



Full wwPDB EM Validation Report ⓘ

Oct 20, 2025 – 03:56 PM EDT

PDB ID : 9DGR / pdb_00009dgr
EMDB ID : EMD-46845
Title : Composite structure of dynein-dynactin on microtubules
Authors : Rao, Q.; Chai, P.; Zhang, K.
Deposited on : 2024-09-03
Resolution : 15.00 Å(reported)

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:

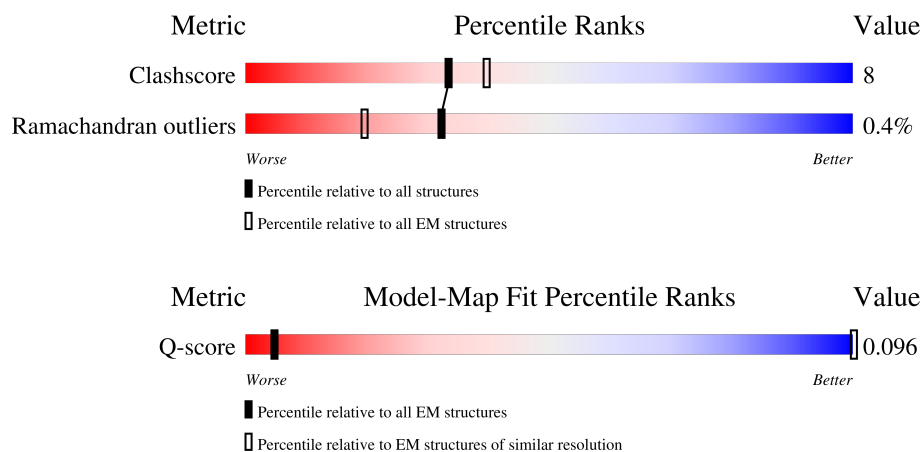
EMDB validation analysis : 0.0.1.dev129
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

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 15.00 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.



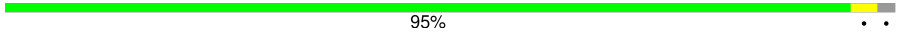
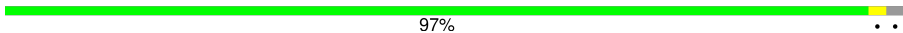
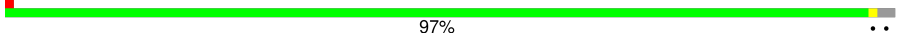
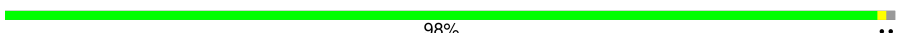











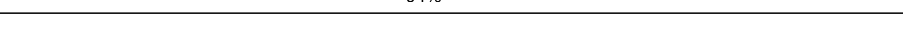





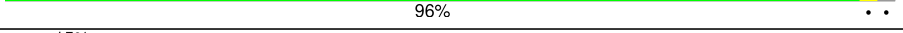
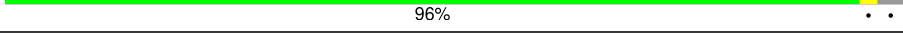


Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Q-score	-	25397	37 (14.50 - 15.50)

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	376	 95% ..
1	B	376	 96% ..
1	C	376	 98% .
1	D	376	 95% ..
1	E	376	 96% ..


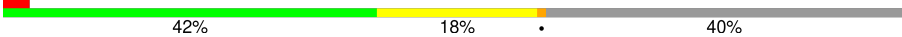
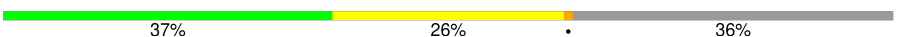






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Mol	Chain	Length	Quality of chain
1	F	376	
1	G	376	
1	I	376	
2	H	375	
3	J	417	
4	K	286	
5	L	272	
6	M	405	
6	N	405	
6	P	405	
6	Q	405	
7	O	186	
7	R	186	
8	U	190	
9	V	182	
10	W	1281	
10	Z	1281	
11	Y	467	
12	e	4646	
12	f	4646	
12	m	4646	
12	n	4646	
13	g	612	
13	h	612	
13	o	612	

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Mol	Chain	Length	Quality of chain
13	p	612	 56%42%
14	i	492	 42%18%40%
14	j	492	 37%26%36%
14	q	492	 60%37%
14	r	492	 57%40%
15	k	96	 66%31%
15	l	96	 67%30%
15	s	96	 97%
15	t	96	 97%

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 131638 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 Alpha-centractin.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	370	Total	C	N	O	0	0
			1822	1082	370	370		
1	B	370	Total	C	N	O	0	0
			1822	1082	370	370		
1	C	375	Total	C	N	O	0	0
			1847	1097	375	375		
1	D	370	Total	C	N	O	0	0
			1822	1082	370	370		
1	E	370	Total	C	N	O	0	0
			1822	1082	370	370		
1	F	370	Total	C	N	O	0	0
			1822	1082	370	370		
1	G	370	Total	C	N	O	0	0
			1822	1082	370	370		
1	I	370	Total	C	N	O	0	0
			1822	1082	370	370		

- Molecule 2 is a protein called Actin, cytoplasmic 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	H	370	Total	C	N	O	0	0
			1822	1082	370	370		

- Molecule 3 is a protein called Actin-related protein 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	J	379	Total	C	N	O	0	0
			1868	1110	379	379		

- Molecule 4 is a protein called F-actin-capping protein subunit alpha-1.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	K	278	Total	C	N	O	0	0
			1378	822	278	278		

- Molecule 5 is a protein called F-actin-capping protein subunit beta.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	L	269	Total	C	N	O	0	0
			1327	789	269	269		

- Molecule 6 is a protein called Dynactin subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	M	340	Total	C	N	O	0	0
			1689	1009	340	340		
6	N	280	Total	C	N	O	0	0
			1394	834	280	280		
6	P	325	Total	C	N	O	0	0
			1612	962	325	325		
6	Q	343	Total	C	N	O	0	0
			1707	1021	343	343		

- Molecule 7 is a protein called Dynactin subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	O	179	Total	C	N	O	0	0
			888	530	179	179		
7	R	170	Total	C	N	O	0	0
			844	504	170	170		

- Molecule 8 is a protein called Dynactin subunit 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	U	167	Total	C	N	O	0	0
			822	488	167	167		

- Molecule 9 is a protein called Dynactin subunit 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	V	179	Total	C	N	O	0	0
			881	523	179	179		

- Molecule 10 is a protein called Dynactin subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	W	152	Total	C	N	O	0	0
			754	450	152	152		
10	Z	192	Total	C	N	O	0	0
			952	568	192	192		

- Molecule 11 is a protein called Dynactin subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	Y	410	Total	C	N	O	0	0
			2038	1218	410	410		

- Molecule 12 is a protein called Cytoplasmic dynein 1 heavy chain 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	e	4569	Total	C	N	O	0	0
			22644	13506	4569	4569		
12	f	4565	Total	C	N	O	0	0
			22625	13495	4565	4565		
12	m	4562	Total	C	N	O	0	0
			18883	9759	4562	4562		
12	n	4526	Total	C	N	O	0	0
			18703	9651	4526	4526		

- Molecule 13 is a protein called Cytoplasmic dynein 1 intermediate chain 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	g	358	Total	C	N	O	0	0
			1767	1051	358	358		
13	h	358	Total	C	N	O	0	0
			1767	1051	358	358		
13	o	358	Total	C	N	O	0	0
			1767	1051	358	358		
13	p	358	Total	C	N	O	0	0
			1767	1051	358	358		

- Molecule 14 is a protein called Dynein light intermediate chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	i	297	Total	C	N	O	0	0
			1472	878	297	297		
14	j	314	Total	C	N	O	0	0
			1555	927	314	314		

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Mol	Chain	Residues	Atoms				AltConf	Trace
14	q	309	Total	C	N	O	0	0
			1241	623	309	309		
14	r	297	Total	C	N	O	0	0
			1193	599	297	297		

- Molecule 15 is a protein called Dynein light chain roadblock.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	k	93	Total	C	N	O	0	0
			462	276	93	93		
15	l	93	Total	C	N	O	0	0
			462	276	93	93		
15	s	93	Total	C	N	O	0	0
			374	188	93	93		
15	t	93	Total	C	N	O	0	0
			374	188	93	93		

- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
16	Y	3	Total	Zn	0
			3	3	

- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
17	m	1	Total	Mg	0
			1	1	
17	n	1	Total	Mg	0
			1	1	

3 Residue-property plots [i](#)

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

- Molecule 1: Alpha-centractin

Chain A:  95%



- Molecule 1: Alpha-centractin

Chain B:  96%



- Molecule 1: Alpha-centractin

Chain C:  98%



- Molecule 1: Alpha-centractin

Chain D:  95%



- Molecule 1: Alpha-centractin

Chain E:  96%



- Molecule 1: Alpha-centractin

Chain F:  95%



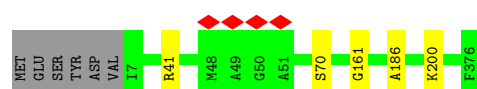
- Molecule 1: Alpha-centractin

Chain G:  97%



- Molecule 1: Alpha-centractin

Chain I:  97%



- Molecule 2: Actin, cytoplasmic 1

Chain H:  98%



- Molecule 3: Actin-related protein 10

Chain J:  89%



- Molecule 4: F-actin-capping protein subunit alpha-1

Chain K:  92%




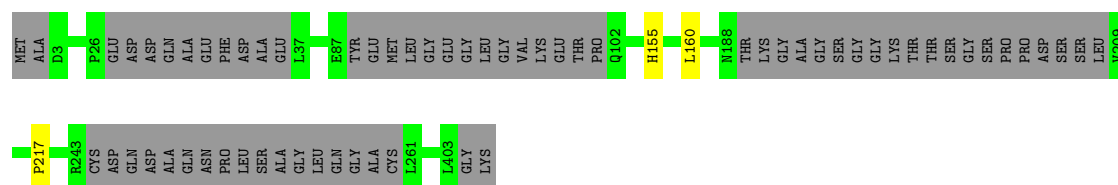
- Molecule 5: F-actin-capping protein subunit beta

Chain L:  96%



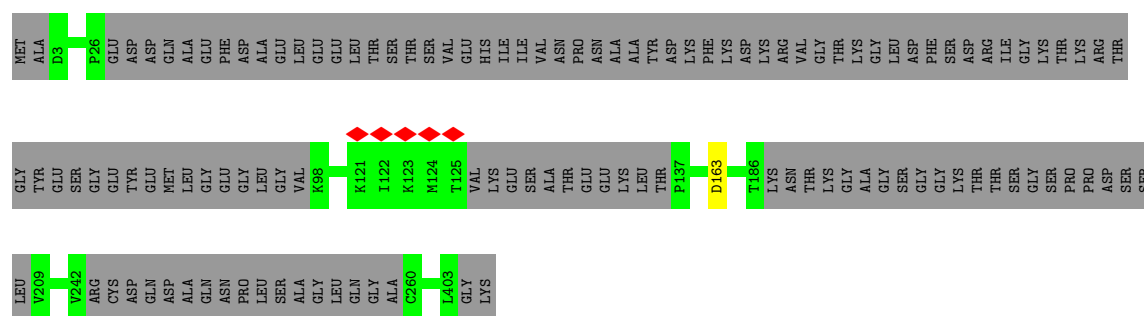
- Molecule 6: Dynactin subunit 2

Chain M: 




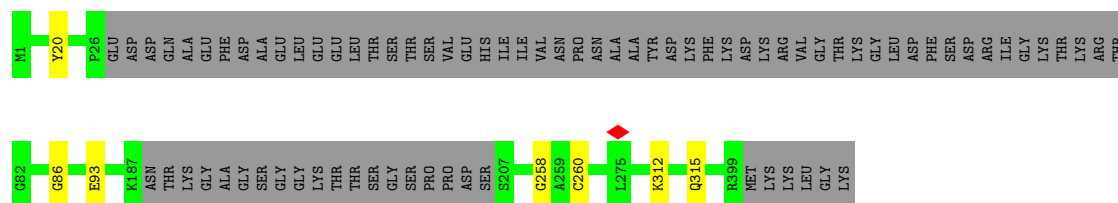
• Molecule 6: Dynactin subunit 2

Chain N: 




