1166:VAL:HG23	1.92	0.52
1:C:3750:THR:HG22	1:C:3795:LEU:HD23	1.92	0.52
1:C:4853:VAL:HA	1:C:4857:LEU:HD12	1.91	0.52
2:G:75:LEU:N	2:G:100:PHE:O	2.42	0.52
1:B:3750:THR:HG22	1:B:3795:LEU:HD23	1.92	0.52
1:A:1434:PRO:HB2	1:A:1502:ASN:HB3	1.91	0.51
1:A:3254:GLU:OE1	1:A:3256:HIS:NE2	2.43	0.51
1:A:4193:GLU:OE1	1:A:4603:LYS:NZ	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:778:MET:N	1:B:778:MET:SD	2.83	0.51
1:B:1100:ARG:HA	1:B:1166:VAL:HG23	1.92	0.51
1:B:3254:GLU:OE1	1:B:3256:HIS:NE2	2.43	0.51
1:C:361:CYS:O	1:C:403:LEU:N	2.38	0.51
1:C:373:THR:HG21	1:C:398:HIS:H	1.75	0.51
1:A:986:ILE:HG12	1:A:1058:LEU:HB3	1.90	0.51
1:B:218:SER:HA	1:B:286:GLY:H	1.75	0.51
1:B:891:GLU:HA	1:B:894:VAL:HG22	1.93	0.51
1:B:1444:GLY:HA3	1:B:1488:VAL:HA	1.92	0.51
1:B:3681:LEU:HD22	1:B:3746:SER:HB2	1.91	0.51
1:A:1444:GLY:HA3	1:A:1488:VAL:HA	1.92	0.51
1:C:778:MET:SD	1:C:778:MET:N	2.83	0.51
1:D:3055:ALA:HB3	1:D:3100:LEU:HD13	1.90	0.51
1:D:3919:LEU:HD22	1:D:3934:LEU:HD21	1.92	0.51
1:A:778:MET:SD	1:A:778:MET:N	2.83	0.51
1:A:1691:GLU:OE1	1:A:1791:LYS:NZ	2.36	0.51
1:A:3919:LEU:HD22	1:A:3934:LEU:HD21	1.92	0.51
1:C:218:SER:HA	1:C:286:GLY:H	1.75	0.51
1:D:218:SER:HA	1:D:286:GLY:H	1.75	0.51
1:D:373:THR:HG21	1:D:398:HIS:H	1.75	0.51
1:B:3058:ALA:HA	1:B:3062:ASN:HB3	1.93	0.51
1:A:3750:THR:HG22	1:A:3795:LEU:HD23	1.92	0.51
1:B:2174:MET:HG2	1:B:2178:LEU:HD23	1.93	0.51
1:B:3919:LEU:HD22	1:B:3934:LEU:HD21	1.92	0.51
1:C:3058:ALA:HA	1:C:3062:ASN:HB3	1.93	0.51
1:D:2162:ARG:NH2	1:D:2208:GLN:OE1	2.44	0.51
1:D:4193:GLU:OE1	1:D:4603:LYS:NZ	2.43	0.51
1:D:4853:VAL:HA	1:D:4857:LEU:HD12	1.91	0.51
1:B:2162:ARG:NH2	1:B:2208:GLN:OE1	2.44	0.51
1:B:4807:ASP:N	1:B:4807:ASP:OD1	2.41	0.51
1:C:891:GLU:HA	1:C:894:VAL:HG22	1.93	0.51
1:C:1723:ASN:ND2	1:C:1914:ASP:OD2	2.41	0.51
1:D:413:SER:OG	1:D:414:ARG:N	2.41	0.51
1:D:3750:THR:HG22	1:D:3795:LEU:HD23	1.92	0.51
1:B:207:PHE:CD2	1:C:2324:ILE:HD13	2.46	0.51
1:B:4853:VAL:HA	1:B:4857:LEU:HD12	1.91	0.51
1:C:2162:ARG:NH2	1:C:2208:GLN:OE1	2.44	0.51
1:C:4193:GLU:OE1	1:C:4603:LYS:NZ	2.43	0.51
1:D:139:SER:O	1:D:198:ASN:ND2	2.44	0.51
1:D:226:GLY:O	1:D:355:LYS:NZ	2.44	0.51
1:D:1100:ARG:HA	1:D:1166:VAL:HG23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4158:GLN:NE2	1:D:4199:MET:O	2.44	0.51
1:A:2174:MET:HG2	1:A:2178:LEU:HD23	1.93	0.51
1:B:2878:ALA:HA	1:B:2881:LYS:HB2	1.93	0.51
1:C:139:SER:O	1:C:198:ASN:ND2	2.44	0.51
1:D:1522:ILE:HD11	1:D:1532:TYR:HB2	1.93	0.51
1:A:2162:ARG:NH2	1:A:2208:GLN:OE1	2.44	0.51
1:B:146:ASP:OD1	1:B:146:ASP:N	2.43	0.51
1:B:4115:GLN:O	1:B:4119:GLU:HG2	2.11	0.51
1:C:728:ASP:OD1	1:C:728:ASP:N	2.44	0.51
1:C:4115:GLN:O	1:C:4119:GLU:HG2	2.11	0.51
2:H:31:LEU:N	2:H:35:LYS:O	2.44	0.51
1:A:33:GLN:HE21	1:A:35:LEU:HD11	1.76	0.50
1:A:192:LEU:O	1:A:212:TRP:NE1	2.39	0.50
1:A:373:THR:HG21	1:A:398:HIS:H	1.75	0.50
1:A:891:GLU:HA	1:A:894:VAL:HG22	1.93	0.50
1:A:508:TYR:HD2	1:A:511:ALA:H	1.60	0.50
1:A:1723:ASN:ND2	1:A:1914:ASP:OD2	2.41	0.50
1:A:4158:GLN:NE2	1:A:4199:MET:O	2.44	0.50
1:B:951:GLY:O	1:B:953:ALA:N	2.44	0.50
1:B:4193:GLU:OE1	1:B:4603:LYS:NZ	2.43	0.50
1:B:4521:SER:HB3	1:B:4558:TYR:HE2	1.76	0.50
1:C:146:ASP:OD1	1:C:146:ASP:N	2.43	0.50
1:D:728:ASP:N	1:D:728:ASP:OD1	2.44	0.50
1:B:1434:PRO:HB2	1:B:1502:ASN:HB3	1.91	0.50
1:D:3254:GLU:OE1	1:D:3256:HIS:NE2	2.43	0.50
1:D:4071:THR:OG1	1:D:4072:ASP:N	2.42	0.50
1:D:4115:GLN:O	1:D:4119:GLU:HG2	2.11	0.50
1:D:4854:ILE:O	1:D:4858:LEU:HB2	2.12	0.50
1:A:500:GLU:OE1	1:A:557:TRP:NE1	2.45	0.50
1:B:4614:LEU:HA	1:B:4618:GLU:HB3	1.94	0.50
1:C:508:TYR:HD2	1:C:511:ALA:H	1.59	0.50
1:C:983:LEU:HD23	1:C:1055:ARG:HD2	1.94	0.50
1:D:3058:ALA:HA	1:D:3062:ASN:HB3	1.93	0.50
1:A:172:GLY:O	1:B:3938:ARG:NH1	2.45	0.50
1:B:500:GLU:OE1	1:B:557:TRP:NE1	2.45	0.50
1:B:508:TYR:HD2	1:B:511:ALA:H	1.60	0.50
1:B:983:LEU:HD23	1:B:1055:ARG:HD2	1.94	0.50
1:B:4158:GLN:NE2	1:B:4199:MET:O	2.44	0.50
1:C:40:GLU:N	1:C:40:GLU:OE1	2.45	0.50
1:C:1522:ILE:HD11	1:C:1532:TYR:HB2	1.94	0.50
1:C:2878:ALA:HA	1:C:2881:LYS:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4158:GLN:NE2	1:C:4199:MET:O	2.44	0.50
1:D:2174:MET:HG2	1:D:2178:LEU:HD23	1.92	0.50
1:A:2405:MET:SD	1:A:2419:ARG:NE	2.85	0.50
1:B:33:GLN:HE21	1:B:35:LEU:HD11	1.76	0.50
1:B:139:SER:O	1:B:198:ASN:ND2	2.44	0.50
1:B:373:THR:HG21	1:B:398:HIS:H	1.75	0.50
1:B:1143:GLN:HA	1:B:1152:TYR:H	1.76	0.50
1:C:3254:GLU:OE1	1:C:3256:HIS:NE2	2.43	0.50
1:D:508:TYR:HD2	1:D:511:ALA:H	1.59	0.50
1:A:40:GLU:N	1:A:40:GLU:OE1	2.45	0.50
1:B:926:GLU:OE2	1:B:930:ASN:ND2	2.40	0.50
1:B:2405:MET:SD	1:B:2419:ARG:NE	2.85	0.50
1:C:4614:LEU:HA	1:C:4618:GLU:HB3	1.94	0.50
1:D:40:GLU:N	1:D:40:GLU:OE1	2.45	0.50
1:A:1100:ARG:HA	1:A:1166:VAL:HG23	1.92	0.50
1:A:1522:ILE:HD11	1:A:1532:TYR:HB2	1.93	0.50
1:A:3058:ALA:HA	1:A:3062:ASN:HB3	1.93	0.50
1:A:4854:ILE:O	1:A:4858:LEU:HB2	2.12	0.50
1:B:40:GLU:OE1	1:B:40:GLU:N	2.45	0.50
1:C:500:GLU:OE1	1:C:557:TRP:NE1	2.45	0.50
1:C:4854:ILE:O	1:C:4858:LEU:HB2	2.12	0.50
1:D:500:GLU:OE1	1:D:557:TRP:NE1	2.45	0.50
1:D:4807:ASP:OD1	1:D:4807:ASP:N	2.41	0.50
1:A:1143:GLN:HA	1:A:1152:TYR:H	1.76	0.50
1:D:983:LEU:HD23	1:D:1055:ARG:HD2	1.94	0.50
1:A:361:CYS:O	1:A:403:LEU:N	2.38	0.49
1:B:1262:PRO:HG3	1:B:1595:VAL:HG12	1.94	0.49
1:D:891:GLU:HA	1:D:894:VAL:HG22	1.93	0.49
1:D:2210:GLN:OE1	1:D:2249:ASN:ND2	2.45	0.49
1:A:139:SER:O	1:A:198:ASN:ND2	2.44	0.49
1:A:146:ASP:OD1	1:A:146:ASP:N	2.43	0.49
1:B:2233:MET:HE3	1:B:2233:MET:HA	1.94	0.49
1:C:951:GLY:O	1:C:953:ALA:N	2.44	0.49
1:C:1791:LYS:O	1:C:1795:MET:HG2	2.13	0.49
1:D:33:GLN:HE21	1:D:35:LEU:HD11	1.76	0.49
1:D:1143:GLN:HA	1:D:1152:TYR:H	1.76	0.49
1:D:4521:SER:HB3	1:D:4558:TYR:HE2	1.76	0.49
1:A:787:LEU:HG	1:A:789:PHE:HE1	1.78	0.49
1:A:983:LEU:HD23	1:A:1055:ARG:HD2	1.94	0.49
1:A:1022:GLN:HG3	1:A:1024:VAL:HG13	1.94	0.49
1:A:1791:LYS:O	1:A:1795:MET:HG2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2210:GLN:OE1	1:A:2249:ASN:ND2	2.46	0.49
1:A:4614:LEU:HA	1:A:4618:GLU:HB3	1.94	0.49
1:B:1791:LYS:O	1:B:1795:MET:HG2	2.13	0.49
1:C:3967:LEU:O	1:C:3971:MET:HG2	2.13	0.49
1:D:548:CYS:HB2	1:D:579:LEU:HD23	1.94	0.49
1:D:915:HIS:HB2	1:D:918:LEU:HB2	1.94	0.49
1:D:3967:LEU:O	1:D:3971:MET:HG2	2.12	0.49
1:A:2471:LEU:O	1:A:2476:GLY:N	2.43	0.49
1:B:2210:GLN:OE1	1:B:2249:ASN:ND2	2.45	0.49
1:B:2490:GLY:O	1:B:2494:ASP:N	2.39	0.49
1:C:226:GLY:O	1:C:355:LYS:NZ	2.44	0.49
1:C:915:HIS:HB2	1:C:918:LEU:HB2	1.94	0.49
1:C:1767:PRO:O	1:C:1769:PHE:N	2.44	0.49
1:C:4521:SER:HB3	1:C:4558:TYR:HE2	1.77	0.49
1:D:926:GLU:OE2	1:D:930:ASN:ND2	2.40	0.49
1:D:1262:PRO:HG3	1:D:1595:VAL:HG12	1.94	0.49
1:D:2233:MET:HE3	1:D:2233:MET:HA	1.94	0.49
1:D:3927:CYS:O	1:D:3929:GLY:N	2.46	0.49
1:D:4614:LEU:HA	1:D:4618:GLU:HB3	1.94	0.49
1:A:1262:PRO:HG3	1:A:1595:VAL:HG12	1.94	0.49
1:A:4115:GLN:O	1:A:4119:GLU:HG2	2.11	0.49
1:A:4518:TYR:OH	1:A:4735:ASN:ND2	2.46	0.49
1:B:361:CYS:O	1:B:403:LEU:N	2.38	0.49
1:B:787:LEU:HG	1:B:789:PHE:HE1	1.78	0.49
1:B:3927:CYS:O	1:B:3929:GLY:N	2.46	0.49
1:C:787:LEU:HG	1:C:789:PHE:HE1	1.78	0.49
1:C:2174:MET:HG2	1:C:2178:LEU:HD23	1.93	0.49
1:D:1136:ALA:O	1:D:1145:TRP:N	2.46	0.49
1:D:2878:ALA:HA	1:D:2881:LYS:HB2	1.93	0.49
1:A:548:CYS:HB2	1:A:579:LEU:HD23	1.94	0.49
1:A:915:HIS:HB2	1:A:918:LEU:HB2	1.94	0.49
1:A:2878:ALA:HA	1:A:2881:LYS:HB2	1.93	0.49
1:B:1136:ALA:O	1:B:1145:TRP:N	2.46	0.49
1:C:1143:GLN:HA	1:C:1152:TYR:H	1.76	0.49
2:E:31:LEU:N	2:E:35:LYS:O	2.44	0.49
1:A:2228:LEU:H	1:A:2237:THR:HG22	1.78	0.49
1:A:4030:THR:O	1:A:4035:ASP:N	2.46	0.49
1:A:4071:THR:OG1	1:A:4072:ASP:N	2.42	0.49
1:B:1522:ILE:HD11	1:B:1532:TYR:HB2	1.94	0.49
1:D:1767:PRO:O	1:D:1769:PHE:N	2.44	0.49
1:D:1791:LYS:O	1:D:1795:MET:HG2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1136:ALA:O	1:A:1145:TRP:N	2.46	0.49
1:C:2210:GLN:OE1	1:C:2249:ASN:ND2	2.45	0.49
1:D:192:LEU:O	1:D:212:TRP:NE1	2.39	0.49
1:D:2405:MET:SD	1:D:2419:ARG:NE	2.85	0.49
1:A:246:THR:N	1:A:261:HIS:O	2.44	0.49
1:A:2876:LEU:HD22	1:A:2880:GLU:HG3	1.95	0.49
1:B:2450:VAL:HG23	1:B:2451:VAL:HG13	1.95	0.49
1:C:801:ARG:NH2	1:C:802:PHE:O	2.45	0.49
1:A:2450:VAL:HG23	1:A:2451:VAL:HG13	1.95	0.49
1:B:2876:LEU:HD22	1:B:2880:GLU:HG3	1.95	0.49
1:B:3954:GLN:O	1:B:3958:SER:OG	2.28	0.49
1:B:4518:TYR:OH	1:B:4735:ASN:ND2	2.46	0.49
1:C:33:GLN:HE21	1:C:35:LEU:HD11	1.76	0.49
1:C:1022:GLN:HG3	1:C:1024:VAL:HG13	1.94	0.49
1:C:1262:PRO:HG3	1:C:1595:VAL:HG12	1.95	0.49
1:C:2405:MET:SD	1:C:2419:ARG:NE	2.85	0.49
1:D:2228:LEU:H	1:D:2237:THR:HG22	1.78	0.49
1:D:2471:LEU:O	1:D:2476:GLY:N	2.43	0.49
1:A:69:LEU:H	1:A:69:LEU:HD23	1.78	0.48
1:B:200:SER:OG	1:B:201:TRP:N	2.46	0.48
1:B:915:HIS:HB2	1:B:918:LEU:HB2	1.94	0.48
1:C:1136:ALA:O	1:C:1145:TRP:N	2.46	0.48
1:C:3927:CYS:O	1:C:3929:GLY:N	2.46	0.48
1:D:801:ARG:NH2	1:D:802:PHE:O	2.45	0.48
1:B:1017:THR:HA	1:B:1025:LYS:HD3	1.95	0.48
1:B:2228:LEU:H	1:B:2237:THR:HG22	1.78	0.48
1:B:4030:THR:O	1:B:4035:ASP:N	2.46	0.48
1:C:200:SER:OG	1:C:201:TRP:N	2.46	0.48
1:C:4030:THR:O	1:C:4035:ASP:N	2.46	0.48
1:D:200:SER:OG	1:D:201:TRP:N	2.46	0.48
1:A:728:ASP:OD1	1:A:728:ASP:N	2.45	0.48
1:A:3927:CYS:O	1:A:3929:GLY:N	2.46	0.48
1:A:4521:SER:HB3	1:A:4558:TYR:HE2	1.77	0.48
1:B:4854:ILE:O	1:B:4858:LEU:HB2	2.12	0.48
1:C:1017:THR:HA	1:C:1025:LYS:HD3	1.95	0.48
1:C:1511:VAL:HG23	1:C:1519:LEU:HD12	1.95	0.48
1:C:2228:LEU:H	1:C:2237:THR:HG22	1.78	0.48
1:D:69:LEU:HD23	1:D:69:LEU:H	1.78	0.48
1:D:787:LEU:HG	1:D:789:PHE:HE1	1.78	0.48
1:A:207:PHE:CD2	1:B:2324:ILE:HD13	2.49	0.48
1:A:1017:THR:HA	1:A:1025:LYS:HD3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2623:PRO:HB3	1:A:2666:PRO:HG3	1.96	0.48
1:C:1505:GLY:O	1:C:1524:ASN:ND2	2.47	0.48
1:C:2450:VAL:HG23	1:C:2451:VAL:HG13	1.95	0.48
1:C:2623:PRO:HB3	1:C:2666:PRO:HG3	1.95	0.48
1:D:1511:VAL:HG23	1:D:1519:LEU:HD12	1.95	0.48
1:D:1723:ASN:ND2	1:D:1914:ASP:OD2	2.41	0.48
1:D:2450:VAL:HG23	1:D:2451:VAL:HG13	1.95	0.48
1:D:2623:PRO:HB3	1:D:2666:PRO:HG3	1.95	0.48
1:B:3967:LEU:O	1:B:3971:MET:HG2	2.12	0.48
1:C:2233:MET:HE3	1:C:2233:MET:HA	1.95	0.48
1:C:4518:TYR:OH	1:C:4735:ASN:ND2	2.46	0.48
1:A:1767:PRO:O	1:A:1769:PHE:N	2.44	0.48
1:A:1769:PHE:O	2:E:83:TYR:OH	2.29	0.48
1:A:3967:LEU:O	1:A:3971:MET:HG2	2.12	0.48
1:B:2471:LEU:O	1:B:2476:GLY:N	2.43	0.48
1:C:926:GLU:OE2	1:C:930:ASN:ND2	2.40	0.48
1:C:2204:ARG:O	1:C:2206:SER:N	2.42	0.48
1:C:2314:GLU:OE2	1:C:3812:LYS:NZ	2.47	0.48
1:A:226:GLY:O	1:A:355:LYS:NZ	2.44	0.48
1:B:192:LEU:O	1:B:212:TRP:NE1	2.39	0.48
1:B:2314:GLU:OE2	1:B:3812:LYS:NZ	2.47	0.48
1:B:4660:TYR:HB3	1:B:4664:ARG:HH12	1.79	0.48
1:C:3954:GLN:O	1:C:3958:SER:OG	2.28	0.48
1:D:619:VAL:HG23	1:D:624:ALA:HB3	1.95	0.48
1:D:1022:GLN:HG3	1:D:1024:VAL:HG13	1.94	0.48
1:D:2314:GLU:OE2	1:D:3812:LYS:NZ	2.47	0.48
1:D:4788:PHE:HB3	1:D:4791:PHE:HD2	1.79	0.48
1:A:2314:GLU:OE2	1:A:3812:LYS:NZ	2.47	0.48
1:A:4136:GLU:OE2	1:A:4146:ARG:NH1	2.47	0.48
1:B:548:CYS:HB2	1:B:579:LEU:HD23	1.94	0.48
1:B:619:VAL:HG23	1:B:624:ALA:HB3	1.95	0.48
1:B:902:TRP:HA	1:B:913:ARG:HB3	1.96	0.48
1:B:1505:GLY:O	1:B:1524:ASN:ND2	2.46	0.48
1:B:1767:PRO:O	1:B:1769:PHE:N	2.44	0.48
1:C:69:LEU:H	1:C:69:LEU:HD23	1.78	0.48
1:C:803:LEU:HD11	1:C:811:PHE:HA	1.96	0.48
1:C:4136:GLU:OE2	1:C:4146:ARG:NH1	2.47	0.48
2:F:31:LEU:N	2:F:35:LYS:O	2.44	0.48
1:B:4136:GLU:OE2	1:B:4146:ARG:NH1	2.47	0.48
1:C:2876:LEU:HD22	1:C:2880:GLU:HG3	1.95	0.48
1:D:1769:PHE:O	2:H:83:TYR:OH	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4030:THR:O	1:D:4035:ASP:N	2.46	0.48
1:A:902:TRP:HA	1:A:913:ARG:HB3	1.96	0.48
1:A:4084:LYS:HE2	1:A:4085:ARG:HG2	1.96	0.48
1:B:2623:PRO:HB3	1:B:2666:PRO:HG3	1.95	0.48
1:C:885:LEU:HD21	1:C:956:HIS:HB2	1.96	0.48
1:C:902:TRP:HA	1:C:913:ARG:HB3	1.96	0.48
1:C:2391:TYR:O	1:C:2395:ILE:HG22	2.13	0.48
1:C:3727:GLN:NE2	1:C:3764:ILE:O	2.32	0.48
1:C:4078:ASP:N	1:C:4078:ASP:OD1	2.47	0.48
1:D:1017:THR:HA	1:D:1025:LYS:HD3	1.95	0.48
1:D:2391:TYR:O	1:D:2395:ILE:HG22	2.13	0.48
2:G:31:LEU:N	2:G:35:LYS:O	2.44	0.48
1:A:482:LEU:HG	1:A:486:GLN:NE2	2.29	0.47
1:A:885:LEU:HD21	1:A:956:HIS:HB2	1.96	0.47
1:A:1165:MET:HE1	1:A:1176:THR:HG23	1.96	0.47
1:A:1505:GLY:O	1:A:1524:ASN:ND2	2.47	0.47