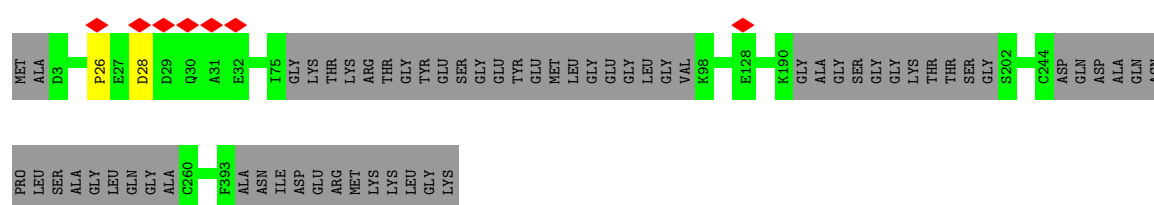
• Molecule 6: Dynactin subunit 2

Chain P: 



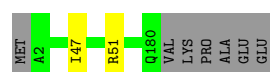
• Molecule 6: Dynactin subunit 2

Chain Q: 

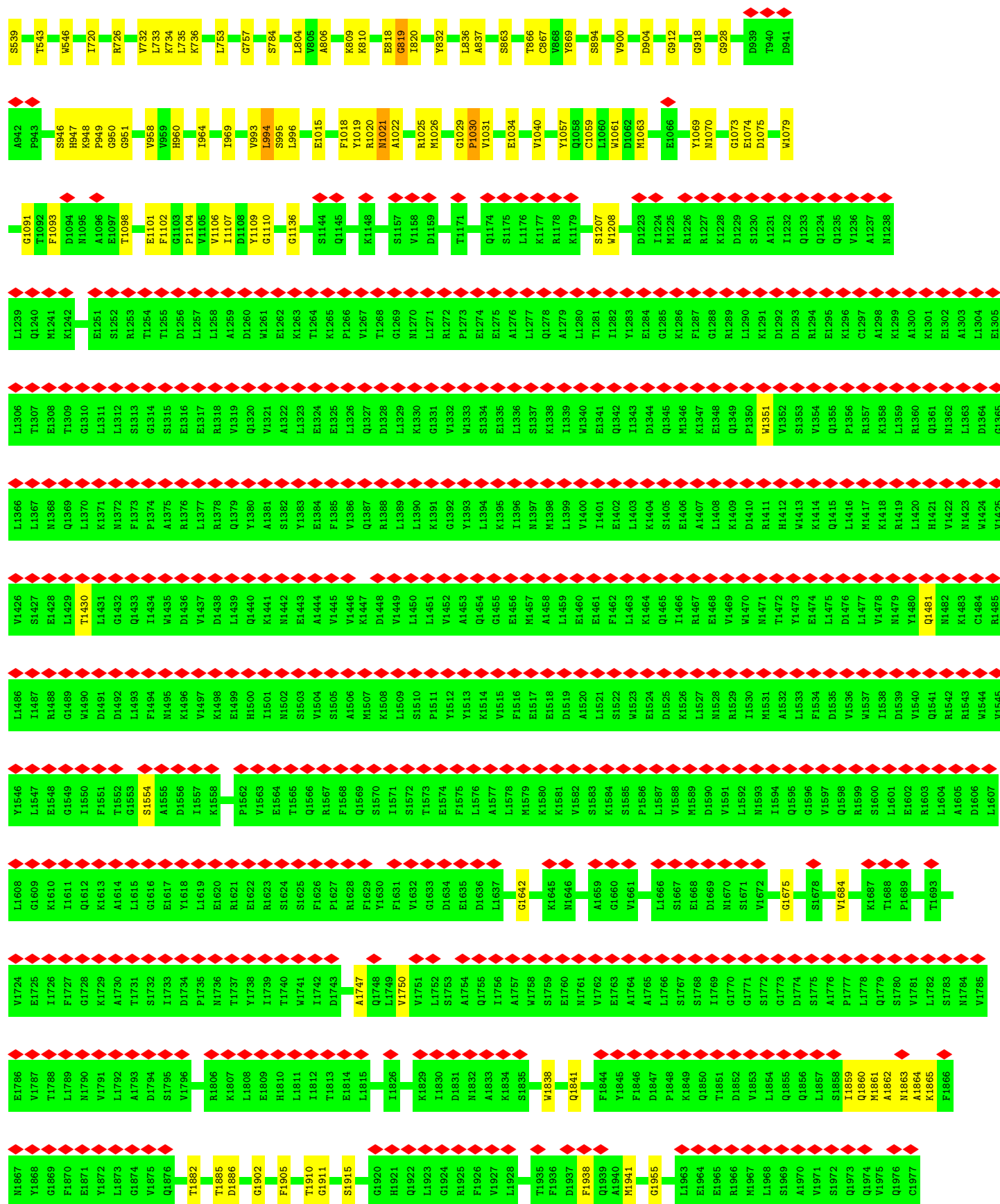


• Molecule 7: Dynactin subunit 3

Chain O: 



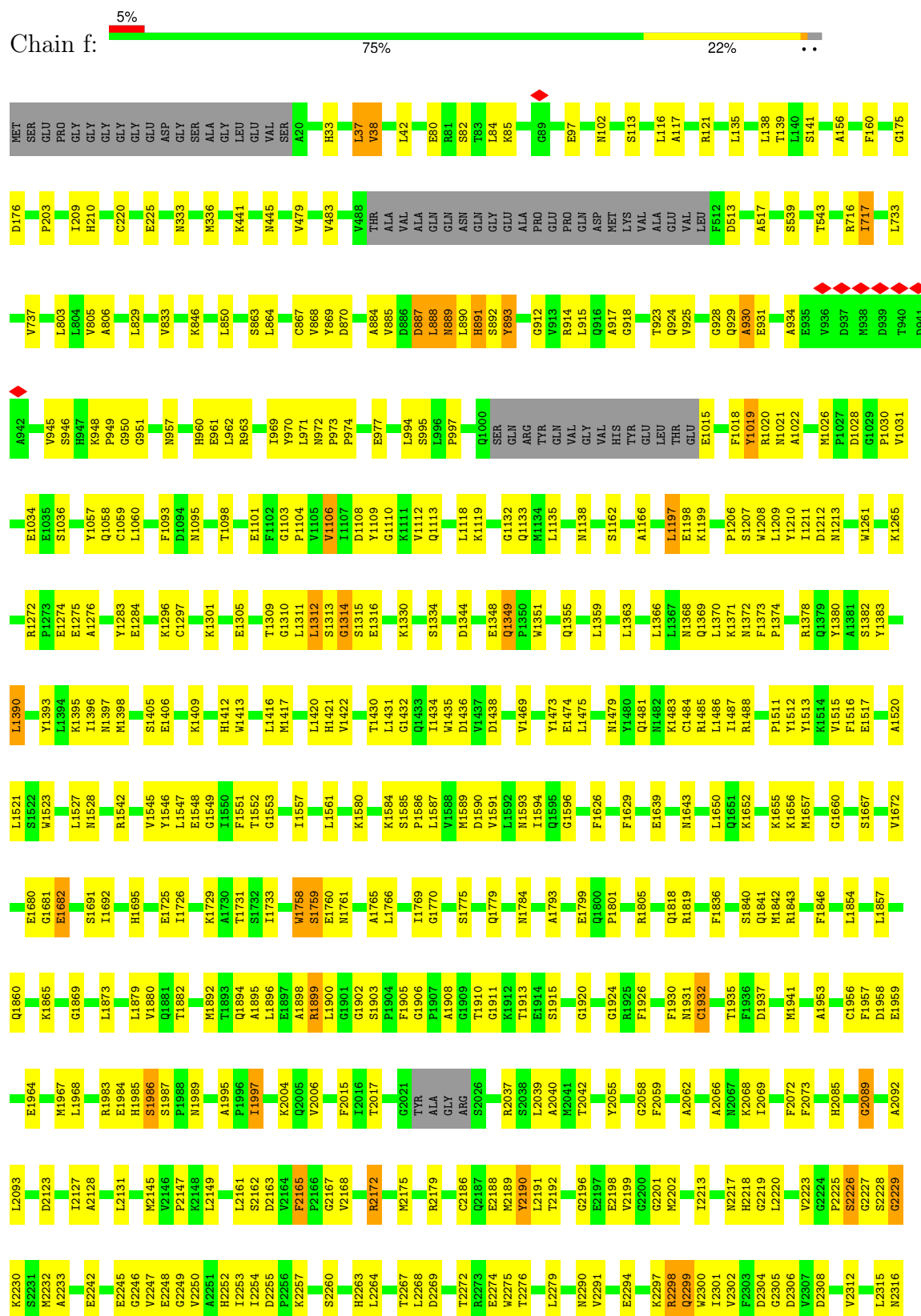




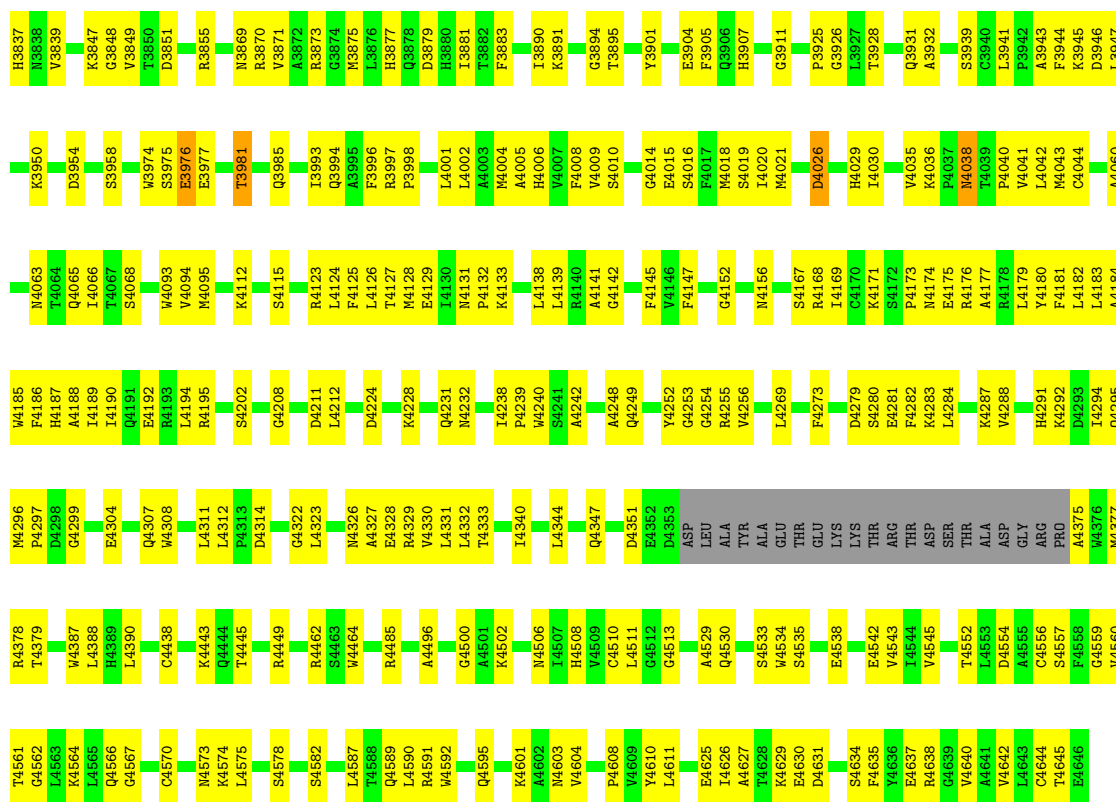


C4556	S4557	F4558	C4559	V4560	T4561	C4562	L4563	K4564	C4570	S4571	N4572	N4573	K4574	L4575	S4576	L4577	L4585	P4586	L4587	T4588	K4589	K4590	L4591	Q4595	A4602	N4603	V4604	V4605	T4606	V4622	D4623	F4624	E4625	I4626	A4627	T4628	E4629	E4630	D4631	F4632	R4633	S4634	F4635	V4636	E4637	C4638	C4639	V4640	T4645	E4646								
R4378	T4379	T4401	V4402	D4403	N4404	I4405	E4439	N4446	G4458	I4459	M4473	T4474	A4496	A4497	S4498	G4499	G4500	A4501	K4502	E4503	L4504	K4505	L4511	G4512	G4513	Y4527	V4528	A4529	Q4530	A4531	N4532	S4533	M4534	S4535	L4536	E4537	E4538	L4539	I4544	V4545	T4546	T4547	S4548	Q4549	S4550	A4551	T4552	L4553	D4554	A4555								
Q4307	V4308	V4309	E4310	L4311	D4312	P4313	D4314	T4315	Q4316	T4317	P4318	S4319	V4320	L4321	G4322	L4323	A4324	N4325	N4326	A4327	L4331	L4332	T4333	T4334	Q4335	G4336	V4337	D4338	M4339	L4340	N4343	D4353	ASP	LEU	ALA	TYR	ALA	GLU	THR	GLU	LYS	THR	THR	THR	ASP	SER	THR	ALA	ASP	GLY	ARG	PRO	A4375	V4376	N4377			
W4222	D4225	T4226	A4227	K4228	C4229	R4230	Q4231	N4232	I4233	S4234	P4235	D4236	K4237	L4238	L4246	M4247	A4248	Q4249	S4250	I4251	Y4252	G4253	C4254	D4255	T4274	S4277	F4278	D4279	S4280	E4281	F4282	K4283	L4284	A4285	C4286	K4287	V4288	D4289	Q4290	H4291	K4292	D4293	I4294	Q4295	M4296	P4297	D4298	G4299	T4300	R4301	R4302	E4303	F4304	F4305	V4306			
P4118	H4119	A4120	C4121	F4122	R4123	L4124	F4125	L4126	T4127	M4128	E4129	I4130	N4131	P4132	K4133	V4134	A4141	V4146	F4147	P4150	P4151	G4152	V4166	S4167	K4171	P4172	S4173	A4177	R4178	L4179	Y4180	F4181	L4182	L4183	A4184	W4185	F4186	H4187	A4188	I4189	I4190	Q4191	E4192	R4193	L4194	R4195	G4208	V4219	D4220	T4221								
S4052	G4053	H4054	V4055	E4056	D4057	L4058	A4059	A4060	E4061	Q4062	N4063	T4064	Q4065	L4066	T4067	S4068	A4069	A4070	L4071	G4072	S4073	A4074	P4075	G4076	F4077	N4078	Q4079	A4080	D4081	K4082	A4083	L4084	N4085	T4086	A4087	V4088	K4089	S4090	G4091	R4092	V4093	V4094	M4095	L4096	K4097	N4098	V4099	H4100	L4101	A4102	P4103	G4104	V4105	K4112	S4115	L4116	Q4117	
E3977	N3978	P3979	A3980	T3981	P3982	L3983	R3873	G3874	N3875	L3876	H3880	V3886	G3887	E3888	P3889	R4000	L4001	L4002	A4005	H4006	V4007	F4008	V4009	S4010	T4011	N4012	G4014	E4015	M4018	S4019	Q4023	P4024	L4025	D4026	L4027	T4028	H4029	I4030	V4031	D4032	T4033	E4034	A4035	K4036	P4037	M4038	T4039	L4042	M4043	C4044	S4045	V4046	P4047					
T3860	K3861	D3862	L3863	R3873	G3874	N3875	L3876	H3880	V3886	G3887	E3888	P3889	Q3906	R3910	K3923	I3924	P3925	G3926	L3927	T3928	V3929	A3932	E3933	A3934	P3942	A3943	K3950	V3951	Q3952	A3953	D3954	E3955	Q3956	P3957	S3958	T3959	V3960	S3964	S3965	E3967	Q3968	T3969	V3970	P3971	H3972	S3975	E3976											
K3774	R3775	E3776	A3777	E3778	E3779	V3780	T3781	R3782	K3783	V3784	E3785	E3786	T3787	D3788	T3789	V3790	L3791	L3792	E3793	V3794	E3795	T3796	V3797	T3798	Q3800	E3816	H3822	F3823	L3824	Y3827	Y3836	H3837	N3838	V3839	L3840	Y3841	E3842	N3843	P3844	N3845	L3846	K3847	G3848	V3849	T3850	D3851	H3852	T3853	Q3854	R3855	L3856	C3857	I3858	I3859				
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S3554	N3555	A3556	D3557	E3558	R3559	L3560	R3561	A3564	P3587	L3588	I3589	T3600	M3601	Y3604	K3605	T3612	D3617	A3618	F3619	E3624	S3625	A3626	L3627	R3628	F3629	G3630	N3631	P3632	V3635	Q3636	D3637	G3657	Q3658	G3665	S3672	P3673	F3675	V3676	I3677	F3678	L3679	S3680	T3685	T3687	T3688	T3689	E3771	N3772	L3773									
S3475	T3476	A3477	L3478	L3479	K3480	S3481	L3482	S3483	A3484	E3485	R3486	E3487	R3488	W3489	A3490	K3491	T3492	S3493	A3494	T3495	F3496	K3497	N3498	Q3499	M3500	S3501	T3502	L3503	A3504	S3510	A3511	A3512	F3513	G3518	D3521	Q3522	M3524	R3525	Q3526	H3536	L3536	Q3537	Q3538	A3539	N3540	F3543	D3546	I3547	A3548	R3549	T3550	E3551						

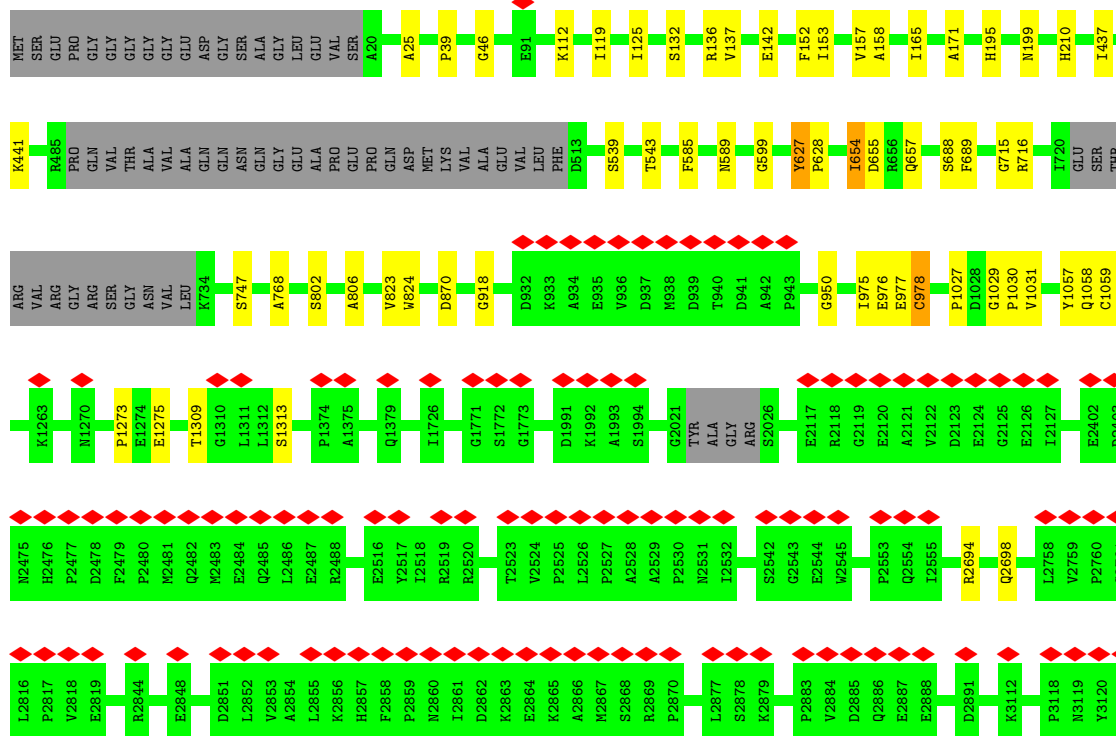
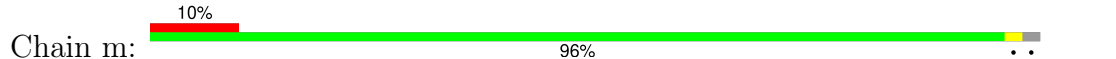
● Molecule 12: Cytoplasmic dynein 1 heavy chain 1