1:A:4660:TYR:HB3	1:A:4664:ARG:HH12	1.79	0.47
1:B:1022:GLN:HG3	1:B:1024:VAL:HG13	1.94	0.47
1:B:3728:ALA:HA	1:B:3731:HIS:CD2	2.49	0.47
1:C:533:LEU:HA	1:C:536:LEU:HB3	1.96	0.47
1:C:2828:SER:OG	1:C:2889:GLN:OE1	2.30	0.47
1:D:803:LEU:HD11	1:D:811:PHE:HA	1.96	0.47
1:D:4136:GLU:OE2	1:D:4146:ARG:NH1	2.47	0.47
1:D:4518:TYR:OH	1:D:4735:ASN:ND2	2.46	0.47
2:E:30:MET:HE3	2:E:36:LYS:HG2	1.96	0.47
1:A:2233:MET:HE3	1:A:2233:MET:HA	1.95	0.47
1:B:69:LEU:HD23	1:B:69:LEU:H	1.78	0.47
1:C:548:CYS:HB2	1:C:579:LEU:HD23	1.94	0.47
1:C:4084:LYS:HE2	1:C:4085:ARG:HG2	1.96	0.47
1:C:4788:PHE:HB3	1:C:4791:PHE:HD2	1.79	0.47
1:D:482:LEU:HG	1:D:486:GLN:NE2	2.29	0.47
1:D:2876:LEU:HD22	1:D:2880:GLU:HG3	1.95	0.47
1:C:1738:THR:OG1	1:C:1740:PHE:O	2.31	0.47
1:C:2795:ASP:OD1	1:C:2795:ASP:N	2.47	0.47
1:D:1505:GLY:O	1:D:1524:ASN:ND2	2.47	0.47
1:A:200:SER:OG	1:A:201:TRP:N	2.46	0.47
1:A:433:LEU:O	1:A:437:SER:N	2.48	0.47
1:A:619:VAL:HG23	1:A:624:ALA:HB3	1.95	0.47
1:A:2391:TYR:O	1:A:2395:ILE:HG22	2.13	0.47
1:A:4890:CYS:SG	1:A:4912:HIS:CE1	3.08	0.47
1:B:2795:ASP:OD1	1:B:2795:ASP:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4660:TYR:HB3	1:C:4664:ARG:HH12	1.79	0.47
1:D:902:TRP:HA	1:D:913:ARG:HB3	1.96	0.47
1:D:951:GLY:O	1:D:953:ALA:N	2.44	0.47
1:D:4092:ASP:OD1	1:D:4092:ASP:N	2.47	0.47
1:A:3728:ALA:HA	1:A:3731:HIS:CD2	2.49	0.47
1:B:4071:THR:OG1	1:B:4072:ASP:N	2.42	0.47
1:D:885:LEU:HD21	1:D:956:HIS:HB2	1.96	0.47
1:D:4084:LYS:HE2	1:D:4085:ARG:HG2	1.96	0.47
1:A:926:GLU:OE2	1:A:930:ASN:ND2	2.40	0.47
1:A:4788:PHE:HB3	1:A:4791:PHE:HD2	1.79	0.47
1:B:2391:TYR:O	1:B:2395:ILE:HG22	2.13	0.47
1:B:3727:GLN:NE2	1:B:3764:ILE:O	2.32	0.47
1:B:4084:LYS:HE2	1:B:4085:ARG:HG2	1.96	0.47
1:B:4890:CYS:SG	1:B:4912:HIS:CE1	3.08	0.47
1:C:482:LEU:HG	1:C:486:GLN:NE2	2.29	0.47
1:A:803:LEU:HD11	1:A:811:PHE:HA	1.96	0.47
1:A:1511:VAL:HG23	1:A:1519:LEU:HD12	1.95	0.47
1:A:1935:LEU:HD13	1:A:2024:ILE:HD13	1.97	0.47
1:B:482:LEU:HG	1:B:486:GLN:NE2	2.29	0.47
1:B:533:LEU:HA	1:B:536:LEU:HB3	1.96	0.47
1:B:885:LEU:HD21	1:B:956:HIS:HB2	1.96	0.47
1:B:2204:ARG:O	1:B:2206:SER:N	2.42	0.47
1:B:4043:SER:O	1:B:4045:ARG:N	2.48	0.47
1:C:474:ASP:OD2	1:C:478:ARG:NH2	2.48	0.47
1:C:3047:THR:HA	1:C:3051:SER:HB3	1.97	0.47
1:C:3728:ALA:HA	1:C:3731:HIS:CD2	2.49	0.47
1:D:474:ASP:OD2	1:D:478:ARG:NH2	2.48	0.47
1:D:4660:TYR:HB3	1:D:4664:ARG:HH12	1.79	0.47
2:F:30:MET:HE3	2:F:36:LYS:HG2	1.96	0.47
1:A:533:LEU:HA	1:A:536:LEU:HB3	1.96	0.47
1:B:474:ASP:OD2	1:B:478:ARG:NH2	2.48	0.47
1:B:1129:GLY:HA3	1:B:1145:TRP:HB3	1.96	0.47
1:C:4092:ASP:N	1:C:4092:ASP:OD1	2.47	0.47
1:D:57:ASN:ND2	1:D:322:ALA:O	2.48	0.47
1:A:3727:GLN:NE2	1:A:3764:ILE:O	2.32	0.47
1:B:803:LEU:HD11	1:B:811:PHE:HA	1.96	0.47
1:B:1935:LEU:HD13	1:B:2024:ILE:HD13	1.97	0.47
1:B:4788:PHE:HB3	1:B:4791:PHE:HD2	1.79	0.47
1:C:57:ASN:ND2	1:C:322:ALA:O	2.48	0.47
1:C:1129:GLY:HA3	1:C:1145:TRP:HB3	1.96	0.47
1:C:2471:LEU:O	1:C:2476:GLY:N	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4890:CYS:SG	1:C:4912:HIS:CE1	3.08	0.47
1:D:146:ASP:OD1	1:D:146:ASP:N	2.43	0.47
1:D:1129:GLY:HA3	1:D:1145:TRP:HB3	1.96	0.47
1:D:1165:MET:HE1	1:D:1176:THR:HG23	1.96	0.47
1:D:3728:ALA:HA	1:D:3731:HIS:CD2	2.49	0.47
1:A:474:ASP:OD2	1:A:478:ARG:NH2	2.48	0.47
1:C:619:VAL:HG23	1:C:624:ALA:HB3	1.96	0.47
1:A:57:ASN:ND2	1:A:322:ALA:O	2.48	0.46
1:A:4653:MET:HA	1:A:4665:ILE:HG21	1.97	0.46
1:B:669:GLN:HB3	1:B:1020:ILE:HG13	1.97	0.46
1:B:1165:MET:HE1	1:B:1176:THR:HG23	1.96	0.46
1:B:1511:VAL:HG23	1:B:1519:LEU:HD12	1.95	0.46
1:D:419:ILE:HG21	1:D:488:LEU:HB3	1.96	0.46
1:D:669:GLN:HB3	1:D:1020:ILE:HG13	1.97	0.46
2:H:30:MET:HE3	2:H:36:LYS:HG2	1.96	0.46
1:B:728:ASP:OD1	1:B:728:ASP:N	2.44	0.46
1:B:2828:SER:OG	1:B:2889:GLN:OE1	2.30	0.46
1:C:1165:MET:HE1	1:C:1176:THR:HG23	1.96	0.46
1:D:246:THR:N	1:D:261:HIS:O	2.44	0.46
1:D:533:LEU:HA	1:D:536:LEU:HB3	1.96	0.46
1:D:555:LEU:HA	1:D:558:LEU:HD12	1.98	0.46
1:D:1935:LEU:HD13	1:D:2024:ILE:HD13	1.97	0.46
1:D:3047:THR:HA	1:D:3051:SER:HB3	1.97	0.46
1:A:234:LEU:HA	1:A:408:SER:HB3	1.98	0.46
1:B:234:LEU:HA	1:B:408:SER:HB3	1.98	0.46
1:B:2012:GLU:O	1:B:2016:LEU:N	2.41	0.46
1:B:4078:ASP:OD1	1:B:4078:ASP:N	2.47	0.46
1:B:4653:MET:HA	1:B:4665:ILE:HG21	1.98	0.46
1:A:1129:GLY:HA3	1:A:1145:TRP:HB3	1.96	0.46
1:A:4078:ASP:OD1	1:A:4078:ASP:N	2.47	0.46
1:C:1089:ARG:O	1:C:1250:TRP:N	2.48	0.46
1:C:1246:ASP:OD1	1:C:1694:TYR:OH	2.30	0.46
1:D:2795:ASP:OD1	1:D:2795:ASP:N	2.47	0.46
1:D:4890:CYS:SG	1:D:4912:HIS:CE1	3.08	0.46
2:G:30:MET:HE3	2:G:36:LYS:HG2	1.96	0.46
1:D:2511:MET:HA	1:D:2511:MET:HE2	1.97	0.46
1:A:419:ILE:HG21	1:A:488:LEU:HB3	1.96	0.46
1:A:4043:SER:O	1:A:4045:ARG:N	2.48	0.46
1:C:555:LEU:HA	1:C:558:LEU:HD12	1.98	0.46
1:C:2509:THR:HA	1:C:2513:LEU:HD11	1.98	0.46
1:D:4078:ASP:OD1	1:D:4078:ASP:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:960:LYS:HG3	1:A:961:VAL:HG23	1.98	0.46
1:A:2795:ASP:OD1	1:A:2795:ASP:N	2.47	0.46
1:B:226:GLY:O	1:B:355:LYS:NZ	2.44	0.46
1:B:801:ARG:NH2	1:B:802:PHE:O	2.45	0.46
1:C:1215:MET:HE3	1:C:1215:MET:HA	1.98	0.46
1:D:1215:MET:HE3	1:D:1215:MET:HA	1.98	0.46
1:D:4653:MET:HA	1:D:4665:ILE:HG21	1.97	0.46
1:A:2324:ILE:HD13	1:D:207:PHE:CD2	2.51	0.46
1:A:2511:MET:HE2	1:A:2511:MET:HA	1.97	0.46
1:A:3262:MET:HE3	1:A:3262:MET:O	2.16	0.46
1:B:657:PRO:HD2	1:B:791:VAL:HG12	1.98	0.46
1:B:719:GLY:O	1:B:724:SER:OG	2.34	0.46
1:C:4043:SER:O	1:C:4045:ARG:N	2.48	0.46
1:D:657:PRO:HD2	1:D:791:VAL:HG12	1.98	0.46
2:H:78:THR:HG23	2:H:80:ASP:HB3	1.98	0.46
1:A:494:MET:HG2	1:A:497:LEU:H	1.81	0.46
1:A:657:PRO:HD2	1:A:791:VAL:HG12	1.98	0.46
1:B:419:ILE:HG21	1:B:488:LEU:HB3	1.96	0.46
1:B:894:VAL:O	1:B:898:ILE:N	2.47	0.46
1:B:1832:MET:HE3	1:B:1832:MET:HB2	1.73	0.46
1:B:3262:MET:O	1:B:3262:MET:HE3	2.16	0.46
1:C:2191:MET:SD	1:C:2191:MET:N	2.89	0.46
1:D:426:PHE:O	1:D:430:ILE:HG12	2.16	0.46
1:D:4566:TYR:O	1:D:4570:THR:OG1	2.26	0.46
2:E:78:THR:HG23	2:E:80:ASP:HB3	1.98	0.46
1:A:3047:THR:HA	1:A:3051:SER:HB3	1.97	0.46
1:C:657:PRO:HD2	1:C:791:VAL:HG12	1.98	0.46
1:C:669:GLN:HB3	1:C:1020:ILE:HG13	1.97	0.46
1:C:1935:LEU:HD13	1:C:2024:ILE:HD13	1.97	0.46
1:D:960:LYS:HG3	1:D:961:VAL:HG23	1.98	0.46
1:A:555:LEU:HA	1:A:558:LEU:HD12	1.98	0.45
1:A:4106:GLU:OE1	1:A:4148:TYR:OH	2.24	0.45
1:B:2509:THR:HA	1:B:2513:LEU:HD11	1.98	0.45
1:B:3808:GLU:HA	1:B:3811:ASN:HD21	1.81	0.45
1:C:419:ILE:HG21	1:C:488:LEU:HB3	1.96	0.45
1:C:2490:GLY:O	1:C:2494:ASP:N	2.39	0.45
1:C:3808:GLU:HA	1:C:3811:ASN:HD21	1.81	0.45
1:C:3843:GLN:HB2	1:C:3918:THR:HA	1.98	0.45
1:C:4071:THR:OG1	1:C:4072:ASP:N	2.42	0.45
1:D:902:TRP:HE3	1:D:913:ARG:HG2	1.82	0.45
1:A:426:PHE:O	1:A:430:ILE:HG12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:669:GLN:HB3	1:A:1020:ILE:HG13	1.97	0.45
1:A:801:ARG:NH2	1:A:802:PHE:O	2.45	0.45
1:A:1103:PHE:O	1:A:1164:CYS:N	2.49	0.45
1:B:233:VAL:HG12	1:B:274:LEU:HD22	1.99	0.45
1:C:426:PHE:O	1:C:430:ILE:HG12	2.16	0.45
1:D:1108:VAL:HG21	1:D:1214:ARG:HH21	1.82	0.45
1:D:2191:MET:SD	1:D:2191:MET:N	2.89	0.45
1:D:3808:GLU:HA	1:D:3811:ASN:HD21	1.81	0.45
1:A:1108:VAL:HG21	1:A:1214:ARG:HH21	1.82	0.45
1:A:4092:ASP:OD1	1:A:4092:ASP:N	2.47	0.45
1:B:433:LEU:O	1:B:437:SER:N	2.47	0.45
1:B:2191:MET:SD	1:B:2191:MET:N	2.89	0.45
1:B:2511:MET:HE2	1:B:2511:MET:HA	1.97	0.45
1:B:3047:THR:HA	1:B:3051:SER:HB3	1.97	0.45
1:B:3985:LEU:HD11	1:B:3998:MET:HE3	1.98	0.45
1:C:246:THR:N	1:C:261:HIS:O	2.44	0.45
1:C:494:MET:HG2	1:C:497:LEU:HD22	1.99	0.45
1:C:1103:PHE:O	1:C:1164:CYS:N	2.49	0.45
1:C:4056:HIS:O	1:C:4062:THR:OG1	2.29	0.45
1:D:1089:ARG:HH21	1:D:1601:PRO:HB3	1.82	0.45
1:B:1215:MET:HE3	1:B:1215:MET:HA	1.98	0.45
1:C:234:LEU:HA	1:C:408:SER:HB3	1.98	0.45
1:C:4653:MET:HA	1:C:4665:ILE:HG21	1.97	0.45
1:D:234:LEU:HA	1:D:408:SER:HB3	1.98	0.45
1:D:494:MET:HG2	1:D:497:LEU:H	1.81	0.45
1:D:995:MET:HE2	1:D:1054:VAL:HG12	1.98	0.45
1:A:1089:ARG:HH21	1:A:1601:PRO:HB3	1.82	0.45
1:A:3808:GLU:HA	1:A:3811:ASN:HD21	1.81	0.45
1:C:995:MET:HE2	1:C:1054:VAL:HG12	1.98	0.45
1:D:2264:VAL:HG21	1:D:2300:PHE:HE2	1.81	0.45
1:D:3985:LEU:HD11	1:D:3998:MET:HE3	1.98	0.45
1:A:347:ASP:N	1:A:347:ASP:OD1	2.50	0.45
1:A:2263:LYS:O	1:A:2267:TYR:HD2	2.00	0.45
1:B:494:MET:HG2	1:B:497:LEU:HD22	1.99	0.45
1:B:555:LEU:HA	1:B:558:LEU:HD12	1.98	0.45
1:B:619:VAL:HA	1:B:624:ALA:HB3	1.99	0.45
1:B:1172:THR:C	1:B:1173:MET:HE2	2.42	0.45
1:B:1173:MET:HE3	1:B:1195:PHE:CZ	2.51	0.45
1:B:2286:ASP:OD1	1:B:2286:ASP:N	2.48	0.45
1:C:207:PHE:CD2	1:D:2324:ILE:HD13	2.51	0.45
1:C:960:LYS:HG3	1:C:961:VAL:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1108:VAL:HG21	1:C:1214:ARG:HH21	1.82	0.45
1:C:1302:TYR:HB2	1:C:1544:VAL:O	2.17	0.45
1:A:995:MET:HE2	1:A:1054:VAL:HG12	1.98	0.45
1:A:3858:ARG:NH1	1:A:3930:ASN:OD1	2.47	0.45
1:A:4056:HIS:O	1:A:4062:THR:OG1	2.29	0.45
1:A:4154:SER:HA	1:A:4157:THR:HG22	1.99	0.45
1:B:960:LYS:HG3	1:B:961:VAL:HG23	1.98	0.45
1:B:1623:LEU:HD23	1:B:1623:LEU:HA	1.86	0.45
1:B:2263:LYS:O	1:B:2267:TYR:HD2	2.00	0.45
1:B:3355:LEU:HB3	1:B:3358:PHE:HB2	1.99	0.45
1:C:902:TRP:HE3	1:C:913:ARG:HG2	1.82	0.45
1:C:2263:LYS:O	1:C:2267:TYR:HD2	2.00	0.45
1:D:494:MET:HG2	1:D:497:LEU:HD22	1.99	0.45
1:D:4043:SER:O	1:D:4045:ARG:N	2.48	0.45
1:A:1215:MET:HA	1:A:1215:MET:HE3	1.98	0.45
1:B:1108:VAL:HG21	1:B:1214:ARG:HH21	1.82	0.45
1:B:1462:VAL:HG12	1:B:1463:ARG:H	1.82	0.45
1:B:1695:MET:HG3	1:B:1696:PRO:HD2	1.99	0.45
1:B:1901:VAL:O	1:B:1905:MET:HG2	2.17	0.45
1:B:2508:ALA:HB2	1:B:2595:VAL:HG21	1.99	0.45
1:B:2876:LEU:HB3	1:B:2880:GLU:HG3	1.99	0.45
1:B:3941:ASP:OD1	1:B:3941:ASP:N	2.50	0.45
1:C:233:VAL:HG12	1:C:274:LEU:HD22	1.99	0.45
1:C:494:MET:HG2	1:C:497:LEU:H	1.81	0.45
1:C:619:VAL:HA	1:C:624:ALA:HB3	1.99	0.45
1:C:1172:THR:C	1:C:1173:MET:HE2	2.42	0.45
1:C:3985:LEU:HD11	1:C:3998:MET:HE3	1.98	0.45
1:D:2490:GLY:O	1:D:2494:ASP:N	2.39	0.45
1:D:3843:GLN:HB2	1:D:3918:THR:HA	1.98	0.45
1:A:902:TRP:HE3	1:A:913:ARG:HG2	1.82	0.45
1:A:2508:ALA:HB2	1:A:2595:VAL:HG21	1.99	0.45
1:A:3843:GLN:HB2	1:A:3918:THR:HA	1.98	0.45
1:B:2716:LEU:HD21	1:B:2771:ARG:HH22	1.82	0.45
1:B:3888:TYR:OH	1:B:3952:HIS:HB3	2.17	0.45
1:B:4908:THR:O	1:B:4913:ASN:ND2	2.49	0.45
1:C:1695:MET:HG3	1:C:1696:PRO:HD2	1.99	0.45
1:C:2508:ALA:HB2	1:C:2595:VAL:HG21	1.99	0.45
1:D:261:HIS:ND1	1:D:388:GLN:OE1	2.44	0.45
1:D:617:LEU:HG	1:D:632:ILE:HG21	1.99	0.45
1:D:936:SER:O	1:D:940:LEU:HD13	2.17	0.45
1:D:1089:ARG:O	1:D:1250:TRP:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1302:TYR:HB2	1:D:1544:VAL:O	2.17	0.45
1:D:3858:ARG:NH1	1:D:3930:ASN:OD1	2.47	0.45
1:A:1089:ARG:O	1:A:1250:TRP:N	2.48	0.45
1:A:2320:VAL:O	1:A:2324:ILE:HG13	2.17	0.45
1:A:2716:LEU:HD21	1:A:2771:ARG:HH22	1.82	0.45
1:A:3985:LEU:HD11	1:A:3998:MET:HE3	1.98	0.45
1:B:57:ASN:ND2	1:B:322:ALA:O	2.48	0.45
1:B:141:ASP:N	1:B:141:ASP:OD1	2.50	0.45
1:B:1089:ARG:O	1:B:1250:TRP:N	2.48	0.45
1:B:1783:PHE:HE2	1:B:1788:LEU:HD22	1.82	0.45
1:B:2264:VAL:HG21	1:B:2300:PHE:HE2	1.81	0.45
1:B:2320:VAL:O	1:B:2324:ILE:HG13	2.17	0.45
1:B:2331:GLY:H	1:B:2339:GLY:HA2	1.82	0.45
1:B:4154:SER:HA	1:B:4157:THR:HG22	1.99	0.45
1:C:753:ASP:OD1	1:C:753:ASP:N	2.50	0.45
1:C:2228:LEU:HG	1:C:2230:SER:H	1.82	0.45
1:C:2264:VAL:HG21	1:C:2300:PHE:HE2	1.81	0.45
1:C:2716:LEU:HD21	1:C:2771:ARG:HH22	1.82	0.45
1:C:2876:LEU:HB3	1:C:2880:GLU:HG3	1.99	0.45
1:D:619:VAL:HA	1:D:624:ALA:HB3	1.99	0.45
1:D:2263:LYS:O	1:D:2267:TYR:HD2	2.00	0.45
1:D:3941:ASP:OD1	1:D:3941:ASP:N	2.50	0.45
1:A:1173:MET:HE3	1:A:1195:PHE:CZ	2.51	0.44
1:A:2331:GLY:H	1:A:2339:GLY:HA2	1.82	0.44
1:A:3857:LEU:HD21	1:A:3869:ILE:HB	2.00	0.44
1:B:73:LEU:O	1:B:118:ALA:N	2.50	0.44
1:B:246:THR:N	1:B:261:HIS:O	2.44	0.44
1:B:995:MET:HE2	1:B:1054:VAL:HG12	1.98	0.44
1:B:4844:ILE:O	1:B:4848:THR:OG1	2.30	0.44
1:C:936:SER:O	1:C:940:LEU:HD13	2.17	0.44
1:C:1783:PHE:HE2	1:C:1788:LEU:HD22	1.82	0.44
1:C:1901:VAL:O	1:C:1905:MET:HG2	2.17	0.44
1:D:347:ASP:N	1:D:347:ASP:OD1	2.50	0.44
1:D:2080:VAL:HA	1:D:2083:MET:HE3	1.99	0.44
1:D:2228:LEU:HG	1:D:2230:SER:H	1.82	0.44
1:D:3262:MET:HE3	1:D:3262:MET:O	2.16	0.44
1:D:3857:LEU:HD21	1:D:3869:ILE:HB	2.00	0.44
1:A:494:MET:HG2	1:A:497:LEU:HD22	1.99	0.44
1:B:753:ASP:OD1	1:B:753:ASP:N	2.50	0.44