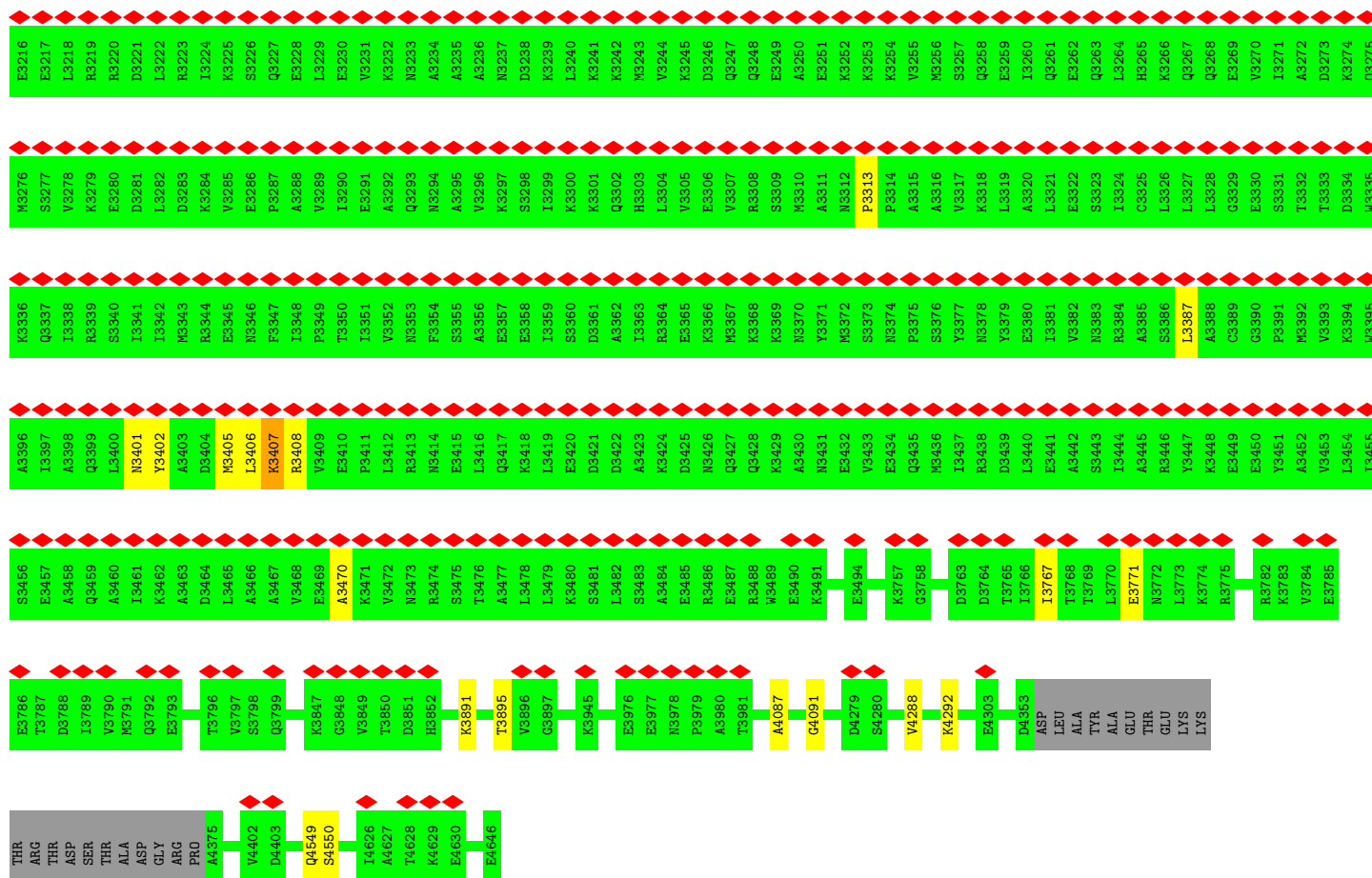


R3682	D3683	P3690	D3691	L3692	C3693	S3694	R3695	L3685	L3688	D3691	N3602	K3605	T3612	S3613	D3617	A3618	F3619	R3620	K3621	N3622	A3626	L3627	G3630	N3631	Q3636	G3758	R3759	I3760	L3761	D3762	D3763	D3764	L3773	R3774	R3775	E3776	G3657	G3658	R3659	V3660	L3661	D3670	L3671	S3672	L3679	S3680	T3681												
L3455	S3456	E3457	A3458	Q3459	A3460	I3461	K3462	A3463	V3472	E3482	S3483	A3484	V3489	E3490	K3491	T3492	S3493	N3498	Q3499	M3500	G3505	D3506	L3509	F3513	I3514	A3515	R3516	A3517	G3518	Y3519	F3520	D3521	R3525	L3528	F3529	Q3542	F3543	E3551	S3554	N3555	A3556	D3557	E3558	R3559	W3562														
S3566	L3567	N3576	A3577	L3580	R3585	L3588	D3591	N3602	K3605	T3612	S3613	D3617	A3618	F3619	R3620	K3621	N3622	A3626	L3627	G3630	N3631	Q3636	G3758	R3759	I3760	L3761	D3762	D3763	D3764	L3645	L3649	R3655	T3656	L3658	F3659	G3657	G3658	R3659	V3660	L3661	D3670	L3671	S3672	L3679	S3680	T3681													
R3682	D3683	P3690	D3691	L3692	C3693	S3694	R3695	L3685	L3688	D3691	N3602	K3605	T3612	S3613	D3617	A3618	F3619	R3620	K3621	N3622	A3626	L3627	G3630	N3631	Q3636	G3758	R3759	I3760	L3761	D3762	D3763	D3764	L3773	R3774	R3775	E3776	G3657	G3658	R3659	V3660	L3661	D3670	L3671	S3672	L3679	S3680	T3681												
P2425	Y2426	P2427	T2428	P2429	M2430	G2431	S2434	L2435	E2438	H2439	V2439	K2442	T2441	L2443	M2473	P2480	M2481	Q2482	Q2485	L2486	Y2489	L2499	W2500	S2501	L2502	S2503	G2504	D2505	V2505	T2518	T2522	P2533	D2536	Y2537	E2538	G2543	P2547	W2548	K2551	V2552	T2555	E2556	V2557	E2558	T2559	D2566	V2569												
P2570	L2591	L2593	G2595	P2596	P2597	G2598	R2705	S2706	K2706	Q2707	K2601	T2602	M2603	T2604	P2613	D2614	S2615	E2616	V2617	V2618	G2619	N2621	F2622	S2623	S2624	A2625	F2635	Y2638	Y2641	T2644	N2645	N2646	V2649	P2652	V2653	M2755	L2756	L2659	L2659	V2660	L2661	F2662	C2663	L2668	N2669	C2675	T2676												
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F2900	Y2901	E2902	E2903	F2912	L2916	R2924	L2925	F2926	H2927	Q2928	P2929	Q2930	T2931	H2932	L2933	I2936	G2937	K2943	T2944	T2945	A2951	W2952	G2955	L2956	V2958	I2961	K2962	V2963	T2968	F2972	R2981	R2982	S2983	K2986	N2987	E2988	K2989	L2990	F2992	E3006	T3010	L3011																	
E3016	G3019	D3024	A3027	A3037	G3041	L3042	D3045	V3058	K3060	N3061	L3062	H3063	V3064	S3065	F3066	T3067	K3068	N3069	P3070	F3086	G3089	V3090	L3091	N3092	K3093	F3094	G3095	S3098	L3102	Y3103	Q3104	G3106	K3107	E3108	F3109	T3110	S3111	V3129	Y3130	D3131	L3132	L3133	P3134	P3136															
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W3335	K3336	Q3337	I3338	R3339	S3340	I3341	I3342	M3343	R3344	E3345	N3346	F3347	I3348	P3349	T3350	I3351	V3352	N3353	F3354	S3355	A3356	E3357	I3358	I3359	D3361	A3362	I3363	R3364	E3365	K3366	M3367	K3368	K3369	N3370	V3371	N3372	S3373	N3374	P3375	P3376	V3377	N3378	V3379	E3380	I3381	V3382	N3383	R3384	A3385	S3386	L3387	A3388	C3389	G3390	P3391	M3392	V3393	K3394	
W3395	A3396	I3397	A3398	Q3399	L3400	I3401	V3402	A3403	D3404	M3405	L3406	K3407	R3408	V3409	E3410	P3411	L3412	R3413	I3414	E3415	L3416	Q3417	K3418	L3419	E3420	D3421	D3422	A3423	K3424	D3425	I3426	Q3427	Q3428	K3429	A3430	R3431	E3432	V3433	E3434	Q3435	H3436	I3437	R3438	D3439	L3440	E3441	A3442	S3443	T3444	A3445	R3446	Y3447	K3448	E3449	E3450	Y3451	A3452	V3453	L3454
L3455	S3456	E3457	A3458	Q3459	A3460	I3461	K3462	A3463	V3472	E3482	S3483	A3484	V3489	E3490	K3491	T3492	S3493	N3498	Q3499	M3500	G3505	D3506	L3509	F3513	I3514	A3515	R3516	A3517	G3518	Y3519	F3520	D3521	R3525	L3528	F3529	Q3542	F3543	E3551	S3554	N3555	A3556	D3557	E3558	R3559	W3562														
S3566	L3567	N3576	A3577	L3580	R3585	L3588	D3591	N3602	K3605	T3612	S3613	D3617	A3618	F3619	R3620	K3621	N3622	A3626	L3627	G3630	N3631	Q3636	G3758	R3759	I3760	L3761	D3762	D3763	D3764	L3645	L3649	R3655	T3656	L3658	F3659	G3657	G3658	R3659	V3660	L3661	D3670	L3671	S3672	L3679	S3680	T3681													

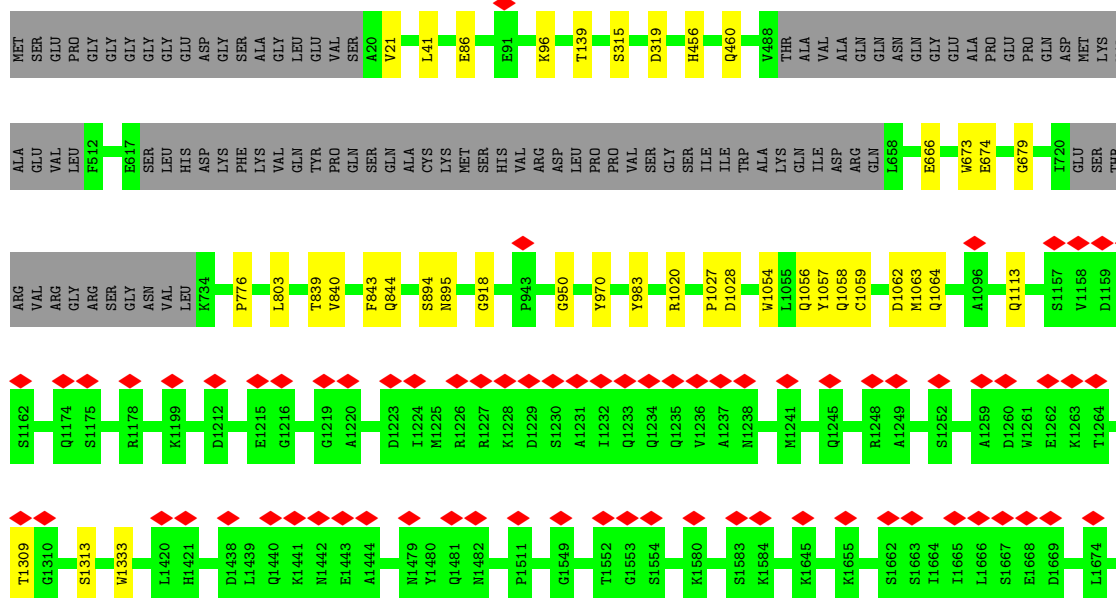


• Molecule 12: Cytoplasmic dynein 1 heavy chain 1





• Molecule 12: Cytoplasmic dynein 1 heavy chain 1

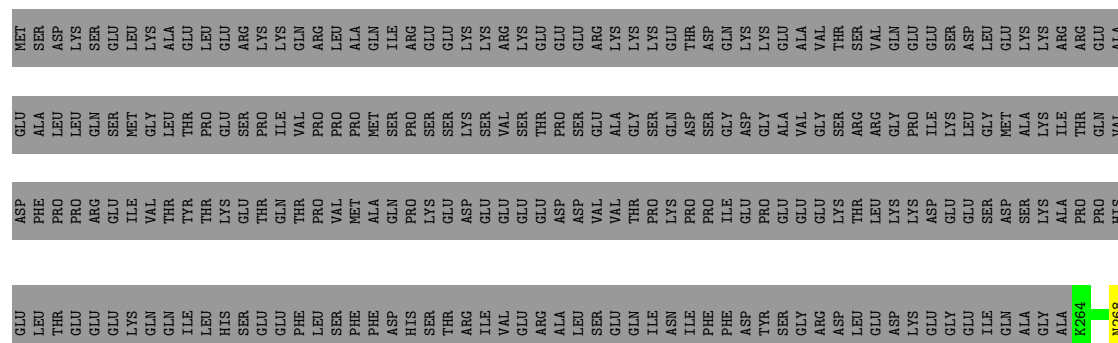






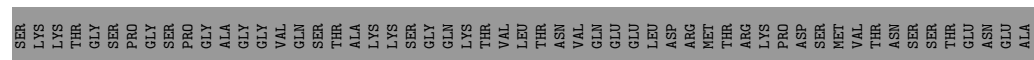
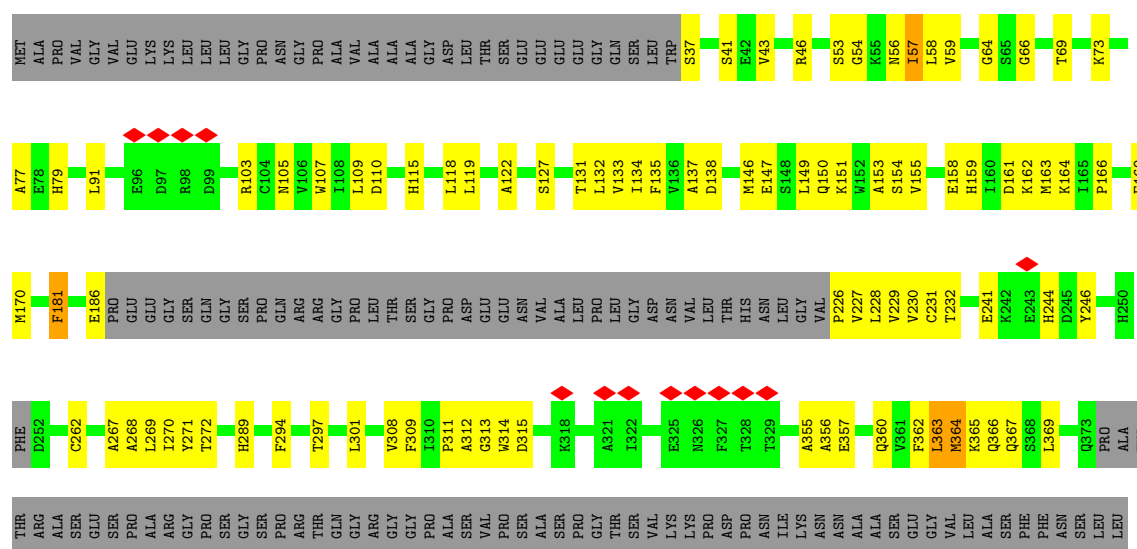
• Molecule 13: Cytoplasmic dynein 1 intermediate chain 2

Chain p: 56% 42%



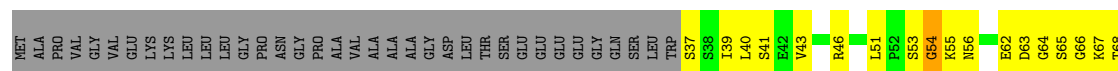
• Molecule 14: Dynein light intermediate chain

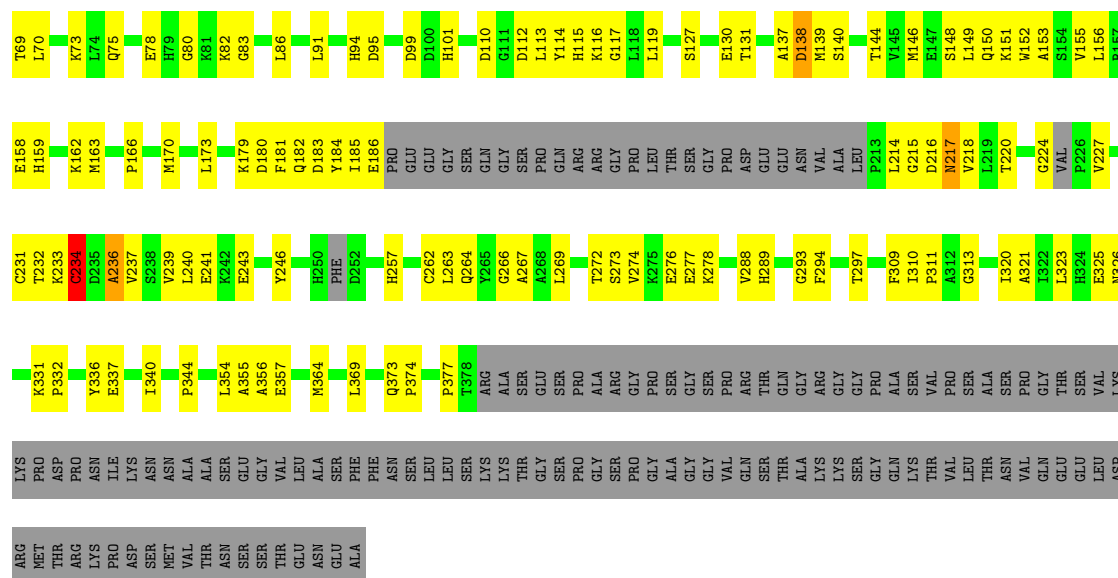
Chain i: 42% 18% 40%



• Molecule 14: Dynein light intermediate chain

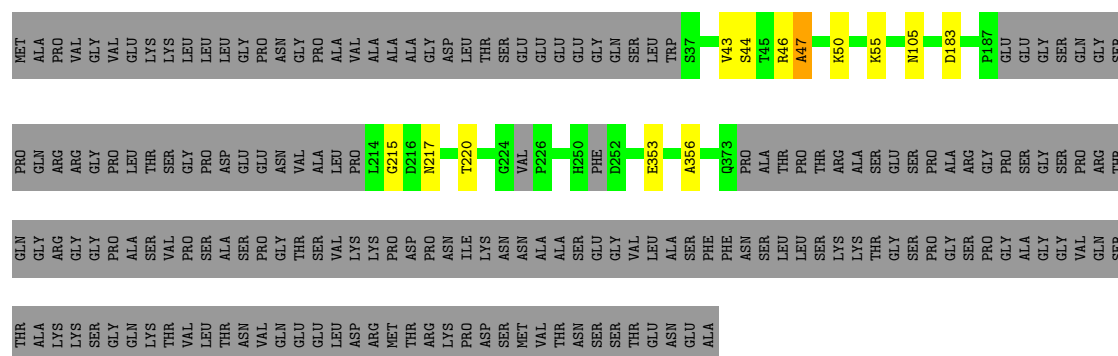
Chain j: 37% 26% 36%





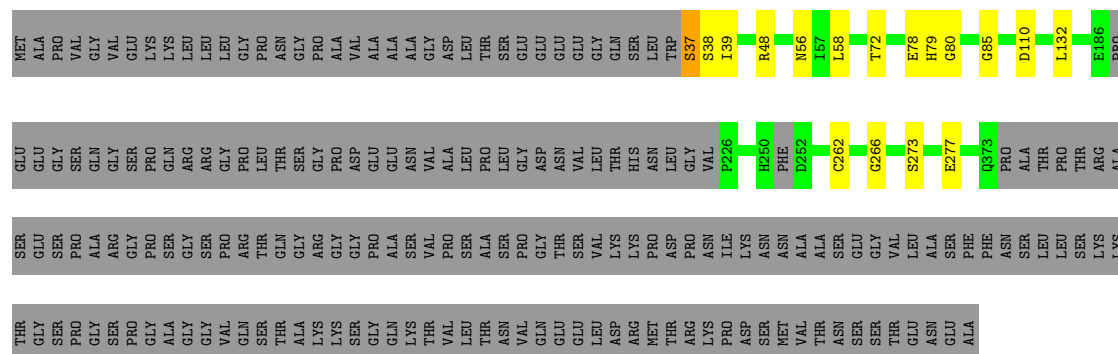
• Molecule 14: Dynein light intermediate chain

Chain q:  60%  37%



• Molecule 14: Dynein light intermediate chain

Chain r:  57%  40%



• Molecule 15: Dynein light chain roadblock

Chain k:  66% 31%



- Molecule 15: Dynein light chain roadblock

Chain l:  67% 30%



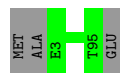
- Molecule 15: Dynein light chain roadblock

Chain s:  97%



- Molecule 15: Dynein light chain roadblock

Chain t:  97%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	16372	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.404	Depositor
Minimum map value	-0.041	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	990.0, 990.0, 990.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	3.3, 3.3, 3.3	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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	0.16	0/1821	0.40	0/2531
1	B	0.18	0/1821	0.48	0/2531
1	C	0.18	0/1846	0.46	0/2566
1	D	0.17	0/1821	0.42	0/2531
1	E	0.17	0/1821	0.46	0/2531
1	F	0.18	0/1821	0.46	0/2531
1	G	0.18	0/1821	0.44	0/2531
1	I	0.15	0/1821	0.43	0/2531
2	H	0.17	0/1821	0.40	0/2531
3	J	0.28	0/1867	0.50	0/2596
4	K	0.16	0/1377	0.40	0/1919
5	L	0.16	0/1326	0.37	0/1844
6	M	0.17	0/1684	0.45	0/2343
6	N	0.15	0/1389	0.40	0/1933
6	P	0.17	0/1609	0.42	0/2240
6	Q	0.16	0/1703	0.39	0/2373
7	O	0.15	0/887	0.44	0/1236
7	R	0.17	0/843	0.49	0/1175
8	U	0.21	0/821	0.54	0/1140
9	V	0.15	0/880	0.42	0/1222
10	W	0.16	0/750	0.45	0/1040
10	Z	0.17	0/951	0.48	0/1325
11	Y	0.40	0/2035	0.58	1/2837 (0.0%)
12	e	0.40	1/22639 (0.0%)	0.72	15/31566 (0.0%)
12	f	0.59	3/22620 (0.0%)	0.91	42/31540 (0.1%)
12	m	0.60	1/18878 (0.0%)	0.82	21/24065 (0.1%)
12	n	0.64	6/18697 (0.0%)	0.86	41/23810 (0.2%)
13	g	0.18	0/1766	0.32	0/2457
13	h	0.14	0/1766	0.40	0/2457
13	o	0.13	0/1766	0.37	1/2457 (0.0%)
13	p	0.14	0/1766	0.37	1/2457 (0.0%)
14	i	0.62	1/1469 (0.1%)	1.38	6/2044 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
14	j	0.79	0/1551	1.16	6/2156 (0.3%)
14	q	1.39	2/1237 (0.2%)	1.68	8/1543 (0.5%)
14	r	0.75	2/1190 (0.2%)	1.12	7/1486 (0.5%)
15	k	0.68	1/461 (0.2%)	0.99	1/642 (0.2%)
15	l	0.78	0/461	1.22	2/642 (0.3%)
15	s	1.02	0/373	1.18	0/466
15	t	1.00	0/373	1.16	0/466
All	All	0.50	17/131549 (0.0%)	0.76	152/178291 (0.1%)

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
12	e	0	2
12	f	0	26
14	j	0	2
14	q	0	1
14	r	0	2
15	l	0	1
All	All	0	34

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	i	362	PHE	C-N	-9.03	1.22	1.33
12	n	1063	MET	C-O	8.29	1.33	1.24
12	n	1062	ASP	C-O	-8.15	1.14	1.24
14	r	79	HIS	C-N	7.88	1.38	1.33
12	f	2715	PRO	CA-CB	-7.72	1.42	1.53
12	n	1020	ARG	C-O	-7.27	1.14	1.24
12	n	1027	PRO	C-O	-6.39	1.16	1.24
12	n	3480	LYS	C-O	6.07	1.31	1.24
12	e	1102	PHE	CA-CB	-5.94	1.45	1.53
12	f	1349	GLN	N-CA	-5.88	1.39	1.46
12	m	1273	PRO	C-O	5.86	1.31	1.24
14	q	353	GLU	C-O	5.60	1.30	1.24
12	f	4202	SER	CA-C	-5.38	1.47	1.53
14	r	58	LEU	C-N	-5.33	1.26	1.33
14	q	43	VAL	C-O	-5.32	1.18	1.24
15	k	79	MET	CA-CB	-5.26	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	n	3381	ILE	C-O	-5.15	1.18	1.24