1:B:936:SER:O	1:B:940:LEU:HD13	2.17	0.44
1:B:1691:GLU:OE1	1:B:1791:LYS:NZ	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2080:VAL:HA	1:B:2083:MET:HE3	1.99	0.44
1:B:4092:ASP:OD1	1:B:4092:ASP:N	2.47	0.44
1:B:4808:MET:HG2	1:C:4516:LEU:HA	1.99	0.44
1:C:1089:ARG:HH21	1:C:1601:PRO:HB3	1.82	0.44
1:C:2065:MET:HE2	1:C:2065:MET:HB2	1.89	0.44
1:C:2461:PRO:HG2	1:C:2514:ALA:HB3	1.99	0.44
1:C:2511:MET:HE2	1:C:2511:MET:HA	1.97	0.44
1:C:3355:LEU:HB3	1:C:3358:PHE:HB2	1.99	0.44
1:C:4176:VAL:HG13	1:C:4879:VAL:HG22	2.00	0.44
1:D:1901:VAL:O	1:D:1905:MET:HG2	2.17	0.44
1:D:2509:THR:HA	1:D:2513:LEU:HD11	1.98	0.44
1:A:161:THR:OG1	1:A:184:VAL:O	2.32	0.44
1:A:1901:VAL:O	1:A:1905:MET:HG2	2.17	0.44
1:A:2228:LEU:HG	1:A:2230:SER:H	1.82	0.44
1:A:2264:VAL:HG21	1:A:2300:PHE:HE2	1.81	0.44
1:B:494:MET:HG2	1:B:497:LEU:H	1.81	0.44
1:B:1924:ILE:HD11	1:B:2035:VAL:HG21	2.00	0.44
1:B:2079:LEU:HG	1:B:2083:MET:HE2	2.00	0.44
1:B:4816:MET:HE3	1:B:4816:MET:HB3	1.80	0.44
1:D:4176:VAL:HG13	1:D:4879:VAL:HG22	2.00	0.44
2:F:78:THR:HG23	2:F:80:ASP:HB3	1.98	0.44
1:A:617:LEU:HG	1:A:632:ILE:HG21	1.99	0.44
1:A:619:VAL:HA	1:A:624:ALA:HB3	1.99	0.44
1:A:2191:MET:SD	1:A:2191:MET:N	2.89	0.44
1:B:1822:LEU:HD23	1:B:1822:LEU:HA	1.84	0.44
1:B:3843:GLN:HB2	1:B:3918:THR:HA	1.98	0.44
1:C:617:LEU:HG	1:C:632:ILE:HG21	1.99	0.44
1:C:719:GLY:O	1:C:724:SER:OG	2.34	0.44
1:C:3262:MET:HE3	1:C:3262:MET:O	2.16	0.44
1:D:1691:GLU:OE1	1:D:1791:LYS:NZ	2.36	0.44
1:D:1832:MET:HE3	1:D:1832:MET:HB2	1.73	0.44
1:D:2320:VAL:O	1:D:2324:ILE:HG13	2.17	0.44
1:A:1783:PHE:HE2	1:A:1788:LEU:HD22	1.82	0.44
1:A:1924:ILE:HD11	1:A:2035:VAL:HG21	2.00	0.44
1:A:2509:THR:HA	1:A:2513:LEU:HD11	1.98	0.44
1:A:2876:LEU:HB3	1:A:2880:GLU:HG3	1.99	0.44
1:A:4176:VAL:HG13	1:A:4879:VAL:HG22	1.99	0.44
1:A:4182:LYS:HE2	1:B:4901:PRO:HB3	1.99	0.44
1:B:4176:VAL:HG13	1:B:4879:VAL:HG22	1.99	0.44
1:C:4768:LEU:HB3	1:D:4752:LEU:HD21	2.00	0.44
2:G:78:THR:HG23	2:G:80:ASP:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:936:SER:O	1:A:940:LEU:HD13	2.17	0.44
1:B:261:HIS:ND1	1:B:388:GLN:OE1	2.44	0.44
1:B:1172:THR:HG22	1:B:1193:LYS:HG2	2.00	0.44
1:B:1302:TYR:HB2	1:B:1544:VAL:O	2.17	0.44
1:C:2080:VAL:HA	1:C:2083:MET:HE3	1.99	0.44
1:C:2395:ILE:HG21	1:C:2467:MET:HE1	2.00	0.44
1:C:3228:THR:HG22	1:C:3347:MET:HE1	2.00	0.44
1:D:233:VAL:HG12	1:D:274:LEU:HD22	1.99	0.44
1:D:1177:LEU:N	1:D:1180:GLU:O	2.51	0.44
1:D:3355:LEU:HB3	1:D:3358:PHE:HB2	1.99	0.44
1:A:233:VAL:HG12	1:A:274:LEU:HD22	1.99	0.44
1:A:894:VAL:O	1:A:898:ILE:N	2.47	0.44
1:A:1177:LEU:N	1:A:1180:GLU:O	2.51	0.44
1:A:1302:TYR:HB2	1:A:1544:VAL:O	2.17	0.44
1:A:1462:VAL:HG12	1:A:1463:ARG:H	1.82	0.44
1:A:1467:VAL:O	1:A:1480:ILE:N	2.39	0.44
1:A:2152:LYS:HA	1:A:2155:TYR:CZ	2.53	0.44
1:A:3941:ASP:N	1:A:3941:ASP:OD1	2.50	0.44
1:B:426:PHE:O	1:B:430:ILE:HG12	2.16	0.44
1:B:1722:MET:HE1	1:B:2119:LEU:HG	2.00	0.44
1:C:1172:THR:HG22	1:C:1193:LYS:HG2	2.00	0.44
1:C:3857:LEU:HD21	1:C:3869:ILE:HB	2.00	0.44
1:D:1172:THR:C	1:D:1173:MET:HE2	2.42	0.44
1:D:1783:PHE:HE2	1:D:1788:LEU:HD22	1.82	0.44
1:D:4154:SER:HA	1:D:4157:THR:HG22	1.99	0.44
1:A:951:GLY:O	1:A:953:ALA:N	2.44	0.44
1:A:1695:MET:HG3	1:A:1696:PRO:HD2	1.99	0.44
1:A:4908:THR:O	1:A:4913:ASN:ND2	2.49	0.44
1:B:18:ASP:HB2	1:B:69:LEU:HD21	2.00	0.44
1:B:2228:LEU:HG	1:B:2230:SER:H	1.82	0.44
1:B:3228:THR:HG22	1:B:3347:MET:HE1	2.00	0.44
1:B:4663:ASP:O	1:B:4667:GLU:HG2	2.18	0.44
1:C:161:THR:OG1	1:C:184:VAL:O	2.32	0.44
1:C:433:LEU:O	1:C:437:SER:N	2.47	0.44
1:C:2034:LYS:HA	1:C:2037:TYR:CE2	2.53	0.44
1:C:2320:VAL:O	1:C:2324:ILE:HG13	2.17	0.44
1:C:4154:SER:HA	1:C:4157:THR:HG22	1.99	0.44
1:D:18:ASP:HB2	1:D:69:LEU:HD21	2.00	0.44
1:D:1927:PHE:CD2	1:D:2031:LEU:HD22	2.53	0.44
1:D:2508:ALA:HB2	1:D:2595:VAL:HG21	1.99	0.44
1:A:1927:PHE:CD2	1:A:2031:LEU:HD22	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2079:LEU:HG	1:A:2083:MET:HE2	2.00	0.44
1:B:68:VAL:HG23	1:B:124:SER:HB3	2.00	0.44
1:B:1089:ARG:HH21	1:B:1601:PRO:HB3	1.82	0.44
1:C:347:ASP:OD1	1:C:347:ASP:N	2.50	0.44
1:C:894:VAL:O	1:C:898:ILE:N	2.47	0.44
1:C:1722:MET:HE1	1:C:2119:LEU:HG	2.00	0.44
1:C:3046:LYS:HD3	1:C:3093:ILE:HD13	2.00	0.44
1:D:73:LEU:O	1:D:118:ALA:N	2.50	0.44
1:D:2716:LEU:HD21	1:D:2771:ARG:HH22	1.82	0.44
1:D:2876:LEU:HB3	1:D:2880:GLU:HG3	1.99	0.44
1:D:3228:THR:HG22	1:D:3347:MET:HE1	2.00	0.44
1:A:949:HIS:NE2	1:A:951:GLY:O	2.51	0.43
1:A:2404:GLU:HB3	1:A:2407:LEU:HB2	2.00	0.43
1:B:347:ASP:OD1	1:B:347:ASP:N	2.50	0.43
1:B:1177:LEU:N	1:B:1180:GLU:O	2.51	0.43
1:B:2511:MET:HB3	1:B:2515:LEU:HD12	2.00	0.43
1:B:3857:LEU:HD21	1:B:3869:ILE:HB	2.00	0.43
1:B:3858:ARG:NH1	1:B:3930:ASN:OD1	2.47	0.43
1:C:1251:LEU:N	1:C:1602:ASN:O	2.47	0.43
1:C:1462:VAL:HG12	1:C:1463:ARG:H	1.82	0.43
1:C:1832:MET:HE3	1:C:1832:MET:HB2	1.73	0.43
1:C:3888:TYR:OH	1:C:3952:HIS:HB3	2.17	0.43
1:D:949:HIS:NE2	1:D:951:GLY:O	2.51	0.43
1:D:2012:GLU:O	1:D:2016:LEU:N	2.41	0.43
1:D:2331:GLY:H	1:D:2339:GLY:HA2	1.82	0.43
1:D:3888:TYR:OH	1:D:3952:HIS:HB3	2.17	0.43
1:D:4663:ASP:O	1:D:4667:GLU:HG2	2.18	0.43
1:A:141:ASP:OD1	1:A:141:ASP:N	2.50	0.43
1:A:1172:THR:C	1:A:1173:MET:HE2	2.42	0.43
1:A:1784:PRO:HB2	1:A:1787:ILE:HG22	1.99	0.43
1:A:3888:TYR:OH	1:A:3952:HIS:HB3	2.17	0.43
1:A:3930:ASN:O	1:A:3934:LEU:HD12	2.18	0.43
1:B:2313:GLU:OE2	1:B:2317:ASN:ND2	2.48	0.43
1:B:2395:ILE:HG21	1:B:2467:MET:HE1	2.00	0.43
1:B:3046:LYS:HD3	1:B:3093:ILE:HD13	2.00	0.43
1:C:248:PRO:HD3	1:C:261:HIS:HD2	1.83	0.43
1:C:949:HIS:NE2	1:C:951:GLY:O	2.51	0.43
1:C:1177:LEU:N	1:C:1180:GLU:O	2.50	0.43
1:C:1927:PHE:CD2	1:C:2031:LEU:HD22	2.53	0.43
1:D:658:ASN:HB2	1:D:835:GLU:N	2.33	0.43
1:D:1695:MET:HG3	1:D:1696:PRO:HD2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2404:GLU:HB3	1:D:2407:LEU:HB2	2.01	0.43
1:D:2511:MET:HB3	1:D:2515:LEU:HD12	2.00	0.43
1:A:19:GLU:O	1:A:217:ILE:HG22	2.18	0.43
1:A:3228:THR:HG22	1:A:3347:MET:HE1	2.00	0.43
1:B:528:SER:O	1:B:532:SER:OG	2.25	0.43
1:B:902:TRP:HE3	1:B:913:ARG:HG2	1.82	0.43
1:B:1927:PHE:CD2	1:B:2031:LEU:HD22	2.53	0.43
1:C:658:ASN:HB2	1:C:835:GLU:N	2.33	0.43
1:C:1307:PRO:HG2	1:C:1308:ILE:HD12	2.01	0.43
1:D:128:MET:HB2	1:D:149:LEU:HD23	2.00	0.43
1:D:1462:VAL:HG12	1:D:1463:ARG:H	1.82	0.43
1:D:1784:PRO:HB2	1:D:1787:ILE:HG22	1.99	0.43
1:A:2395:ILE:HG21	1:A:2467:MET:HE1	1.99	0.43
1:A:3000:LYS:HD2	1:A:3066:ASP:HB3	2.01	0.43
1:A:4663:ASP:O	1:A:4667:GLU:HG2	2.18	0.43
1:B:248:PRO:HD3	1:B:261:HIS:HD2	1.83	0.43
1:B:617:LEU:HG	1:B:632:ILE:HG21	1.99	0.43
1:B:1251:LEU:N	1:B:1602:ASN:O	2.47	0.43
1:B:1784:PRO:HB2	1:B:1787:ILE:HG22	1.99	0.43
1:B:2152:LYS:HA	1:B:2155:TYR:CZ	2.53	0.43
1:C:68:VAL:HG23	1:C:124:SER:HB3	2.00	0.43
1:C:1784:PRO:HB2	1:C:1787:ILE:HG22	1.99	0.43
1:D:1769:PHE:HE1	2:H:91:VAL:HG21	1.84	0.43
1:A:18:ASP:HB2	1:A:69:LEU:HD21	2.00	0.43
1:A:658:ASN:HB2	1:A:835:GLU:N	2.33	0.43
1:A:2080:VAL:HA	1:A:2083:MET:HE3	1.99	0.43
1:B:64:ILE:H	1:B:64:ILE:HG12	1.63	0.43
1:C:1173:MET:HE3	1:C:1195:PHE:CZ	2.51	0.43
1:C:1261:VAL:HA	1:C:1262:PRO:HD3	1.91	0.43
1:C:2079:LEU:HG	1:C:2083:MET:HE2	2.00	0.43
1:C:4807:ASP:OD1	1:C:4807:ASP:N	2.41	0.43
1:D:115:TYR:CZ	1:D:175:VAL:HG22	2.54	0.43
1:D:753:ASP:OD1	1:D:753:ASP:N	2.50	0.43
1:D:1172:THR:HG22	1:D:1193:LYS:HG2	2.00	0.43
1:D:2152:LYS:HA	1:D:2155:TYR:CZ	2.53	0.43
1:D:3000:LYS:HD2	1:D:3066:ASP:HB3	2.01	0.43
2:F:77:CYS:N	2:F:98:LEU:O	2.49	0.43
1:A:185:SER:OG	1:A:186:VAL:N	2.50	0.43
1:A:1172:THR:HG22	1:A:1193:LYS:HG2	2.00	0.43
1:A:2461:PRO:HG2	1:A:2514:ALA:HB3	2.00	0.43
1:A:2643:LEU:O	1:A:2647:ILE:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4752:LEU:HD21	1:D:4768:LEU:HB3	2.01	0.43
1:A:4807:ASP:OD1	1:A:4807:ASP:N	2.41	0.43
1:B:949:HIS:NE2	1:B:951:GLY:O	2.51	0.43
1:B:1832:MET:HB3	1:B:1834:ILE:HG12	2.01	0.43
1:C:18:ASP:HB2	1:C:69:LEU:HD21	2.00	0.43
1:C:128:MET:HB2	1:C:149:LEU:HD23	2.00	0.43
1:C:554:SER:O	1:C:554:SER:OG	2.37	0.43
1:C:1924:ILE:HD11	1:C:2035:VAL:HG21	2.00	0.43
1:C:3930:ASN:O	1:C:3934:LEU:HD12	2.18	0.43
1:C:4182:LYS:HE2	1:D:4901:PRO:HB3	2.01	0.43
1:D:1251:LEU:N	1:D:1602:ASN:O	2.47	0.43
1:D:2079:LEU:HG	1:D:2083:MET:HE2	2.00	0.43
1:D:2643:LEU:O	1:D:2647:ILE:HG12	2.18	0.43
1:D:3930:ASN:O	1:D:3934:LEU:HD12	2.18	0.43
1:A:73:LEU:O	1:A:118:ALA:N	2.50	0.43
1:A:1832:MET:HB3	1:A:1834:ILE:HG12	2.01	0.43
1:B:19:GLU:O	1:B:217:ILE:HG22	2.18	0.43
1:B:2461:PRO:HG2	1:B:2514:ALA:HB3	2.00	0.43
1:D:699:SER:OG	1:D:789:PHE:O	2.30	0.43
1:D:2395:ILE:HG21	1:D:2467:MET:HE1	2.00	0.43
1:A:115:TYR:CZ	1:A:175:VAL:HG22	2.54	0.43
1:B:128:MET:HB2	1:B:149:LEU:HD23	2.00	0.43
1:B:1307:PRO:HG2	1:B:1308:ILE:HD12	2.01	0.43
1:B:2034:LYS:HA	1:B:2037:TYR:CE2	2.53	0.43
1:B:3930:ASN:O	1:B:3934:LEU:HD12	2.18	0.43
1:B:4749:PHE:HB2	1:B:4752:LEU:HD23	2.01	0.43
1:C:1117:TRP:CD1	1:C:1135:PHE:HB2	2.54	0.43
1:D:1924:ILE:HD11	1:D:2035:VAL:HG21	2.00	0.43
1:D:2034:LYS:HA	1:D:2037:TYR:CE2	2.53	0.43
1:A:719:GLY:O	1:A:724:SER:OG	2.34	0.43
1:A:1832:MET:HE3	1:A:1832:MET:HB2	1.73	0.43
1:A:4799:ASP:OD1	1:A:4799:ASP:N	2.52	0.43
1:B:554:SER:O	1:B:554:SER:OG	2.37	0.43
1:C:73:LEU:O	1:C:118:ALA:N	2.50	0.43
1:C:1769:PHE:HE1	2:G:91:VAL:HG21	1.84	0.43
1:C:2331:GLY:H	1:C:2339:GLY:HA2	1.82	0.43
1:C:4799:ASP:OD1	1:C:4799:ASP:N	2.52	0.43
1:D:719:GLY:O	1:D:724:SER:OG	2.34	0.43
1:D:1173:MET:HE3	1:D:1195:PHE:CZ	2.51	0.43
1:D:1722:MET:HE1	1:D:2119:LEU:HG	2.00	0.43
1:D:4799:ASP:N	1:D:4799:ASP:OD1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1117:TRP:CD1	1:B:1135:PHE:HB2	2.54	0.43
1:B:1769:PHE:HE1	2:F:91:VAL:HG21	1.84	0.43
1:B:2450:VAL:HG23	1:B:2451:VAL:HG22	2.01	0.43
1:C:19:GLU:O	1:C:217:ILE:HG22	2.18	0.43
1:C:2152:LYS:HA	1:C:2155:TYR:CZ	2.53	0.43
1:C:2643:LEU:O	1:C:2647:ILE:HG12	2.18	0.43
1:C:3645:LYS:HZ3	1:C:3663:LEU:HB2	1.84	0.43
1:C:4663:ASP:O	1:C:4667:GLU:HG2	2.18	0.43
1:D:19:GLU:O	1:D:217:ILE:HG22	2.18	0.43
1:D:370:LEU:HD23	1:D:370:LEU:HA	1.93	0.43
1:A:1722:MET:HE1	1:A:2119:LEU:HG	2.00	0.42
1:A:3355:LEU:HB3	1:A:3358:PHE:HB2	1.99	0.42
1:A:4749:PHE:HB2	1:A:4752:LEU:HD23	2.01	0.42
1:B:430:ILE:HB	1:B:502:ILE:HD11	2.01	0.42
1:B:658:ASN:HB2	1:B:835:GLU:N	2.33	0.42
1:B:2643:LEU:O	1:B:2647:ILE:HG12	2.18	0.42
1:B:3000:LYS:HD2	1:B:3066:ASP:HB3	2.01	0.42
1:B:4768:LEU:HB3	1:C:4752:LEU:HD21	2.01	0.42
1:C:115:TYR:CZ	1:C:175:VAL:HG22	2.54	0.42
1:C:2404:GLU:HB3	1:C:2407:LEU:HB2	2.00	0.42
1:C:2511:MET:HB3	1:C:2515:LEU:HD12	2.00	0.42
1:D:433:LEU:O	1:D:437:SER:N	2.48	0.42
1:D:1117:TRP:CD1	1:D:1135:PHE:HB2	2.54	0.42
1:A:68:VAL:HG23	1:A:124:SER:HB3	2.00	0.42
1:A:2034:LYS:HA	1:A:2037:TYR:CE2	2.53	0.42
1:C:33:GLN:NE2	1:C:35:LEU:HD11	2.34	0.42
1:D:141:ASP:N	1:D:141:ASP:OD1	2.50	0.42
1:D:248:PRO:HD3	1:D:261:HIS:HD2	1.83	0.42
1:D:1307:PRO:HG2	1:D:1308:ILE:HD12	2.01	0.42
1:D:2334:LEU:O	1:D:2336:GLY:N	2.53	0.42
1:D:3046:LYS:HD3	1:D:3093:ILE:HD13	2.00	0.42
1:D:3645:LYS:HZ3	1:D:3663:LEU:HB2	1.85	0.42
1:A:2204:ARG:O	1:A:2206:SER:N	2.42	0.42
1:A:2604:MET:SD	1:A:2604:MET:N	2.85	0.42
1:A:4180:GLY:O	1:A:4182:LYS:N	2.52	0.42
1:A:4901:PRO:HB3	1:D:4182:LYS:HE2	2.01	0.42
1:B:801:ARG:HA	1:B:1619:LEU:HA	2.01	0.42
1:B:963:LYS:O	1:B:964:MET:HG2	2.19	0.42
1:C:141:ASP:OD1	1:C:141:ASP:N	2.50	0.42
1:C:801:ARG:HA	1:C:1619:LEU:HA	2.01	0.42
1:C:4749:PHE:HB2	1:C:4752:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4596:LEU:HD12	1:D:4596:LEU:HA	1.89	0.42
1:A:963:LYS:O	1:A:964:MET:HG2	2.19	0.42
1:A:1822:LEU:HD23	1:A:1822:LEU:HA	1.84	0.42
1:A:4816:MET:HE3	1:A:4816:MET:HB3	1.80	0.42
1:B:2404:GLU:HB3	1:B:2407:LEU:HB2	2.00	0.42
1:C:2385:ASN:ND2	1:C:2456:SER:O	2.52	0.42
1:C:3000:LYS:HD2	1:C:3066:ASP:HB3	2.01	0.42
1:A:2450:VAL:HG23	1:A:2451:VAL:HG22	2.01	0.42
1:A:3046:LYS:HD3	1:A:3093:ILE:HD13	2.00	0.42
1:B:1103:PHE:O	1:B:1164:CYS:N	2.49	0.42
1:B:3777:LEU:HD12	1:B:3777:LEU:HA	1.92	0.42
1:C:879:GLU:O	1:C:883:GLU:N	2.51	0.42
1:C:2286:ASP:OD1	1:C:2286:ASP:N	2.48	0.42
1:D:2461:PRO:HG2	1:D:2514:ALA:HB3	2.00	0.42
1:A:248:PRO:HD3	1:A:261:HIS:HD2	1.83	0.42
1:A:314:LEU:HD11	1:A:365:HIS:HE1	1.85	0.42
1:A:430:ILE:HB	1:A:502:ILE:HD11	2.02	0.42
1:A:2511:MET:HB3	1:A:2515:LEU:HD12	2.00	0.42
1:B:932:ASN:O	1:B:936:SER:OG	2.32	0.42
1:B:4056:HIS:O	1:B:4062:THR:OG1	2.29	0.42
1:C:963:LYS:O	1:C:964:MET:HG2	2.19	0.42
1:C:2450:VAL:HG23	1:C:2451:VAL:HG22	2.01	0.42
1:A:801:ARG:HA	1:A:1619:LEU:HA	2.01	0.42
1:A:2334:LEU:O	1:A:2336:GLY:N	2.52	0.42
1:A:2828:SER:OG	1:A:2889:GLN:OE1	2.30	0.42
1:B:67:PHE:HB3	1:B:121:LEU:HD12	2.02	0.42
1:B:185:SER:OG	1:B:186:VAL:N	2.50	0.42
1:B:314:LEU:HD11	1:B:365:HIS:HE1	1.85	0.42
1:B:483:LYS:HD2	1:B:483:LYS:HA	1.86	0.42
1:B:4799:ASP:OD1	1:B:4799:ASP:N	2.52	0.42
1:C:67:PHE:HB3	1:C:121:LEU:HD12	2.02	0.42
1:D:554:SER:O	1:D:554:SER:OG	2.37	0.42
1:D:2385:ASN:ND2	1:D:2456:SER:O	2.52	0.42
1:D:4756:LEU:HD23	1:D:4756:LEU:HA	1.93	0.42
1:A:495:ILE:O	1:A:499:LEU:N	2.48	0.42
1:A:695:VAL:O	1:A:727:PHE:N	2.48	0.42
1:A:1307:PRO:HG2	1:A:1308:ILE:HD12	2.01	0.42
1:A:2385:ASN:ND2	1:A:2456:SER:O	2.53	0.42
1:B:114:LEU:HB2	1:B:117:HIS:HD2	1.85	0.42
1:C:1769:PHE:O	2:G:83:TYR:OH	2.29	0.42
1:D:68:VAL:HG23	1:D:124:SER:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3727:GLN:NE2	1:D:3764:ILE:O	2.32	0.42
1:D:4844:ILE:O	1:D:4848:THR:OG1	2.30	0.42
1:A:128:MET:HB2	1:A:149:LEU:HD23	2.00	0.42
1:A:1117:TRP:CD1	1:A:1135:PHE:HB2	2.54	0.42
1:A:1769:PHE:HE1	2:E:91:VAL:HG21	1.84	0.42
1:B:2385:ASN:ND2	1:B:2456:SER:O	2.53	0.42
1:C:488:LEU:HD12	1:C:488:LEU:HA	1.90	0.42
1:C:2334:LEU:O	1:C:2336:GLY:N	2.52	0.42
1:C:3941:ASP:OD1	1:C:3941:ASP:N	2.50	0.42
1:D:64:ILE:H	1:D:64:ILE:HG12	1.63	0.42
1:A:33:GLN:NE2	1:A:35:LEU:HD11	2.34	0.42
1:A:2197:ARG:O	1:A:2201:TYR:HB2	2.20	0.42
1:D:300:VAL:HG23	1:D:301:THR:HG23	2.02	0.42
1:D:1832:MET:HB3	1:D:1834:ILE:HG12	2.01	0.42
1:D:4908:THR:O	1:D:4913:ASN:ND2	2.49	0.42
1:A:114:LEU:HB2	1:A:117:HIS:HD2	1.85	0.41
1:A:1269:GLU:H	1:A:1290:PHE:HE2	1.68	0.41
1:B:115:TYR:CZ	1:B:175:VAL:HG22	2.54	0.41
1:B:499:LEU:HA	1:B:502:ILE:HD12	2.02	0.41
1:B:1905:MET:HA	1:B:1905:MET:HE3	2.02	0.41
1:C:430:ILE:HB	1:C:502:ILE:HD11	2.02	0.41
1:C:499:LEU:HA	1:C:502:ILE:HD12	2.02	0.41
1:C:1832:MET:HB3	1:C:1834:ILE:HG12	2.01	0.41
1:C:3792:LEU:HD23	1:C:3792:LEU:HA	1.93	0.41
1:C:3795:LEU:HD22	1:C:3834:PHE:HZ	1.85	0.41
1:D:63:SER:HB3	1:D:276:ARG:HH12	1.85	0.41
1:D:234:LEU:HD12	1:D:234:LEU:HA	1.94	0.41
1:D:488:LEU:HD12	1:D:488:LEU:HA	1.90	0.41
1:D:963:LYS:O	1:D:964:MET:HG2	2.19	0.41
1:D:1273:ILE:HG13	1:D:1287:GLN:N	2.35	0.41
1:D:1446:ILE:HD11	1:D:1450:PHE:CD2	2.56	0.41
1:D:1905:MET:HE3	1:D:1905:MET:HA	2.02	0.41
1:D:2197:ARG:O	1:D:2201:TYR:HB2	2.20	0.41
2:F:77:CYS:HB2	2:F:98:LEU:HB2	2.02	0.41
1:A:63:SER:HB3	1:A:276:ARG:HH12	1.85	0.41
1:B:323:ASP:O	1:B:327:THR:OG1	2.31	0.41
1:B:1269:GLU:H	1:B:1290:PHE:HE2	1.68	0.41
1:B:1769:PHE:O	2:F:83:TYR:OH	2.29	0.41
1:C:300:VAL:HG23	1:C:301:THR:HG23	2.02	0.41
1:C:1170:GLU:N	1:C:1170:GLU:OE1	2.53	0.41
1:C:1905:MET:HE3	1:C:1905:MET:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2122:LEU:HD22	1:C:2164:LEU:HD23	2.02	0.41
1:C:3322:MET:HE2	1:C:3365:LEU:HD13	2.02	0.41
1:D:297:LEU:HD12	1:D:297:LEU:HA	1.92	0.41
1:D:495:ILE:O	1:D:499:LEU:N	2.48	0.41
1:D:2065:MET:HG3	1:D:2083:MET:HG2	2.03	0.41
1:D:4749:PHE:HB2	1:D:4752:LEU:HD23	2.01	0.41
2:E:77:CYS:HB2	2:E:98:LEU:HB2	2.02	0.41
1:A:627:SER:HB3	1:A:2130:SER:C	2.46	0.41
1:A:2012:GLU:O	1:A:2016:LEU:N	2.41	0.41
1:A:2278:MET:HB3	1:A:2288:GLY:HA2	2.02	0.41
1:B:1170:GLU:N	1:B:1170:GLU:OE1	2.53	0.41
1:B:4182:LYS:HE2	1:C:4901:PRO:HB3	2.02	0.41
1:C:63:SER:HB3	1:C:276:ARG:HH12	1.85	0.41
1:C:2197:ARG:O	1:C:2201:TYR:HB2	2.20	0.41
1:D:33:GLN:NE2	1:D:35:LEU:HD11	2.34	0.41
1:D:430:ILE:HB	1:D:502:ILE:HD11	2.02	0.41
1:D:695:VAL:O	1:D:727:PHE:N	2.48	0.41
1:D:894:VAL:O	1:D:898:ILE:N	2.47	0.41
1:D:932:ASN:O	1:D:936:SER:OG	2.32	0.41
1:D:1103:PHE:O	1:D:1164:CYS:N	2.49	0.41
1:D:1170:GLU:N	1:D:1170:GLU:OE1	2.53	0.41
1:D:1467:VAL:O	1:D:1480:ILE:N	2.39	0.41
1:D:2836:LEU:HD22	1:D:2895:LEU:HD23	2.02	0.41
1:D:3795:LEU:HD22	1:D:3834:PHE:HZ	1.85	0.41
1:A:67:PHE:HB3	1:A:121:LEU:HD12	2.02	0.41
1:A:1261:VAL:HA	1:A:1262:PRO:HD3	1.91	0.41
1:A:1273:ILE:HG13	1:A:1287:GLN:N	2.35	0.41
1:A:1905:MET:HE3	1:A:1905:MET:HA	2.02	0.41
1:A:2122:LEU:HD22	1:A:2164:LEU:HD23	2.02	0.41
1:A:4851:PHE:O	1:A:4855:VAL:HB	2.20	0.41
1:B:33:GLN:NE2	1:B:35:LEU:HD11	2.34	0.41
1:B:300:VAL:HG23	1:B:301:THR:HG23	2.02	0.41
1:B:879:GLU:O	1:B:883:GLU:N	2.51	0.41
1:B:2278:MET:HB3	1:B:2288:GLY:HA2	2.02	0.41
1:B:3891:TYR:OH	1:B:3898:ASP:OD1	2.24	0.41
1:C:1446:ILE:HD11	1:C:1450:PHE:CD2	2.56	0.41
1:D:323:ASP:O	1:D:327:THR:OG1	2.31	0.41
1:D:2122:LEU:HD22	1:D:2164:LEU:HD23	2.02	0.41
1:A:1170:GLU:OE1	1:A:1170:GLU:N	2.53	0.41
1:A:1446:ILE:HD11	1:A:1450:PHE:CD2	2.56	0.41
1:B:63:SER:HB3	1:B:276:ARG:HH12	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2334:LEU:O	1:B:2336:GLY:N	2.53	0.41
1:C:1426:TYR:HB2	1:C:1511:VAL:HG12	2.02	0.41
1:D:627:SER:HB3	1:D:2130:SER:C	2.46	0.41
1:D:879:GLU:O	1:D:883:GLU:N	2.51	0.41
1:D:2450:VAL:HG23	1:D:2451:VAL:HG22	2.01	0.41
1:A:499:LEU:HA	1:A:502:ILE:HD12	2.03	0.41
1:A:1223:THR:O	1:A:1225:LYS:NZ	2.54	0.41
1:B:1223:THR:O	1:B:1225:LYS:NZ	2.54	0.41
1:B:2122:LEU:HD22	1:B:2164:LEU:HD23	2.02	0.41
1:B:2701:ASN:O	1:B:2849:ASN:ND2	2.54	0.41
1:B:4601:ARG:HD2	1:B:4711:VAL:HG21	2.02	0.41
1:D:67:PHE:HB3	1:D:121:LEU:HD12	2.02	0.41
1:A:370:LEU:HD23	1:A:370:LEU:HA	1.93	0.41
1:A:2701:ASN:O	1:A:2849:ASN:ND2	2.54	0.41
1:B:1217:PHE:HB3	1:B:1239:PHE:HB3	2.03	0.41
1:B:1273:ILE:HG13	1:B:1287:GLN:N	2.35	0.41
1:B:1446:ILE:HD11	1:B:1450:PHE:CD2	2.56	0.41
1:C:185:SER:OG	1:C:186:VAL:N	2.50	0.41
1:D:2101:LEU:HA	1:D:2101:LEU:HD23	1.85	0.41
1:D:2218:SER:O	1:D:2222:GLU:HB2	2.21	0.41
1:D:4106:GLU:OE1	1:D:4148:TYR:OH	2.24	0.41
2:G:77:CYS:HB2	2:G:98:LEU:HB2	2.02	0.41
1:A:1738:THR:OG1	1:A:1740:PHE:O	2.31	0.41
1:A:1788:LEU:O	1:A:1792:THR:OG1	2.31	0.41
1:B:650:ASN:OD1	1:B:650:ASN:N	2.54	0.41
1:C:650:ASN:OD1	1:C:650:ASN:N	2.54	0.41
1:C:1223:THR:O	1:C:1225:LYS:NZ	2.54	0.41
1:C:2065:MET:HG3	1:C:2083:MET:HG2	2.03	0.41
1:C:3943:VAL:O	1:C:3947:LEU:HD12	2.21	0.41
1:C:4601:ARG:HD2	1:C:4711:VAL:HG21	2.02	0.41
1:D:1217:PHE:HB3	1:D:1239:PHE:HB3	2.03	0.41
1:D:1843:ILE:HD13	1:D:1843:ILE:HA	1.97	0.41
1:D:3943:VAL:O	1:D:3947:LEU:HD12	2.21	0.41
1:D:4816:MET:HE3	1:D:4816:MET:HB3	1.80	0.41
1:A:228:LEU:HG	1:A:289:ILE:HD12	2.03	0.41
1:A:753:ASP:OD1	1:A:753:ASP:N	2.50	0.41
1:A:1737:ILE:HD13	1:A:1754:LEU:HB3	2.03	0.41
1:A:2385:ASN:O	1:A:2389:THR:OG1	2.29	0.41
1:B:745:ASN:ND2	1:B:771:ASN:O	2.54	0.41
1:B:2197:ARG:O	1:B:2201:TYR:HB2	2.20	0.41
1:B:2218:SER:O	1:B:2222:GLU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3795:LEU:HD22	1:B:3834:PHE:HZ	1.85	0.41
1:B:3958:SER:O	1:B:4085:ARG:NH1	2.54	0.41
1:B:4180:GLY:O	1:B:4182:LYS:N	2.52	0.41
1:C:510:SER:HG	1:C:513:HIS:HD1	1.64	0.41
1:C:1273:ILE:HG13	1:C:1287:GLN:N	2.35	0.41
1:C:2701:ASN:O	1:C:2849:ASN:ND2	2.54	0.41
1:D:228:LEU:HG	1:D:289:ILE:HD12	2.03	0.41
1:D:499:LEU:HA	1:D:502:ILE:HD12	2.03	0.41
1:D:801:ARG:HA	1:D:1619:LEU:HA	2.01	0.41
1:D:1223:THR:O	1:D:1225:LYS:NZ	2.54	0.41
1:D:1426:TYR:HB2	1:D:1511:VAL:HG12	2.02	0.41
1:D:3322:MET:HE2	1:D:3365:LEU:HD13	2.02	0.41
1:D:3508:ILE:O	1:D:3551:LEU:N	2.54	0.41
1:D:4735:ASN:OD1	1:D:4735:ASN:N	2.54	0.41
1:D:4851:PHE:O	1:D:4855:VAL:HB	2.21	0.41
2:G:77:CYS:N	2:G:98:LEU:O	2.49	0.41
2:H:77:CYS:HB2	2:H:98:LEU:HB2	2.02	0.41
1:A:488:LEU:HD12	1:A:488:LEU:HA	1.90	0.41
1:C:228:LEU:HG	1:C:289:ILE:HD12	2.03	0.41
1:C:494:MET:C	1:C:496:ASN:H	2.29	0.41
1:C:1788:LEU:O	1:C:1792:THR:OG1	2.31	0.41
1:C:2278:MET:HB3	1:C:2288:GLY:HA2	2.02	0.41
1:C:2526:LEU:O	1:C:2527:LEU:HD23	2.21	0.41
1:C:4808:MET:HG2	1:D:4516:LEU:HA	2.03	0.41
1:D:114:LEU:HB2	1:D:117:HIS:HD2	1.85	0.41
1:D:314:LEU:HD11	1:D:365:HIS:HE1	1.85	0.41
1:D:1269:GLU:H	1:D:1290:PHE:HE2	1.68	0.41
1:A:300:VAL:HG23	1:A:301:THR:HG23	2.02	0.40
1:A:688:ALA:HA	2:E:41:ARG:CZ	2.52	0.40
1:A:3795:LEU:HD22	1:A:3834:PHE:HZ	1.85	0.40
1:A:4099:VAL:HG22	1:A:4132:LEU:HD13	2.03	0.40
1:B:3508:ILE:O	1:B:3551:LEU:N	2.54	0.40
1:C:745:ASN:ND2	1:C:771:ASN:O	2.54	0.40
1:C:1217:PHE:HB3	1:C:1239:PHE:HB3	2.03	0.40
1:C:1269:GLU:H	1:C:1290:PHE:HE2	1.68	0.40
1:C:2836:LEU:HD22	1:C:2895:LEU:HD23	2.03	0.40
1:C:3696:LYS:HD3	1:C:3696:LYS:HA	1.86	0.40
1:C:3769:ASN:O	1:C:3773:GLN:NE2	2.54	0.40
1:C:4660:TYR:HB3	1:C:4664:ARG:NH1	2.36	0.40
1:C:4851:PHE:O	1:C:4855:VAL:HB	2.21	0.40
1:D:483:LYS:HD2	1:D:483:LYS:HA	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:745:ASN:ND2	1:D:771:ASN:O	2.54	0.40
1:D:997:ASP:O	1:D:1001:GLU:HG2	2.22	0.40
1:D:2701:ASN:O	1:D:2849:ASN:ND2	2.54	0.40
1:D:3730:LEU:HD23	1:D:3730:LEU:HA	1.87	0.40
1:A:650:ASN:OD1	1:A:650:ASN:N	2.54	0.40
1:A:4516:LEU:HA	1:D:4808:MET:HG2	2.03	0.40
1:A:4601:ARG:HD2	1:A:4711:VAL:HG21	2.02	0.40
1:B:495:ILE:O	1:B:499:LEU:N	2.48	0.40
1:B:4515:LEU:HA	1:B:4518:TYR:CD2	2.56	0.40
1:B:4660:TYR:HB3	1:B:4664:ARG:NH1	2.36	0.40
1:B:4851:PHE:O	1:B:4855:VAL:HB	2.21	0.40
1:C:3958:SER:O	1:C:4085:ARG:NH1	2.54	0.40
1:D:351:THR:OG1	1:D:352:SER:N	2.55	0.40
1:D:540:LEU:HG	1:D:547:ASN:OD1	2.22	0.40
1:D:2526:LEU:O	1:D:2527:LEU:HD23	2.21	0.40
1:A:61:ASP:HB3	1:A:64:ILE:HD11	2.03	0.40
1:A:699:SER:OG	1:A:789:PHE:O	2.30	0.40
1:A:1246:ASP:OD1	1:A:1694:TYR:OH	2.30	0.40
1:A:2010:LEU:HA	1:A:2013:ASP:HB2	2.03	0.40
1:A:3958:SER:O	1:A:4085:ARG:NH1	2.54	0.40
1:A:4735:ASN:OD1	1:A:4735:ASN:N	2.54	0.40
1:B:540:LEU:HG	1:B:547:ASN:OD1	2.22	0.40
1:B:4099:VAL:HG22	1:B:4132:LEU:HD13	2.03	0.40
1:B:4735:ASN:OD1	1:B:4735:ASN:N	2.54	0.40
1:C:483:LYS:HD2	1:C:483:LYS:HA	1.87	0.40
1:C:627:SER:HB3	1:C:2130:SER:C	2.46	0.40
1:C:1467:VAL:O	1:C:1480:ILE:N	2.39	0.40
1:C:1623:LEU:HD23	1:C:1623:LEU:HA	1.86	0.40
1:C:2218:SER:O	1:C:2222:GLU:HB2	2.21	0.40
1:C:4816:MET:HE3	1:C:4816:MET:HB3	1.80	0.40
1:D:185:SER:OG	1:D:186:VAL:N	2.50	0.40
1:D:1737:ILE:HD13	1:D:1754:LEU:HB3	2.03	0.40
1:D:3690:TYR:O	1:D:3694:MET:HE3	2.21	0.40
1:D:4601:ARG:HD2	1:D:4711:VAL:HG21	2.02	0.40
1:A:533:LEU:HD12	1:A:536:LEU:HD22	2.04	0.40
1:A:648:LEU:HD11	1:A:1685:GLN:CD	2.47	0.40
1:A:745:ASN:ND2	1:A:771:ASN:O	2.54	0.40
1:A:1217:PHE:HB3	1:A:1239:PHE:HB3	2.03	0.40
1:A:2836:LEU:HD22	1:A:2895:LEU:HD23	2.02	0.40
1:A:4949:GLU:OE1	1:A:4949:GLU:N	2.55	0.40
1:B:2526:LEU:O	1:B:2527:LEU:HD23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4949:GLU:N	1:B:4949:GLU:OE1	2.55	0.40
1:C:1843:ILE:HD13	1:C:1843:ILE:HA	1.97	0.40
1:C:2010:LEU:HA	1:C:2013:ASP:HB2	2.03	0.40
1:C:3508:ILE:O	1:C:3551:LEU:N	2.54	0.40
1:C:4515:LEU:HA	1:C:4518:TYR:CD2	2.56	0.40
1:D:533:LEU:HD12	1:D:536:LEU:HD22	2.04	0.40
1:D:648:LEU:HD11	1:D:1685:GLN:CD	2.47	0.40
1:D:688:ALA:HA	2:H:41:ARG:CZ	2.52	0.40
1:D:1028:ARG:NH2	1:D:1029:ASN:O	2.55	0.40
1:D:3958:SER:O	1:D:4085:ARG:NH1	2.54	0.40
1:D:4663:ASP:N	1:D:4663:ASP:OD1	2.55	0.40
2:E:101:ASP:OD1	2:E:101:ASP:N	2.54	0.40
1:A:294:PRO:HB3	1:A:328:ALA:HB1	2.03	0.40
1:A:540:LEU:HG	1:A:547:ASN:OD1	2.22	0.40
1:A:997:ASP:O	1:A:1001:GLU:HG2	2.22	0.40
1:A:1028:ARG:NH2	1:A:1029:ASN:O	2.55	0.40
1:A:2218:SER:O	1:A:2222:GLU:HB2	2.21	0.40
1:A:3322:MET:HE2	1:A:3365:LEU:HD13	2.02	0.40
1:A:3792:LEU:HD23	1:A:3792:LEU:HA	1.93	0.40
1:A:4663:ASP:OD1	1:A:4663:ASP:N	2.55	0.40
1:B:351:THR:OG1	1:B:352:SER:N	2.55	0.40
1:B:1028:ARG:NH2	1:B:1029:ASN:O	2.55	0.40
1:B:3943:VAL:O	1:B:3947:LEU:HD12	2.21	0.40
1:C:114:LEU:HB2	1:C:117:HIS:HD2	1.85	0.40
1:C:314:LEU:HD11	1:C:365:HIS:HE1	1.85	0.40
1:C:370:LEU:O	1:C:372:LEU:N	2.52	0.40
1:C:3860:GLN:HE22	1:C:3867:VAL:HG23	1.87	0.40
1:C:4908:THR:O	1:C:4913:ASN:ND2	2.49	0.40
1:D:650:ASN:OD1	1:D:650:ASN:N	2.54	0.40
1:D:2278:MET:HB3	1:D:2288:GLY:HA2	2.02	0.40
1:D:4660:TYR:HB3	1:D:4664:ARG:NH1	2.36	0.40
1:D:4949:GLU:N	1:D:4949:GLU:OE1	2.55	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	3818/4966 (77%)	3361 (88%)	436 (11%)	21 (1%)	21	52
1	B	3818/4966 (77%)	3361 (88%)	436 (11%)	21 (1%)	21	52
1	C	3818/4966 (77%)	3363 (88%)	435 (11%)	20 (0%)	24	56
1	D	3818/4966 (77%)	3362 (88%)	436 (11%)	20 (0%)	24	56
2	E	105/107 (98%)	96 (91%)	9 (9%)	0	100	100
2	F	105/107 (98%)	96 (91%)	9 (9%)	0	100	100
2	G	105/107 (98%)	96 (91%)	9 (9%)	0	100	100
2	H	105/107 (98%)	96 (91%)	9 (9%)	0	100	100
All	All	15692/20292 (77%)	13831 (88%)	1779 (11%)	82 (0%)	26	56