All (152) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	i	363	LEU	N-CA-CB	-42.24	48.73	109.98
14	r	79	HIS	CA-C-N	-14.07	108.83	122.20
14	r	79	HIS	C-N-CA	-14.07	108.83	122.20
14	i	362	PHE	CA-C-N	-13.45	102.34	120.63
14	i	362	PHE	C-N-CA	-13.45	102.34	120.63
12	m	1030	PRO	N-CA-C	-12.64	99.88	114.92
12	f	3976	GLU	N-CA-C	-11.95	97.03	112.93
12	n	3407	LYS	N-CA-C	-10.63	99.69	111.07
12	f	3977	GLU	N-CA-C	-10.08	102.05	114.75
12	m	3407	LYS	N-CA-C	-9.94	100.43	111.07
12	e	4038	ASN	N-CA-C	-9.70	99.80	112.41
12	f	889	ASN	N-CA-C	-9.62	100.87	111.36
15	l	82	PRO	CA-C-N	-9.41	103.56	121.54
15	l	82	PRO	C-N-CA	-9.41	103.56	121.54
12	f	1515	VAL	N-CA-C	-9.34	103.58	112.83
14	j	86	LEU	CA-C-N	-9.27	108.84	122.65
14	j	86	LEU	C-N-CA	-9.27	108.84	122.65
12	n	3470	ALA	N-CA-C	-9.15	100.13	111.11
12	n	1062	ASP	CA-C-N	9.01	136.61	122.74
12	n	1062	ASP	C-N-CA	9.01	136.61	122.74
12	m	3470	ALA	N-CA-C	-8.75	100.61	111.11
12	f	4133	LYS	N-CA-C	-8.69	102.69	113.28
14	j	80	GLY	N-CA-C	-8.39	102.58	110.21
12	f	2387	LEU	N-CA-C	-8.23	103.26	113.38
12	n	1027	PRO	CA-C-N	-8.15	109.38	122.66
12	n	1027	PRO	C-N-CA	-8.15	109.38	122.66
12	m	1313	SER	CA-C-O	-8.08	112.99	121.55
12	f	3758	GLY	N-CA-C	-8.01	104.16	115.30
12	f	1986	SER	CA-C-N	-7.88	109.94	120.65
12	f	1986	SER	C-N-CA	-7.88	109.94	120.65
12	m	978	CYS	N-CA-C	-7.79	102.87	111.36
12	e	3618	ALA	N-CA-C	-7.69	104.82	112.97
14	q	217	ASN	N-CA-C	-7.67	101.36	110.41
12	f	1935	THR	N-CA-C	-7.61	104.00	113.28
12	e	1074	GLU	N-CA-C	-7.55	103.52	112.89
12	n	1313	SER	CA-C-O	-7.43	113.68	121.55
14	i	314	TRP	N-CA-C	-7.41	103.97	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	i	363	LEU	CB-CA-C	7.32	122.30	110.95
12	e	2033	LYS	N-CA-C	-7.31	105.53	114.75
12	f	1209	LEU	CA-C-N	-7.00	110.77	120.71
12	f	1209	LEU	C-N-CA	-7.00	110.77	120.71
14	q	215	GLY	CA-C-O	-6.98	115.50	121.57
12	e	2600	GLY	N-CA-C	-6.94	105.64	115.43
15	k	67	THR	N-CA-C	-6.87	104.90	113.28
12	f	1681	GLY	N-CA-C	-6.86	106.29	115.21
12	n	3405	MET	CA-C-O	-6.73	113.41	120.55
12	f	888	LEU	N-CA-C	-6.68	104.14	112.90
12	f	4026	ASP	N-CA-C	-6.68	103.07	113.02
12	f	887	ASP	N-CA-C	-6.61	105.08	113.01
12	n	1058	GLN	N-CA-C	-6.56	105.39	113.19
14	q	47	ALA	CA-C-N	6.55	130.45	120.82
14	q	47	ALA	C-N-CA	6.55	130.45	120.82
12	e	1021	ASN	N-CA-C	-6.51	104.95	114.39
12	f	893	TYR	CB-CA-C	6.39	123.14	110.42
12	n	3346	ASN	N-CA-C	-6.36	105.00	112.89
14	r	48	ARG	N-CA-C	-6.36	99.99	109.15
12	f	2713	ASN	N-CA-C	-6.35	99.70	109.41
12	f	4038	ASN	N-CA-C	-6.27	106.60	114.56
12	m	3405	MET	CA-C-O	-6.27	113.01	120.10
12	e	2322	ASN	N-CA-C	-6.24	105.57	113.43
14	i	363	LEU	CA-C-O	-6.16	114.56	120.90
12	n	3313	PRO	N-CA-C	6.09	118.13	110.70
12	m	1058	GLN	N-CA-C	-6.08	104.98	113.37
14	j	234	CYS	CA-C-N	-6.06	109.96	121.54
14	j	234	CYS	C-N-CA	-6.06	109.96	121.54
12	e	4018	MET	N-CA-C	-6.02	105.89	113.72
12	m	1027	PRO	N-CA-C	6.00	121.87	113.53
12	e	2257	LYS	N-CA-C	-5.99	107.79	114.62
12	e	2646	ASN	N-CA-C	-5.99	107.21	114.75
12	f	891	HIS	N-CA-C	-5.97	105.18	112.88
12	n	3405	MET	O-C-N	5.96	128.43	122.12
12	n	1281	THR	N-CA-C	-5.95	104.18	112.45
12	f	2229	GLY	N-CA-C	-5.92	99.14	113.18
12	f	1932	CYS	N-CA-C	-5.92	98.19	110.80
12	f	1483	LYS	N-CA-C	-5.91	106.11	113.55
12	m	3405	MET	N-CA-C	-5.86	104.97	111.71
12	m	3313	PRO	N-CA-C	5.86	117.85	110.70
12	n	3224	ILE	CA-C-O	-5.85	114.86	120.95
12	f	3129	VAL	N-CA-C	-5.85	106.02	113.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	m	1069	TYR	CA-C-O	-5.84	114.89	120.90
12	n	3394	LYS	N-CA-C	-5.84	104.92	111.28
14	r	79	HIS	O-C-N	5.84	130.75	123.28
12	m	1275	GLU	CA-C-N	-5.81	110.98	121.14
12	m	1275	GLU	C-N-CA	-5.81	110.98	121.14
14	q	183	ASP	N-CA-C	-5.79	106.55	113.21
12	f	2305	GLY	N-CA-C	-5.75	99.54	113.18
12	e	1030	PRO	N-CA-C	-5.74	106.97	114.03
12	f	2391	GLU	N-CA-C	-5.71	104.99	112.41
12	n	3402	TYR	CA-C-O	-5.69	114.52	120.55
12	m	1273	PRO	CA-C-O	5.68	130.94	120.60
12	e	1910	THR	N-CA-C	-5.61	104.07	112.54
12	n	3431	ASN	CA-C-O	-5.55	114.66	120.55
12	f	2350	TYR	N-CA-C	-5.55	105.11	112.94
12	f	2362	VAL	CA-C-N	-5.53	113.20	120.95
12	f	2362	VAL	C-N-CA	-5.53	113.20	120.95
12	m	3401	ASN	N-CA-C	-5.49	105.29	111.28
12	n	1063	MET	N-CA-C	-5.47	99.51	108.76
12	n	3407	LYS	CA-C-N	-5.47	112.95	120.28
12	n	3407	LYS	C-N-CA	-5.47	112.95	120.28
12	n	3401	ASN	N-CA-C	-5.42	105.37	111.28
12	n	970	TYR	CA-C-N	-5.41	115.47	123.05
12	n	970	TYR	C-N-CA	-5.41	115.47	123.05
12	e	3617	ASP	N-CA-C	-5.41	106.56	112.72
12	f	2089	GLY	CA-C-O	-5.41	118.42	122.37
12	n	3406	LEU	CA-C-N	-5.40	113.42	120.44
12	n	3406	LEU	C-N-CA	-5.40	113.42	120.44
12	m	3405	MET	CA-C-N	5.37	127.92	120.29
12	m	3405	MET	C-N-CA	5.37	127.92	120.29
12	n	1272	ARG	CA-C-O	-5.37	113.94	120.54
12	n	3401	ASN	O-C-N	5.36	127.81	122.12
14	r	72	THR	O-C-N	5.36	127.80	122.12
12	f	928	GLY	N-CA-C	-5.36	107.96	114.92
14	q	47	ALA	CA-C-O	-5.34	115.27	121.15
12	m	3406	LEU	CA-C-N	-5.33	113.51	120.44
12	m	3406	LEU	C-N-CA	-5.33	113.51	120.44
12	n	3224	ILE	O-C-N	5.33	127.04	121.87
14	j	215	GLY	N-CA-C	-5.30	103.04	110.88
12	n	1064	GLN	CA-C-N	5.30	127.64	120.38
12	n	1064	GLN	C-N-CA	5.30	127.64	120.38
12	n	1333	TRP	N-CA-C	-5.28	106.70	112.72
12	f	1019	TYR	CA-C-N	-5.28	114.72	123.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	f	1019	TYR	C-N-CA	-5.28	114.72	123.37
12	n	3461	ILE	CA-C-O	-5.27	115.47	120.95
14	q	50	LYS	CA-C-O	-5.27	115.50	121.72
12	e	2368	VAL	N-CA-C	-5.27	107.69	112.96
12	n	1028	ASP	N-CA-C	-5.25	107.40	112.97
12	f	1349	GLN	N-CA-C	-5.25	97.94	109.11
14	q	217	ASN	CA-C-O	-5.24	116.31	121.02
12	n	983	TYR	N-CA-C	-5.23	105.75	111.82
12	n	1027	PRO	N-CA-C	5.22	120.79	113.53
12	n	3230	GLU	CA-C-O	-5.22	115.34	120.82
14	r	78	GLU	CA-C-N	-5.21	114.69	122.39
14	r	78	GLU	C-N-CA	-5.21	114.69	122.39
12	n	3444	ILE	CA-C-O	-5.19	115.56	120.95
12	m	3402	TYR	CA-C-O	-5.16	115.08	120.55
12	e	1993	ALA	N-CA-C	-5.15	108.02	114.56
12	f	2196	GLY	N-CA-C	-5.15	100.97	113.18
13	o	428	GLN	CB-CA-C	-5.15	110.62	116.54
13	p	428	GLN	CB-CA-C	-5.14	110.63	116.54
12	f	3045	ASP	N-CA-C	-5.13	104.66	112.04
12	n	3401	ASN	CA-C-O	-5.12	115.12	120.55
12	n	1113	GLN	N-CA-C	-5.11	106.74	112.87
12	f	2675	GLY	N-CA-C	-5.09	106.57	113.24
12	f	3639	GLU	N-CA-C	-5.08	107.75	114.31
12	m	3387	LEU	N-CA-C	-5.07	106.87	113.16
12	n	3461	ILE	O-C-N	5.07	126.79	121.87
12	f	3567	LEU	N-CA-C	-5.05	101.48	108.76
12	n	3405	MET	N-CA-C	-5.05	105.78	111.28
12	f	37	LEU	CA-C-N	5.03	131.44	122.13
12	f	37	LEU	C-N-CA	5.03	131.44	122.13
11	Y	51	CYS	CB-CA-C	5.03	116.37	108.63
12	f	2299	GLN	N-CA-C	-5.01	103.86	110.43

There are no chirality outliers.

All (34) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	e	3079	ALA	Peptide
12	e	4316	GLN	Peptide
12	f	1106	VAL	Peptide
12	f	1118	LEU	Peptide
12	f	1207	SER	Peptide
12	f	1312	LEU	Peptide

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Mol	Chain	Res	Type	Group
12	f	1436	ASP	Peptide
12	f	1596	GLY	Peptide
12	f	2165	PHE	Peptide
12	f	2172	ARG	Peptide
12	f	2226	SER	Peptide
12	f	2230	LYS	Peptide
12	f	2427	PHE	Peptide
12	f	2713	ASN	Peptide
12	f	2760	PRO	Peptide
12	f	2874	SER	Peptide
12	f	2876	TRP	Peptide
12	f	3068	MET	Peptide
12	f	3110	THR	Peptide
12	f	3585	ARG	Peptide
12	f	3757	LYS	Peptide
12	f	3761	LEU	Peptide
12	f	3762	ASP	Peptide
12	f	3974	TRP	Peptide
12	f	4094	VAL	Peptide
12	f	4128	MET	Peptide
12	f	4552	THR	Peptide
12	f	934	ALA	Peptide
14	j	234	CYS	Peptide
14	j	331	LYS	Peptide
15	l	53	ALA	Peptide
14	q	44	SER	Mainchain
14	r	37	SER	Mainchain
14	r	80	GLY	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1822	0	820	7	0
1	B	1822	0	820	7	0
1	C	1847	0	830	5	0
1	D	1822	0	820	9	0
1	E	1822	0	820	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1822	0	820	6	0
1	G	1822	0	820	4	0
1	I	1822	0	820	3	0
2	H	1822	0	835	3	0
3	J	1868	0	823	4	0
4	K	1378	0	611	7	0
5	L	1327	0	585	4	0
6	M	1689	0	765	1	0
6	N	1394	0	632	0	0
6	P	1612	0	747	6	0
6	Q	1707	0	769	1	0
7	O	888	0	413	1	0
7	R	844	0	385	1	0
8	U	822	0	370	2	0
9	V	881	0	379	4	0
10	W	754	0	336	1	0
10	Z	952	0	434	3	0
11	Y	2038	0	886	6	0
12	e	22644	0	10062	295	0
12	f	22625	0	10053	725	0
12	m	18883	0	5554	44	0
12	n	18703	0	5475	38	0
13	g	1767	0	796	10	0
13	h	1767	0	796	12	0
13	o	1767	0	796	7	0
13	p	1767	0	796	11	0
14	i	1472	0	645	91	0
14	j	1555	0	681	99	0
14	q	1241	0	329	10	0
14	r	1193	0	315	6	0
15	k	462	0	192	23	0
15	l	462	0	192	24	0
15	s	374	0	95	0	0
15	t	374	0	95	0	0
16	Y	3	0	0	0	0
17	m	1	0	0	0	0
17	n	1	0	0	0	0
All	All	131638	0	52412	1411	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 8.