All (82) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1462	VAL
1	B	1462	VAL
1	C	1462	VAL
1	D	1462	VAL
1	A	411	GLU
1	A	654	SER
1	A	1032	LEU
1	A	1523	ALA
1	A	1848	GLU
1	A	3660	VAL
1	A	4042	ILE
1	B	411	GLU
1	B	654	SER
1	B	1032	LEU
1	B	1523	ALA
1	B	1848	GLU
1	B	3660	VAL
1	B	4042	ILE
1	C	411	GLU
1	C	654	SER
1	C	1032	LEU
1	C	1523	ALA
1	C	1848	GLU

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Mol	Chain	Res	Type
1	C	3660	VAL
1	C	4042	ILE
1	D	411	GLU
1	D	654	SER
1	D	1032	LEU
1	D	1523	ALA
1	D	1848	GLU
1	D	3660	VAL
1	D	4042	ILE
1	A	186	VAL
1	A	722	LEU
1	B	186	VAL
1	B	722	LEU
1	C	186	VAL
1	C	722	LEU
1	D	186	VAL
1	D	722	LEU
1	A	289	ILE
1	B	289	ILE
1	C	289	ILE
1	D	289	ILE
1	A	392	ILE
1	A	979	ALA
1	A	1299	ILE
1	A	1465	VAL
1	A	2444	ILE
1	B	392	ILE
1	B	979	ALA
1	B	1299	ILE
1	B	1465	VAL
1	B	2444	ILE
1	C	392	ILE
1	C	979	ALA
1	C	1299	ILE
1	C	1465	VAL
1	C	2444	ILE
1	D	392	ILE
1	D	979	ALA
1	D	1299	ILE
1	D	1465	VAL
1	D	2444	ILE
1	A	82	LEU

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Mol	Chain	Res	Type
1	A	371	TRP
1	A	1472	GLU
1	B	82	LEU
1	B	371	TRP
1	B	1472	GLU
1	C	82	LEU
1	C	371	TRP
1	D	82	LEU
1	D	371	TRP
1	A	4700	ILE
1	B	4700	ILE
1	C	4700	ILE
1	D	4700	ILE
1	A	495	ILE
1	B	495	ILE
1	C	495	ILE
1	D	495	ILE

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	2915/4355 (67%)	2906 (100%)	9 (0%)	86	83
1	B	2915/4355 (67%)	2907 (100%)	8 (0%)	86	83
1	C	2915/4355 (67%)	2907 (100%)	8 (0%)	86	83
1	D	2915/4355 (67%)	2906 (100%)	9 (0%)	86	83
2	E	76/88 (86%)	76 (100%)	0	100	100
2	F	76/88 (86%)	76 (100%)	0	100	100
2	G	76/88 (86%)	75 (99%)	1 (1%)	61	70
2	H	76/88 (86%)	76 (100%)	0	100	100
All	All	11964/17772 (67%)	11929 (100%)	35 (0%)	84	83

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	153	THR
1	A	186	VAL
1	A	459	LEU
1	A	686	VAL
1	A	1195	PHE
1	A	1538	THR
1	A	2330	PHE
1	A	2477	ILE
1	A	2997	ASN
1	B	153	THR
1	B	186	VAL
1	B	459	LEU
1	B	686	VAL
1	B	1195	PHE
1	B	2083	MET
1	B	2330	PHE
1	B	2997	ASN
1	C	153	THR
1	C	186	VAL
1	C	459	LEU
1	C	586	LEU
1	C	686	VAL
1	C	1195	PHE
1	C	2330	PHE
1	C	2997	ASN
1	D	153	THR
1	D	186	VAL
1	D	459	LEU
1	D	686	VAL
1	D	1195	PHE
1	D	1538	THR
1	D	2330	PHE
1	D	2477	ILE
1	D	2997	ASN
2	G	30	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (151) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	GLN
1	A	225	GLN
1	A	472	HIS
1	A	484	ASN

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Mol	Chain	Res	Type
1	A	496	ASN
1	A	506	HIS
1	A	607	ASN
1	A	608	HIS
1	A	658	ASN
1	A	669	GLN
1	A	932	ASN
1	A	969	ASN
1	A	971	GLN
1	A	1147	GLN
1	A	1264	ASN
1	A	1440	ASN
1	A	1524	ASN
1	A	1627	GLN
1	A	1632	HIS
1	A	1724	ASN
1	A	2599	ASN
1	A	2628	ASN
1	A	2703	GLN
1	A	2753	GLN
1	A	2801	ASN
1	A	2896	GLN
1	A	3317	HIS
1	A	3446	GLN
1	A	3811	ASN
1	A	3868	ASN
1	A	3931	GLN
1	A	4054	HIS
1	A	4190	ASN
1	A	4487	GLN
1	A	4578	HIS
1	A	4698	ASN
1	A	4932	HIS
1	A	4960	GLN
1	B	150	GLN
1	B	225	GLN
1	B	484	ASN
1	B	506	HIS
1	B	607	ASN
1	B	608	HIS
1	B	658	ASN
1	B	669	GLN

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Mol	Chain	Res	Type
1	B	716	ASN
1	B	932	ASN
1	B	971	GLN
1	B	1147	GLN
1	B	1440	ASN
1	B	1524	ASN
1	B	1632	HIS
1	B	1724	ASN
1	B	2599	ASN
1	B	2628	ASN
1	B	2703	GLN
1	B	2753	GLN
1	B	2801	ASN
1	B	2849	ASN
1	B	2896	GLN
1	B	3317	HIS
1	B	3446	GLN
1	B	3811	ASN
1	B	3868	ASN
1	B	3900	GLN
1	B	3904	ASN
1	B	3931	GLN
1	B	4054	HIS
1	B	4190	ASN
1	B	4487	GLN
1	B	4578	HIS
1	B	4698	ASN
1	B	4932	HIS
1	B	4960	GLN
1	C	150	GLN
1	C	225	GLN
1	C	484	ASN
1	C	506	HIS
1	C	607	ASN
1	C	608	HIS
1	C	658	ASN
1	C	669	GLN
1	C	716	ASN
1	C	932	ASN
1	C	969	ASN
1	C	971	GLN
1	C	1147	GLN

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Mol	Chain	Res	Type
1	C	1440	ASN
1	C	1524	ASN
1	C	1627	GLN
1	C	1632	HIS
1	C	1724	ASN
1	C	2599	ASN
1	C	2703	GLN
1	C	2753	GLN
1	C	2801	ASN
1	C	3317	HIS
1	C	3446	GLN
1	C	3811	ASN
1	C	3868	ASN
1	C	3900	GLN
1	C	3931	GLN
1	C	4054	HIS
1	C	4190	ASN
1	C	4487	GLN
1	C	4578	HIS
1	C	4698	ASN
1	C	4786	ASN
1	C	4960	GLN
1	D	150	GLN
1	D	225	GLN
1	D	484	ASN
1	D	506	HIS
1	D	607	ASN
1	D	608	HIS
1	D	658	ASN
1	D	669	GLN
1	D	932	ASN
1	D	969	ASN
1	D	971	GLN
1	D	1440	ASN
1	D	1524	ASN
1	D	1627	GLN
1	D	1632	HIS
1	D	1724	ASN
1	D	2599	ASN
1	D	2703	GLN
1	D	2753	GLN
1	D	2801	ASN

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Mol	Chain	Res	Type
1	D	3317	HIS
1	D	3446	GLN
1	D	3811	ASN
1	D	3868	ASN
1	D	3900	GLN
1	D	3931	GLN
1	D	4054	HIS
1	D	4190	ASN
1	D	4487	GLN
1	D	4578	HIS
1	D	4698	ASN
1	D	4862	GLN
1	D	4960	GLN
2	E	88	HIS
2	E	95	ASN
2	F	88	HIS
2	F	95	ASN
2	G	88	HIS
2	G	95	ASN
2	H	88	HIS
2	H	95	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

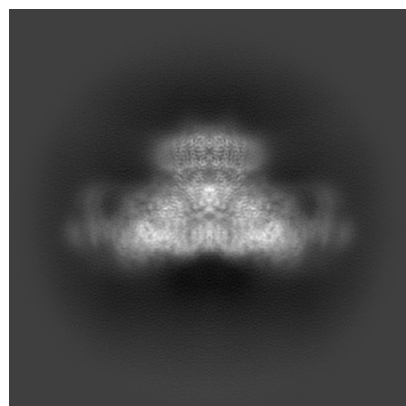
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27746. These allow visual inspection of the internal detail of the map and identification of artifacts.

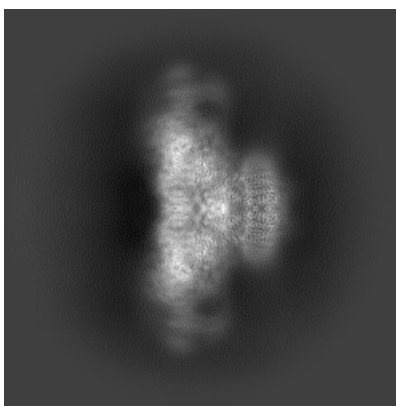
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

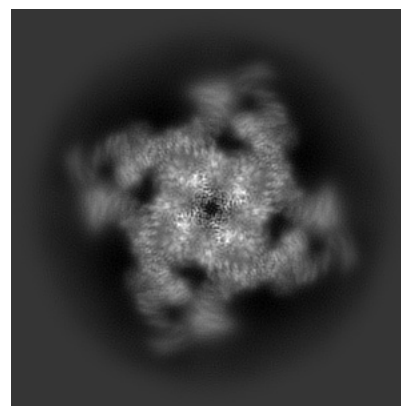
6.1.1 Primary map



X

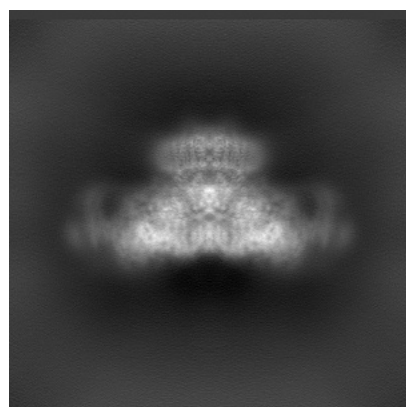


Y

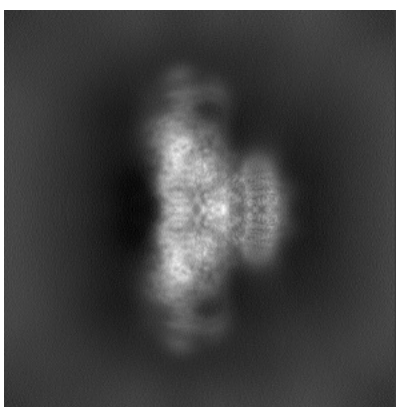


Z

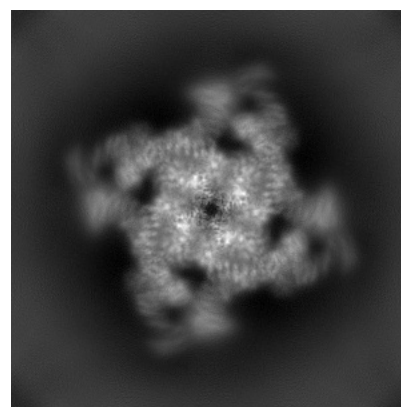
6.1.2 Raw map



X



Y

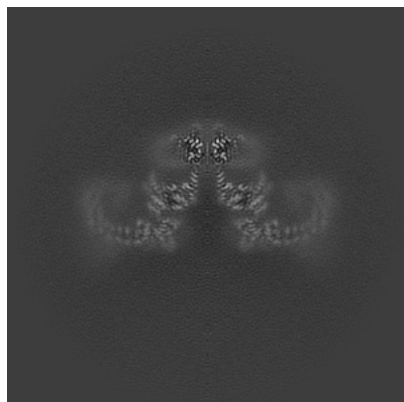


Z

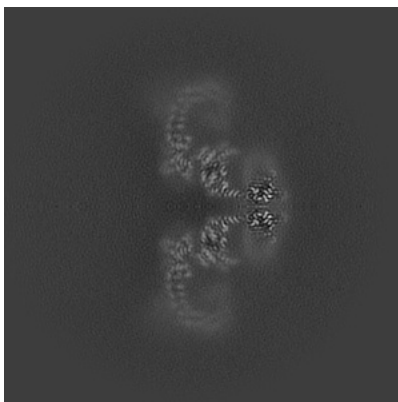
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