All (1411) 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)
12:e:733:LEU:CB	14:i:360:GLN:HA	1.53	1.37
12:e:806:ALA:HA	14:i:356:ALA:N	1.45	1.32
12:n:776:PRO:CB	13:p:375:LEU:O	1.81	1.29
12:f:2645:PRO:O	14:q:220:THR:O	1.60	1.18
12:f:2645:PRO:O	14:q:220:THR:C	1.88	1.15
12:n:803:LEU:O	12:n:894:SER:O	1.62	1.15
12:m:806:ALA:HB1	14:q:356:ALA:N	1.60	1.14
12:n:803:LEU:C	12:n:894:SER:O	1.90	1.12
12:f:890:LEU:HA	12:m:689:PHE:HA	1.27	1.11
12:f:963:ARG:O	12:f:969:ILE:HA	1.51	1.08
12:e:4332:LEU:O	12:e:4336:GLY:N	1.87	1.06
12:e:733:LEU:CB	14:i:360:GLN:CA	2.33	1.05
12:f:1660:GLY:HA3	12:f:1873:LEU:HA	1.39	1.04
12:f:2600:GLY:O	12:f:2604:THR:N	1.91	1.03
12:f:2983:SER:HA	12:f:2988:GLU:H	1.25	1.02
12:f:995:SER:HA	12:f:1020:ARG:HA	1.38	1.01
12:e:4180:TYR:O	12:e:4184:ALA:N	1.93	1.01
12:f:2218:HIS:H	12:f:2321:ASP:HA	1.21	1.00
12:f:3801:TYR:O	12:f:3805:SER:N	1.94	1.00
12:f:4564:LYS:O	12:f:4642:VAL:HA	1.59	0.99
12:f:2773:MET:O	12:f:2777:TYR:N	1.95	0.99
12:m:806:ALA:CB	14:q:356:ALA:H	1.74	0.99
12:f:2229:GLY:O	12:f:2233:ALA:N	1.96	0.98
12:f:3981:THR:O	12:f:3985:GLN:N	1.96	0.98
14:j:180:ASP:O	14:j:184:TYR:N	1.97	0.98
12:m:806:ALA:HB1	14:q:356:ALA:H	1.16	0.97
15:l:58:ARG:HA	15:l:62:PRO:HA	1.45	0.97
12:e:1911:GLY:O	12:e:1915:SER:N	1.98	0.97
12:e:4019:SER:O	12:e:4023:GLN:N	1.97	0.97
14:j:152:TRP:O	14:j:156:LEU:N	1.97	0.96
12:e:806:ALA:CB	14:i:355:ALA:C	2.39	0.95
12:n:918:GLY:HA2	12:n:950:GLY:HA2	1.48	0.95
12:e:720:ILE:HA	12:e:735:LEU:HA	1.48	0.95
12:e:806:ALA:HB2	14:i:355:ALA:HA	1.46	0.94
12:e:806:ALA:O	14:i:356:ALA:HA	1.65	0.94
12:f:1474:GLU:HA	12:f:1587:LEU:HA	1.47	0.94
12:f:1964:GLU:O	12:f:1968:LEU:N	1.98	0.94
12:e:4333:THR:O	12:e:4337:VAL:N	2.01	0.94
12:f:2659:LEU:O	12:f:2706:ILE:HA	1.68	0.93
12:f:4183:LEU:O	12:f:4187:HIS:N	2.01	0.93
12:f:1479:ASN:HA	12:f:1485:ARG:HA	1.48	0.93
12:f:4566:GLN:O	12:f:4640:VAL:HA	1.67	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:l:23:VAL:HA	15:l:29:PRO:HA	1.50	0.93
12:e:806:ALA:HB1	14:i:355:ALA:C	1.94	0.93
12:m:918:GLY:HA2	12:m:950:GLY:HA2	1.49	0.93
12:e:806:ALA:HB2	14:i:355:ALA:CA	1.99	0.92
12:f:2089:GLY:O	12:f:2093:LEU:N	2.03	0.92
12:f:4208:GLY:O	12:f:4212:LEU:N	2.02	0.92
14:i:127:SER:O	14:i:131:THR:N	2.02	0.92
12:f:3521:ASP:O	12:f:3525:ARG:N	2.01	0.92
13:g:366:LYS:HA	15:l:3:GLU:HA	1.50	0.92
12:f:1589:MET:O	12:f:1593:ASN:N	2.02	0.92
12:f:4174:ASN:N	12:f:4231:GLN:O	2.03	0.92
12:e:1075:ASP:O	12:e:1079:TRP:N	2.02	0.91
12:f:917:ALA:C	12:f:950:GLY:HA3	1.95	0.91
12:f:4138:LEU:O	12:f:4142:GLY:N	2.03	0.91
12:e:4181:PHE:O	12:e:4185:TRP:N	2.02	0.91
12:f:2740:GLY:O	12:f:2744:LEU:N	2.04	0.91
12:e:1882:THR:O	12:e:1886:ASP:N	2.03	0.91
12:f:2776:PHE:O	12:f:2780:SER:N	2.03	0.91
12:f:3939:SER:HA	12:f:3945:LYS:HA	1.53	0.91
12:e:806:ALA:CB	14:i:355:ALA:CA	2.49	0.91
12:f:3946:ASP:O	12:f:3950:LYS:N	2.03	0.91
12:f:4610:TYR:N	12:f:4642:VAL:O	2.02	0.91
12:f:2263:HIS:O	12:f:2279:LEU:N	2.04	0.90
15:k:68:PHE:HA	15:k:81:ALA:HA	1.53	0.90
12:f:1098:THR:O	12:f:1110:GLY:N	2.04	0.90
14:j:73:LYS:HA	14:j:78:GLU:HA	1.53	0.90
12:f:4575:LEU:O	12:f:4627:ALA:N	2.05	0.90
14:j:273:SER:O	14:j:277:GLU:N	2.05	0.90
12:f:2829:ALA:O	12:f:2834:GLN:N	2.04	0.89
12:f:2370:SER:O	12:f:2374:ILE:N	2.04	0.89
12:e:806:ALA:CA	14:i:356:ALA:N	2.33	0.89
12:f:923:THR:HA	12:f:1036:SER:HA	1.52	0.89
12:f:4004:MET:O	12:f:4008:PHE:N	2.06	0.88
14:j:144:THR:O	14:j:148:SER:N	2.06	0.88
12:e:2164:VAL:HA	12:e:4536:LEU:H	1.39	0.88
12:f:2641:TYR:HA	12:f:2649:VAL:O	1.73	0.88
12:n:803:LEU:O	12:n:894:SER:C	2.15	0.88
14:j:217:ASN:O	14:j:264:GLN:N	2.07	0.87
12:f:2924:ARG:O	12:f:2928:GLN:N	2.07	0.87
12:e:958:VAL:N	12:e:1104:PRO:O	2.07	0.87
12:f:2290:ASN:HA	12:f:2294:GLU:H	1.39	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:4190:ILE:O	12:f:4194:LEU:N	2.07	0.87
12:e:3906:GLN:O	12:e:3910:ARG:N	2.06	0.87
14:j:66:GLY:O	14:j:70:LEU:N	2.08	0.87
12:e:4336:GLY:O	12:e:4340:ILE:N	2.08	0.87
12:m:806:ALA:HB1	14:q:356:ALA:CA	2.03	0.87
12:e:918:GLY:CA	12:e:950:GLY:HA2	2.05	0.87
12:e:1030:PRO:O	12:e:1034:GLU:N	2.07	0.86
12:e:1059:CYS:O	12:e:1063:MET:N	2.08	0.86
12:f:2252:HIS:O	12:f:2302:VAL:N	2.08	0.86
14:i:147:GLU:O	14:i:151:LYS:N	2.08	0.86
12:f:82:SER:HA	12:f:113:SER:HA	1.56	0.86
12:f:3086:PHE:O	12:f:3089:CYS:N	2.09	0.86
12:n:803:LEU:CB	12:n:895:ASN:O	2.24	0.85
12:e:4327:ALA:O	12:e:4331:LEU:N	2.09	0.85
12:e:3876:LEU:O	12:e:3880:HIS:N	2.08	0.85
12:f:2367:ASP:HA	12:f:2370:SER:HA	1.57	0.85
12:f:4175:GLU:O	12:f:4179:LEU:N	2.08	0.85
12:f:3879:ASP:O	12:f:3883:PHE:N	2.10	0.85
14:i:115:HIS:O	14:i:119:LEU:N	2.09	0.85
14:j:112:ASP:O	14:j:116:LYS:N	2.08	0.85
12:e:806:ALA:HA	14:i:356:ALA:H	1.42	0.84
12:e:918:GLY:HA2	12:e:950:GLY:HA2	1.56	0.84
12:f:2724:SER:O	12:f:2728:LEU:N	2.09	0.84
14:i:166:PRO:O	14:i:170:MET:N	2.10	0.84
14:j:262:CYS:O	14:j:267:ALA:N	2.10	0.84
15:k:69:LEU:N	15:k:80:VAL:O	2.10	0.84
12:f:4557:SER:HA	12:f:4591:ARG:HA	1.59	0.84
12:n:803:LEU:CB	12:n:895:ASN:C	2.51	0.84
12:e:2929:PRO:HA	12:e:3060:ARG:HA	1.58	0.84
12:f:2299:GLN:O	12:f:2339:VAL:HA	1.77	0.84
14:j:179:LYS:O	14:j:183:ASP:N	2.09	0.84
12:f:3555:ASN:O	12:f:3559:ARG:N	2.09	0.84
12:f:2161:LEU:O	12:f:2165:PHE:N	2.09	0.83
12:e:4335:GLN:O	12:e:4339:MET:N	2.11	0.83
12:f:2830:LEU:O	12:f:2835:ASP:N	2.11	0.83
14:j:158:GLU:O	14:j:162:LYS:N	2.10	0.83
12:e:806:ALA:HA	14:i:355:ALA:C	2.03	0.83
12:e:1101:GLU:HA	12:e:1106:VAL:HA	1.60	0.83
12:f:1349:GLN:O	12:f:1431:LEU:N	2.10	0.82
14:j:127:SER:O	14:j:131:THR:N	2.11	0.82
12:f:4016:SER:O	12:f:4020:ILE:N	2.12	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:1801:PRO:O	12:f:1805:ARG:N	2.11	0.82
14:j:146:MET:O	14:j:150:GLN:N	2.11	0.82
12:f:3993:ILE:O	12:f:3997:ARG:N	2.12	0.82
14:j:336:TYR:O	14:j:340:ILE:N	2.12	0.82
12:f:1672:VAL:HA	12:f:1691:SER:HA	1.61	0.81
12:f:2198:GLU:O	12:f:2202:MET:N	2.13	0.81
12:e:1955:GLY:O	12:e:2015:PHE:N	2.11	0.81
12:f:1836:PHE:O	12:f:1840:SER:N	2.14	0.81
12:e:995:SER:HA	12:e:1018:PHE:HA	1.62	0.81
12:f:2198:GLU:H	12:f:2202:MET:N	1.78	0.81
12:e:1069:TYR:O	12:e:1073:GLY:N	2.14	0.81
12:f:2219:GLY:HA3	12:f:2319:LEU:HA	1.63	0.81
12:f:3219:ARG:HA	12:f:3472:VAL:HA	1.62	0.80
12:f:4249:GLN:O	12:f:4254:GLY:N	2.14	0.80
14:j:37:SER:O	14:j:41:SER:N	2.11	0.80
12:f:2218:HIS:H	12:f:2321:ASP:CA	1.94	0.80
12:f:2499:LEU:O	12:f:2503:SER:N	2.14	0.80
12:f:3037:ALA:O	12:f:3042:LEU:N	2.14	0.80
12:f:3612:THR:O	12:f:3636:GLN:N	2.11	0.80
12:f:4282:PHE:O	12:f:4296:MET:N	2.13	0.80
12:e:1481:GLN:HA	12:e:2272:THR:HA	1.62	0.80
12:f:2614:ASP:O	12:f:2658:TRP:N	2.15	0.80
12:e:4549:GLN:O	12:e:4550:SER:CB	2.30	0.79
12:f:1101:GLU:HA	12:f:1106:VAL:HA	1.63	0.79
12:f:3098:SER:O	12:f:3102:LEU:N	2.16	0.79
12:f:1430:THR:O	12:f:1434:ILE:N	2.15	0.79
14:i:146:MET:O	14:i:150:GLN:N	2.12	0.79
12:f:3661:LEU:HA	12:f:3671:LEU:H	1.48	0.79
12:f:85:LYS:HA	12:f:97:GLU:HA	1.65	0.79
12:f:1368:ASN:O	12:f:1372:ASN:N	2.12	0.79
12:f:4611:LEU:O	12:f:4645:THR:N	2.16	0.79
14:j:95:ASP:O	14:j:99:ASP:N	2.15	0.79
12:f:1549:GLY:O	12:f:1553:GLY:N	2.16	0.79
12:f:2250:VAL:N	12:f:2298:ARG:O	2.13	0.79
12:f:2269:ASP:N	12:f:2274:GLU:O	2.15	0.79
12:f:2616:GLU:N	12:f:2658:TRP:O	2.16	0.79
14:j:321:ALA:O	14:j:325:GLU:N	2.14	0.79
12:f:1580:LYS:O	12:f:1584:LYS:N	2.14	0.78
12:f:4065:GLN:O	12:f:4093:TRP:N	2.15	0.78
12:f:4556:CYS:O	12:f:4592:TRP:N	2.16	0.78
12:f:4608:PRO:O	12:f:4642:VAL:N	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:e:733:LEU:CB	14:i:360:GLN:O	2.31	0.78
12:e:806:ALA:O	14:i:356:ALA:CA	2.31	0.78
12:f:1548:GLU:O	12:f:1552:THR:N	2.16	0.78
12:e:4317:THR:O	12:e:4319:SER:N	2.15	0.78