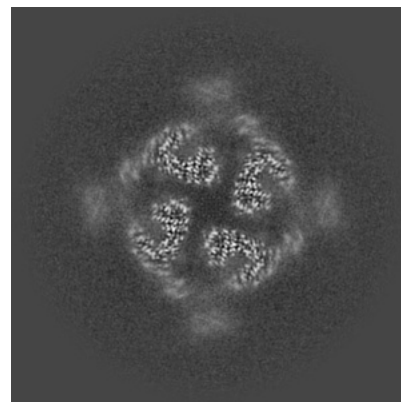
6.2.1 Primary map



X Index: 230

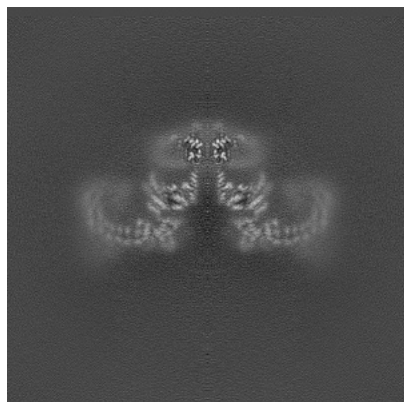


Y Index: 230

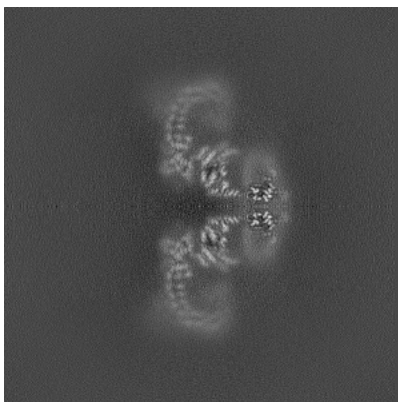


Z Index: 230

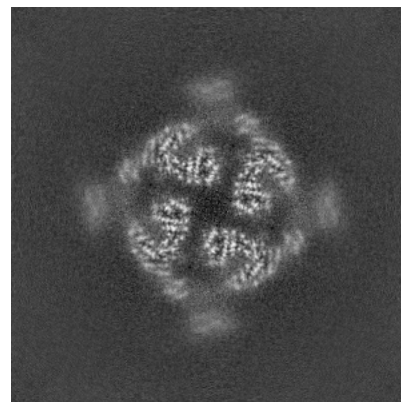
6.2.2 Raw map



X Index: 230



Y Index: 230

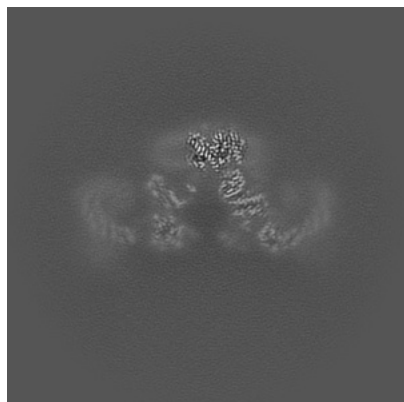


Z Index: 230

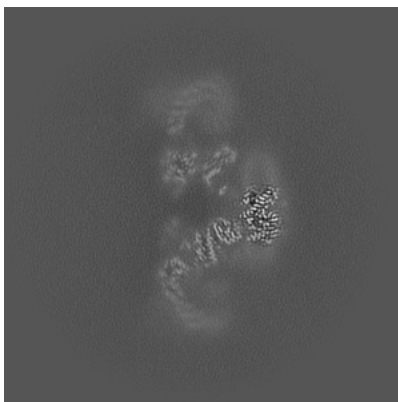
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

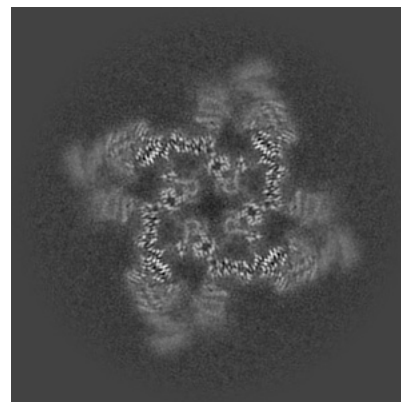
6.3.1 Primary map



X Index: 222

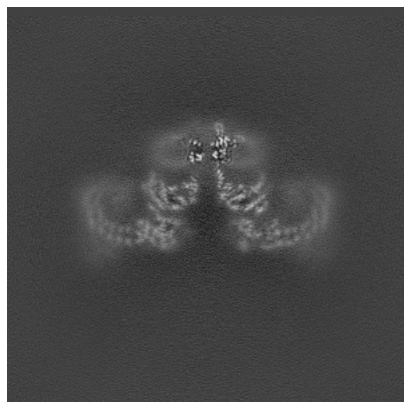


Y Index: 222

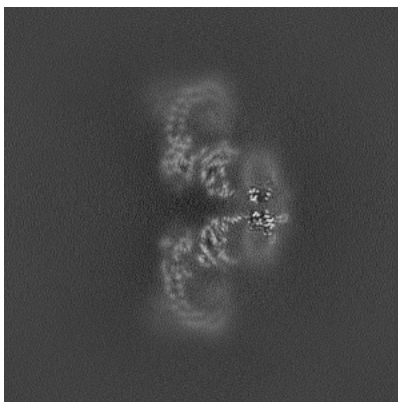


Z Index: 203

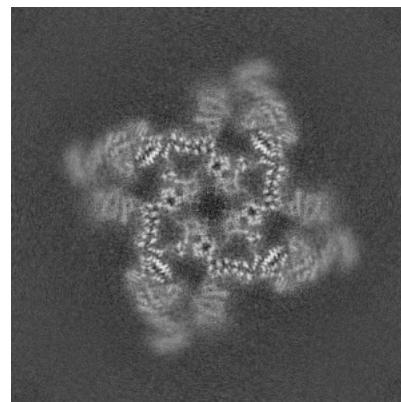
6.3.2 Raw map



X Index: 228



Y Index: 228

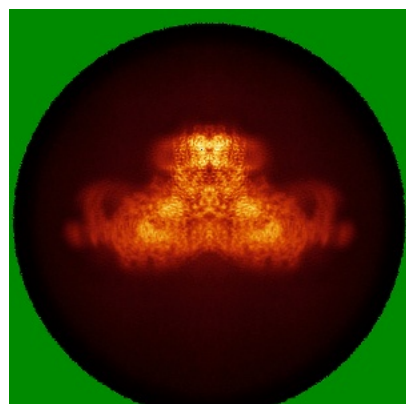


Z Index: 203

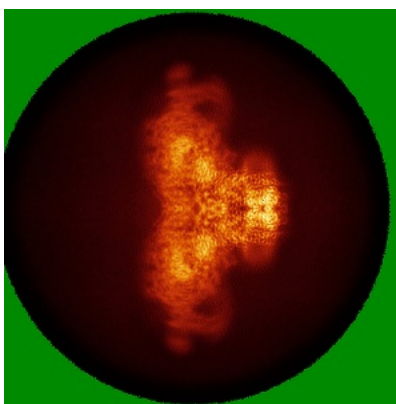
The images above show the largest variance slices of the map in three orthogonal directions.

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

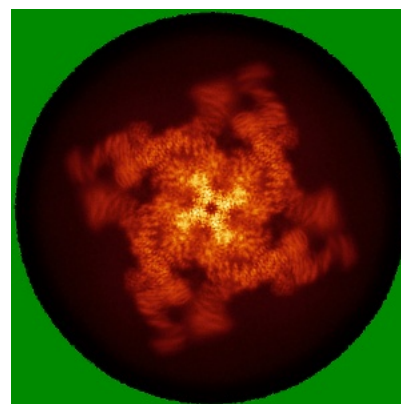
6.4.1 Primary map



X

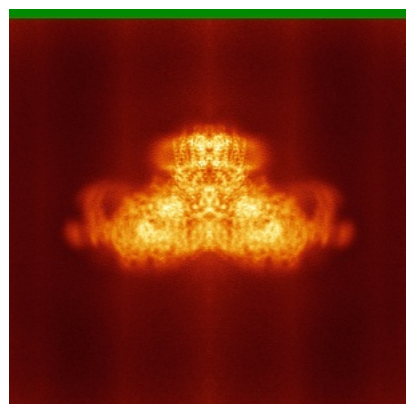


Y

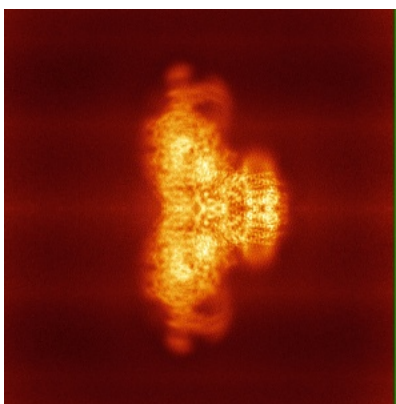


Z

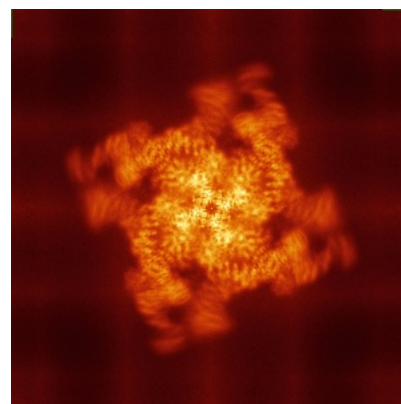
6.4.2 Raw map



X



Y

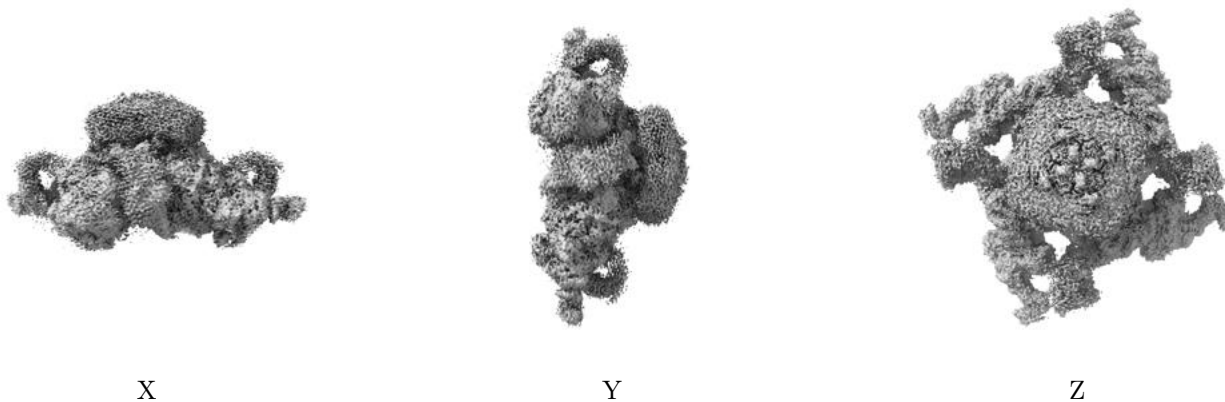


Z

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.

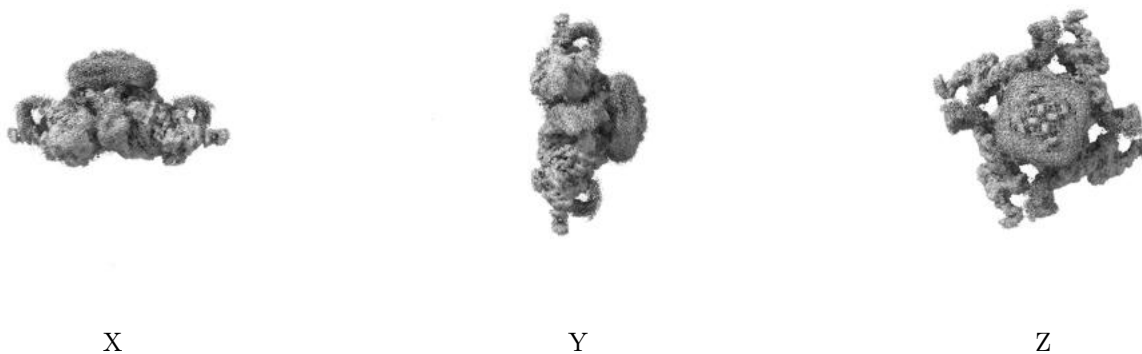
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. 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.

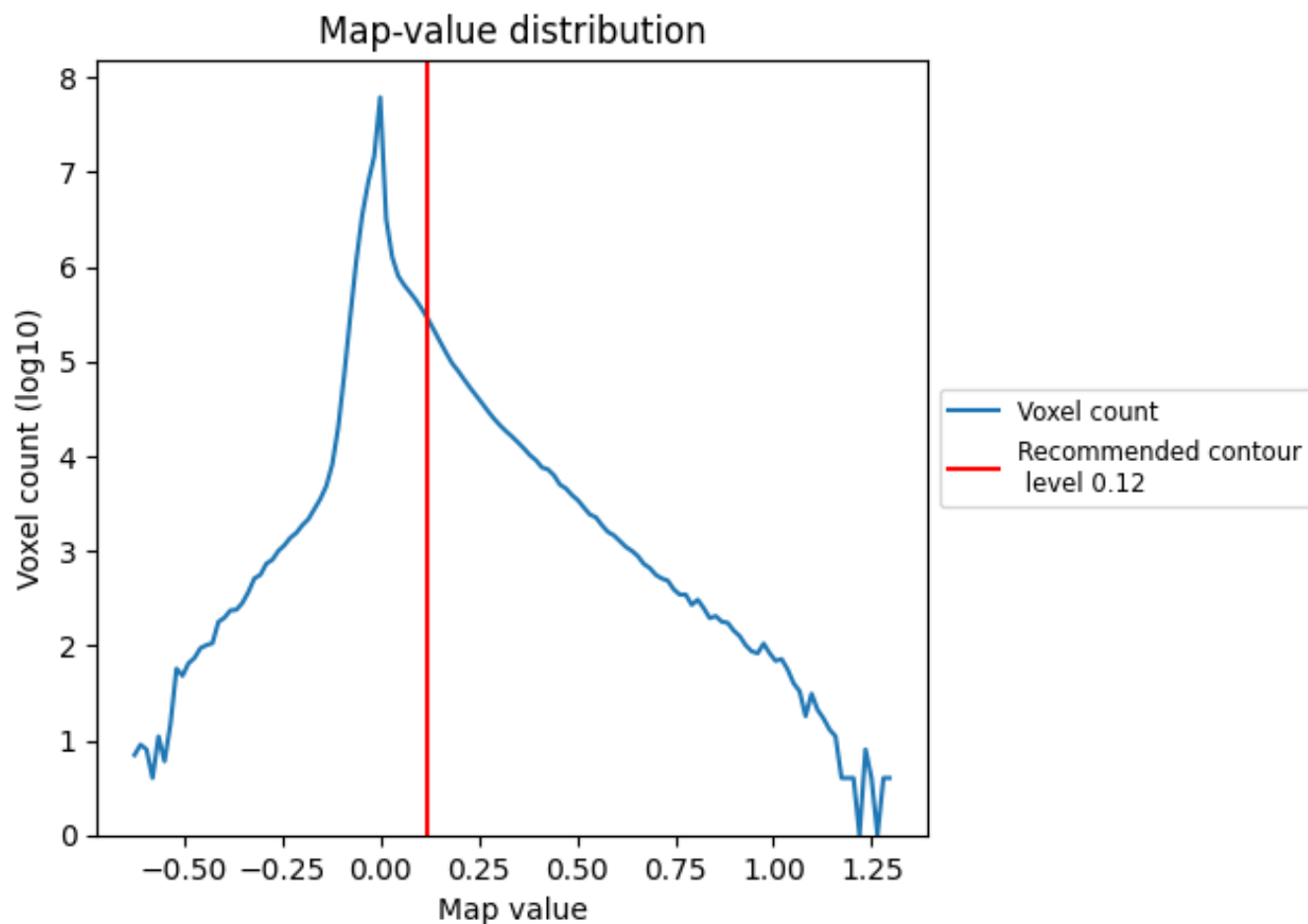
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

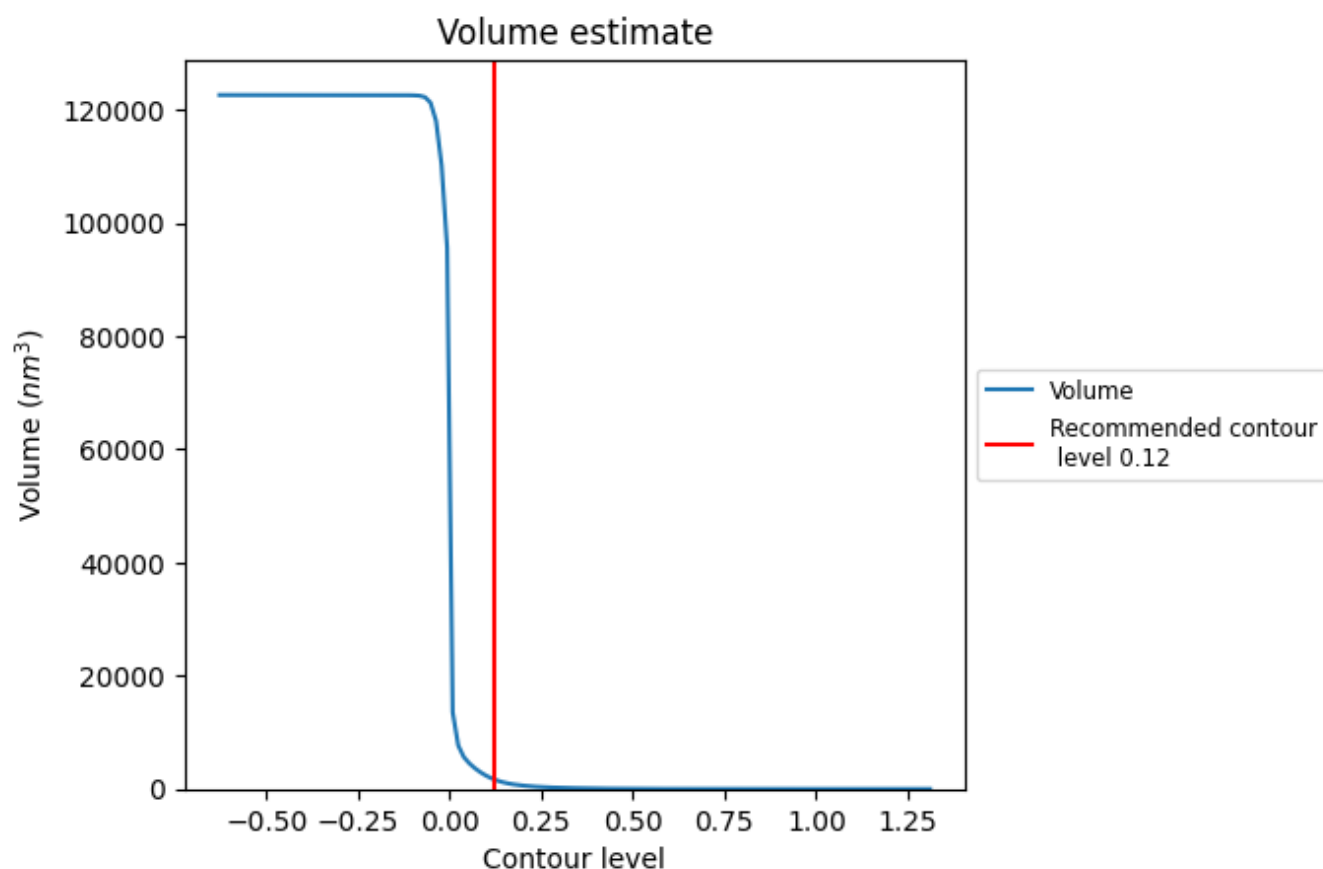
This section contains the results of statistical analysis of the map.

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.

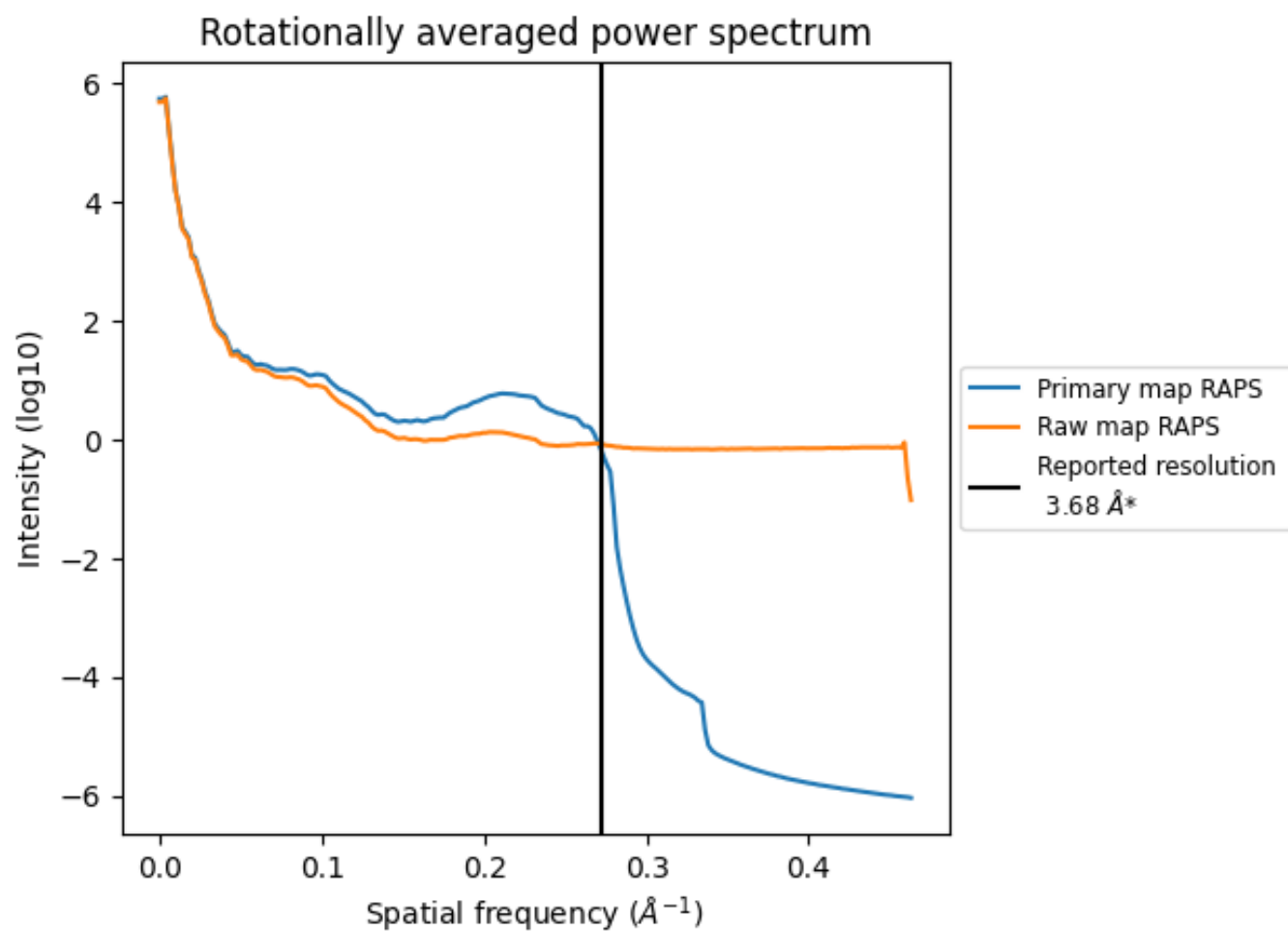
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1734 nm^3 ; this corresponds to an approximate mass of 1567 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 ⓘ

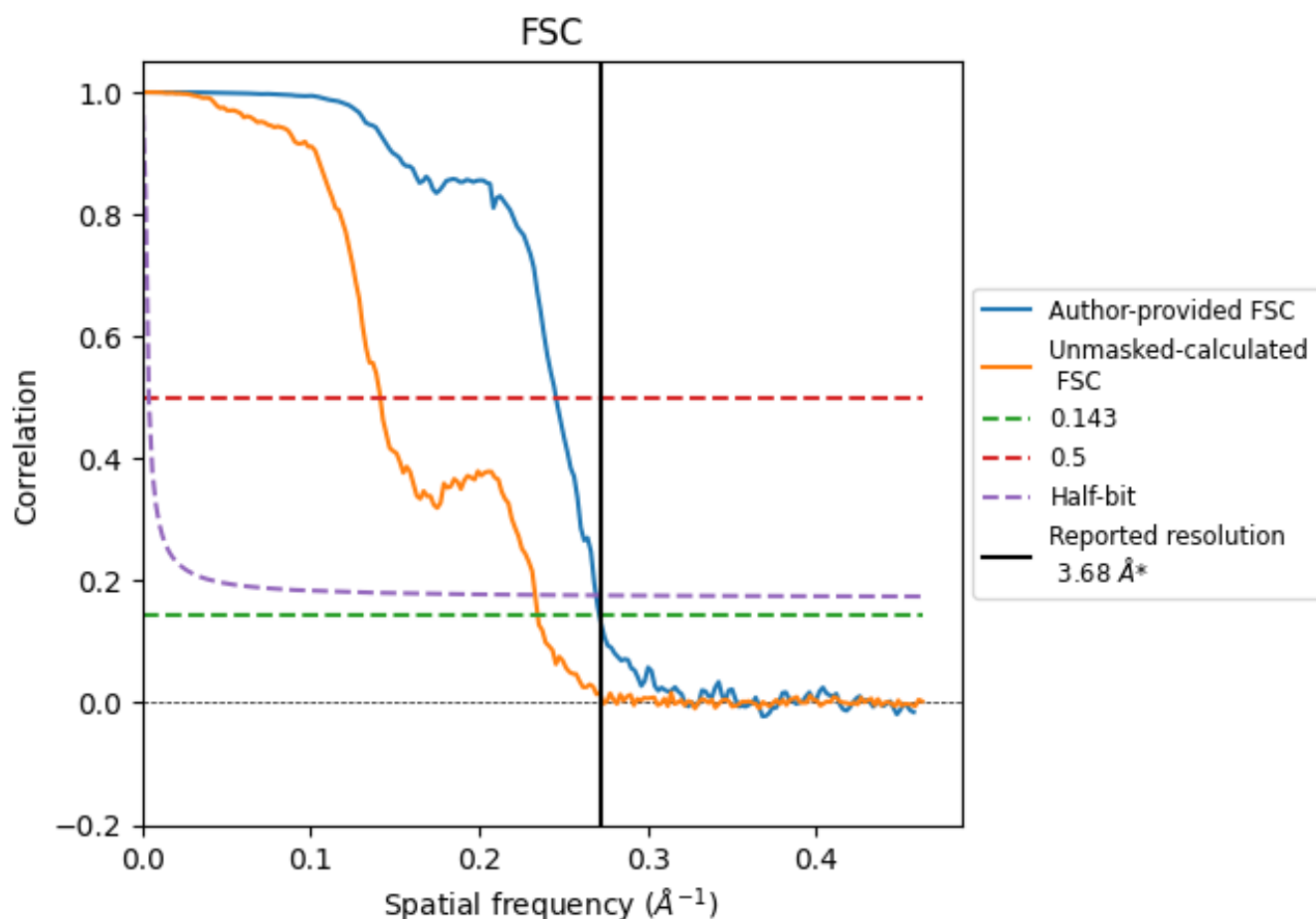


*Reported resolution corresponds to spatial frequency of 0.272 Å⁻¹

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 0.272 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

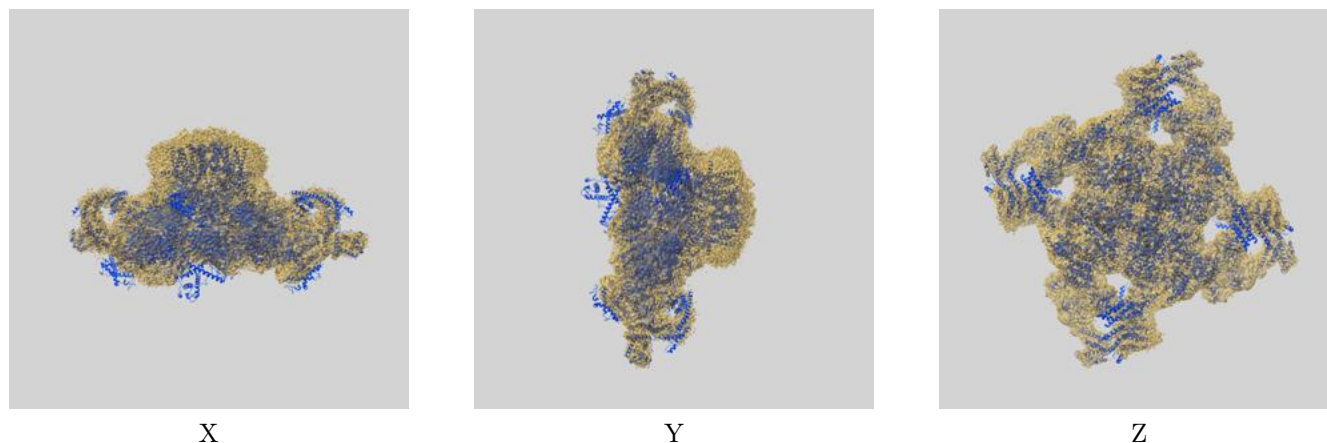
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.68	-	-
Author-provided FSC curve	3.68	4.07	3.71
Unmasked-calculated*	4.26	7.08	4.29

*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 4.26 differs from the reported value 3.68 by more than 10 %

9 Map-model fit [i](#)

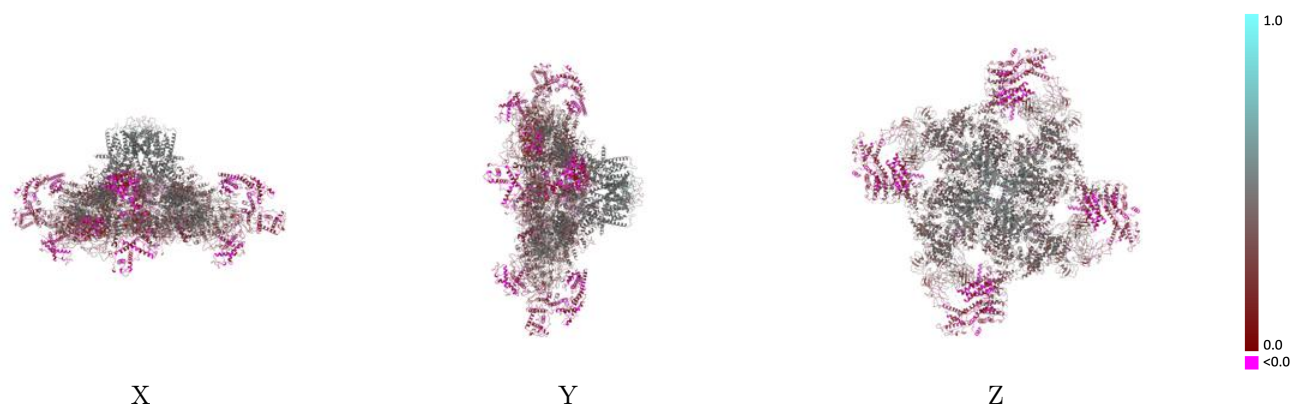
This section contains information regarding the fit between EMDB map EMD-27746 and PDB model 8DVV. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



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

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

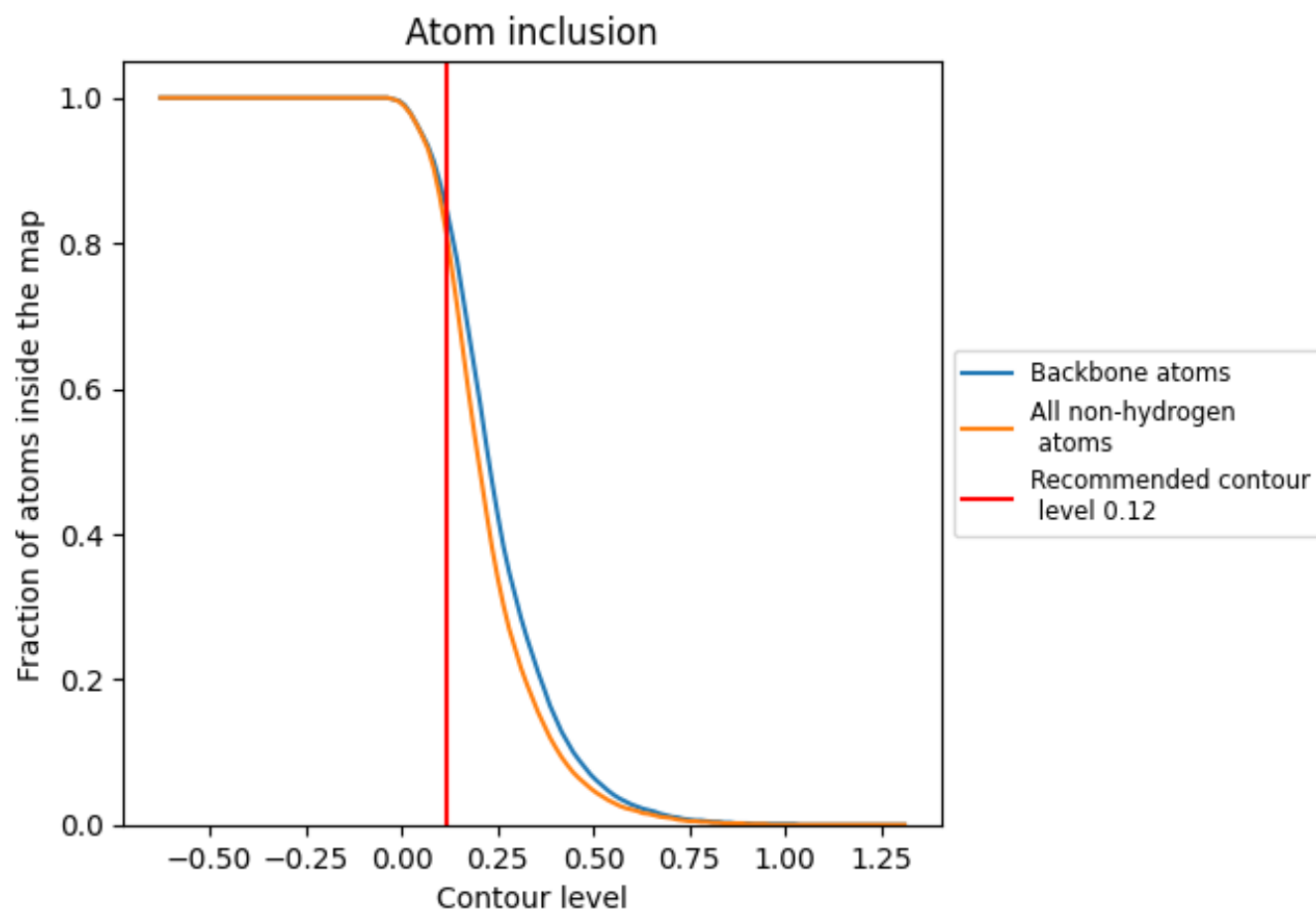


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8050	0.3180
A	0.8010	0.3150
B	0.8010	0.3160
C	0.8010	0.3160
D	0.8010	0.3160
E	0.9510	0.3910
F	0.9510	0.3940
G	0.9520	0.3930
H	0.9520	0.3910

1.0

0.0

<0.0