12:f:2220:LEU:O	12:f:2343:PHE:N	2.17	0.78
12:n:918:GLY:HA2	12:n:950:GLY:CA	2.13	0.78
12:m:918:GLY:HA2	12:m:950:GLY:CA	2.13	0.78
12:e:806:ALA:CA	14:i:355:ALA:C	2.56	0.78
12:f:3851:ASP:O	12:f:3855:ARG:N	2.14	0.78
14:i:133:VAL:O	14:i:228:LEU:N	2.14	0.78
12:f:4375:ALA:O	12:f:4379:THR:N	2.13	0.78
14:i:58:LEU:N	14:i:132:LEU:O	2.17	0.78
14:i:270:ILE:HA	14:i:309:PHE:HA	1.65	0.78
12:e:3956:GLN:O	12:e:3960:TRP:N	2.16	0.77
12:e:2773:MET:O	12:e:2777:TYR:N	2.17	0.77
12:e:4001:LEU:O	12:e:4005:ALA:N	2.12	0.77
12:f:3871:VAL:O	12:f:3875:MET:N	2.18	0.77
12:f:4182:LEU:O	12:f:4186:PHE:N	2.16	0.77
12:f:1765:ALA:O	12:f:1769:ILE:CB	2.33	0.77
12:f:3655:ARG:HA	12:f:3660:VAL:HA	1.66	0.77
12:e:2439:HIS:O	12:e:2443:LEU:N	2.16	0.77
12:f:2595:GLY:O	12:f:2713:ASN:HA	1.84	0.77
12:f:2639:CYS:HA	12:f:2652:PRO:HA	1.66	0.77
12:e:2034:LYS:HA	12:e:4208:GLY:HA3	1.66	0.77
12:f:4545:VAL:O	12:f:4573:ASN:N	2.17	0.77
12:f:961:GLU:N	12:f:972:ASN:O	2.18	0.76
12:f:2355:THR:O	12:f:2359:CYS:N	2.19	0.76
12:f:2438:GLU:O	12:f:2442:LYS:CB	2.33	0.76
12:f:3519:TYR:HA	12:f:3698:PHE:O	1.85	0.76
12:f:4288:VAL:N	12:f:4292:LYS:O	2.19	0.76
14:i:363:LEU:O	14:i:366:GLN:N	2.18	0.76
12:e:4559:GLY:HA2	12:e:4588:THR:O	1.86	0.76
12:f:3704:THR:O	12:f:3708:LEU:N	2.16	0.76
12:e:733:LEU:O	14:i:363:LEU:C	2.29	0.76
12:f:2677:GLN:O	12:f:2681:SER:N	2.15	0.76
14:i:151:LYS:O	14:i:155:VAL:N	2.18	0.76
12:f:2482:GLN:O	12:f:2486:LEU:N	2.18	0.75
12:e:1861:MET:O	12:e:1863:ASN:N	2.16	0.75
12:e:3535:HIS:O	12:e:3539:ALA:N	2.19	0.75
12:f:1409:LYS:O	12:f:1413:TRP:N	2.20	0.75
14:j:166:PRO:O	14:j:170:MET:N	2.17	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:j:181:PHE:HA	14:j:313:GLY:HA2	1.68	0.75
12:f:3950:LYS:O	12:f:3954:ASP:N	2.19	0.74
14:r:85:GLY:O	14:r:110:ASP:N	2.21	0.74
12:f:997:PRO:HA	12:f:1019:TYR:H	1.51	0.74
12:f:2779:MET:O	12:f:2783:ARG:N	2.20	0.74
12:f:3726:GLU:O	12:f:3730:ASP:N	2.20	0.74
12:f:4066:ILE:HA	12:f:4093:TRP:O	1.87	0.74
12:f:997:PRO:HA	12:f:1019:TYR:N	2.02	0.74
12:f:1380:TYR:O	12:f:1383:TYR:N	2.20	0.74
12:f:4566:GLN:HA	12:f:4582:SER:HA	1.69	0.74
15:l:69:LEU:O	15:l:79:MET:HA	1.88	0.74
12:e:3083:PRO:O	12:e:3086:PHE:N	2.20	0.74
12:f:2267:THR:O	12:f:2276:THR:N	2.14	0.74
12:f:3037:ALA:O	12:f:3041:GLY:N	2.21	0.74
12:f:1416:LEU:O	12:f:1420:LEU:N	2.17	0.74
12:f:4005:ALA:O	12:f:4009:VAL:N	2.17	0.74
9:V:73:PHE:HA	9:V:82:PHE:HA	1.70	0.73
12:f:4347:GLN:O	12:f:4351:ASP:N	2.21	0.73
12:e:4564:LYS:HA	12:e:4585:LEU:H	1.53	0.73
15:k:24:ASN:N	15:k:28:ILE:O	2.20	0.73
12:f:1469:VAL:O	12:f:1473:TYR:N	2.22	0.73
12:f:1766:LEU:O	12:f:1770:GLY:N	2.20	0.73
12:f:4603:ASN:O	12:f:4626:ILE:N	2.20	0.73
12:e:4177:ALA:O	12:e:4181:PHE:N	2.18	0.73
12:f:2218:HIS:N	12:f:2321:ASP:HA	2.00	0.73
12:f:2123:ASP:O	12:f:2127:ILE:N	2.16	0.73
12:f:1587:LEU:O	12:f:1591:VAL:N	2.21	0.73
12:f:4015:GLU:O	12:f:4019:SER:N	2.22	0.73
12:f:890:LEU:HA	12:m:689:PHE:CA	2.13	0.72
12:f:1330:LYS:O	12:f:1334:SER:N	2.20	0.72
12:e:1998:THR:HA	12:e:2008:VAL:H	1.54	0.72
12:e:2160:LEU:O	12:e:2163:ASP:N	2.20	0.72
14:j:236:ALA:O	14:j:240:LEU:N	2.17	0.72
12:f:1775:SER:O	12:f:1779:GLN:N	2.22	0.72
14:j:227:VAL:O	14:j:267:ALA:HA	1.89	0.72
12:f:1557:ILE:O	12:f:1561:LEU:N	2.23	0.72
12:m:1057:TYR:C	12:m:1059:CYS:H	1.97	0.72
12:e:344:LEU:HA	12:e:356:ALA:HB1	1.71	0.72
12:f:2312:VAL:O	12:f:2316:ASN:N	2.20	0.72
12:f:2623:SER:C	12:f:2625:ALA:H	1.96	0.72
14:i:135:PHE:O	14:i:230:VAL:N	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:i:229:VAL:N	14:i:268:ALA:O	2.23	0.72
14:i:363:LEU:O	14:i:364:MET:C	2.28	0.72
12:n:456:HIS:O	12:n:460:GLN:N	2.19	0.72
12:f:994:LEU:HA	12:f:1022:ALA:H	1.55	0.72
12:f:1351:TRP:N	12:f:1430:THR:HA	2.04	0.72
12:f:1374:PRO:O	12:f:1378:ARG:N	2.17	0.72
12:f:2765:TYR:O	12:f:2769:LEU:N	2.17	0.72
12:f:2839:GLU:O	12:f:2843:ARG:N	2.23	0.72
9:V:58:GLY:HA3	9:V:89:ASP:HA	1.70	0.72
12:f:4328:GLU:O	12:f:4332:LEU:N	2.19	0.72
12:f:2937:GLY:N	12:f:3068:MET:O	2.19	0.71
15:l:72:ARG:HA	15:l:77:GLU:HA	1.71	0.71
14:j:69:THR:HA	14:j:78:GLU:O	1.89	0.71
14:j:137:ALA:O	14:j:232:THR:N	2.22	0.71
12:f:4042:LEU:O	12:f:4145:PHE:N	2.19	0.71
14:i:231:CYS:N	14:i:270:ILE:O	2.23	0.71
12:f:1210:TYR:O	12:f:1213:ASN:N	2.24	0.71
12:f:1272:ARG:O	12:f:1276:ALA:N	2.18	0.71
12:f:2248:GLU:O	12:f:2298:ARG:N	2.24	0.71
14:j:75:GLN:HA	14:j:91:LEU:HA	1.72	0.71
12:f:2424:GLN:O	12:f:2428:THR:N	2.18	0.71
12:e:2393:GLU:O	12:e:2397:ARG:N	2.24	0.71
12:f:1660:GLY:HA3	12:f:1873:LEU:CA	2.18	0.71
12:f:2754:ALA:O	12:f:2756:LEU:N	2.23	0.71
15:k:72:ARG:HA	15:k:77:GLU:HA	1.72	0.71
12:n:918:GLY:CA	12:n:950:GLY:HA2	2.20	0.71
12:f:2473:ASN:HA	12:f:2480:PRO:HA	1.72	0.70
12:f:3618:ALA:O	12:f:3622:ASN:N	2.24	0.70
12:f:4340:ILE:O	12:f:4344:LEU:N	2.23	0.70
12:e:2817:PRO:O	12:e:2821:LEU:N	2.24	0.70
12:e:733:LEU:O	14:i:363:LEU:CA	2.39	0.70
12:e:810:LYS:N	14:i:357:GLU:H	1.89	0.70
12:f:4529:ALA:O	12:f:4534:TRP:N	2.18	0.70
14:i:154:SER:O	14:i:158:GLU:N	2.17	0.70
12:f:1930:PHE:O	12:f:1958:ASP:N	2.25	0.70
12:f:4269:LEU:O	12:f:4273:PHE:N	2.25	0.70
14:i:271:TYR:N	14:i:308:VAL:O	2.25	0.70
12:f:4288:VAL:O	12:f:4292:LYS:N	2.25	0.70
12:e:806:ALA:HB1	14:i:355:ALA:O	1.90	0.70
15:l:27:GLY:O	15:l:44:ASN:N	2.25	0.70
12:f:1435:TRP:O	12:f:1438:ASP:HA	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:m:918:GLY:CA	12:m:950:GLY:HA2	2.20	0.69
12:f:4184:ALA:O	12:f:4188:ALA:N	2.26	0.69
12:f:4043:MET:O	12:f:4127:THR:HA	1.93	0.69
12:e:720:ILE:CA	12:e:735:LEU:HA	2.21	0.69
12:e:733:LEU:CB	14:i:360:GLN:C	2.66	0.69
12:e:1021:ASN:O	12:e:1025:ARG:N	2.25	0.69
12:f:1906:GLY:HA3	12:f:2042:THR:HA	1.72	0.69
12:f:2933:LEU:O	12:f:3066:PHE:N	2.18	0.69
12:m:4288:VAL:N	12:m:4292:LYS:O	2.26	0.69
12:n:4288:VAL:N	12:n:4292:LYS:O	2.26	0.69
14:r:262:CYS:O	14:r:266:GLY:N	2.26	0.68
14:i:53:SER:O	14:i:105:ASN:N	2.21	0.68
12:e:486:PRO:HA	12:e:512:PHE:HA	1.75	0.68
12:e:3873:ARG:O	12:e:4146:VAL:N	2.23	0.68
12:f:2686:MET:HA	12:f:2691:GLY:O	1.94	0.68
12:f:4152:GLY:O	12:f:4156:ASN:N	2.25	0.68
12:f:994:LEU:O	12:f:1021:ASN:N	2.26	0.68
12:f:1898:ALA:HA	12:f:1986:SER:HA	1.75	0.68
10:W:1130:ALA:O	10:W:1134:LEU:N	2.25	0.68
12:e:2614:ASP:O	12:e:2658:TRP:N	2.26	0.68
12:e:3926:GLY:O	12:e:3958:SER:HA	1.92	0.68
12:f:2315:LEU:O	12:f:2319:LEU:N	2.17	0.68
15:k:69:LEU:HA	15:l:71:ILE:HA	1.74	0.68
15:l:23:VAL:HA	15:l:29:PRO:CA	2.23	0.68
12:f:2175:MET:O	12:f:2179:ARG:N	2.22	0.68
12:f:2489:TYR:HA	12:f:2543:GLY:HA2	1.76	0.68
12:f:3928:THR:O	12:f:3932:ALA:N	2.25	0.68
12:f:4631:ASP:O	12:f:4635:PHE:N	2.22	0.68
12:f:3637:ASP:N	12:f:3680:SER:O	2.27	0.68
14:j:181:PHE:O	14:j:313:GLY:HA2	1.94	0.68
12:f:4152:GLY:HA3	12:f:4314:ASP:O	1.93	0.67
15:l:27:GLY:HA3	15:l:44:ASN:HA	1.75	0.67
12:f:1057:TYR:O	12:f:1060:LEU:N	2.28	0.67
12:f:1481:GLN:HA	12:f:2272:THR:H	1.58	0.67
12:e:918:GLY:HA2	12:e:950:GLY:CA	2.24	0.67
12:f:2223:VAL:O	12:f:2364:PHE:N	2.21	0.67
12:f:2595:GLY:HA3	12:f:2736:VAL:O	1.94	0.67
12:f:2951:ALA:O	12:f:2956:LEU:N	2.21	0.67
12:e:2142:CYS:O	12:e:2146:VAL:N	2.25	0.67
12:f:3926:GLY:HA3	12:f:3958:SER:CB	2.25	0.67
14:j:233:LYS:N	14:j:273:SER:HA	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:k:23:VAL:HA	15:k:29:PRO:HA	1.76	0.67
15:k:70:ARG:O	15:l:70:ARG:N	2.28	0.67
12:f:3617:ASP:O	12:f:3620:ARG:N	2.25	0.67
15:k:26:GLU:O	15:k:44:ASN:HA	1.94	0.67
12:e:3589:ILE:HA	12:e:3699:VAL:O	1.95	0.66
12:e:2836:ARG:HA	12:e:3093:TRP:H	1.59	0.66
12:f:2068:LYS:O	12:f:2072:PHE:N	2.28	0.66
12:f:4496:ALA:O	12:f:4500:GLY:N	2.25	0.66
14:i:159:HIS:O	14:i:163:MET:N	2.16	0.66
12:f:960:HIS:O	12:f:1108:ASP:N	2.29	0.66
12:f:1512:TYR:O	12:f:1516:PHE:N	2.29	0.66
12:e:2985:CYS:O	12:e:3036:GLY:HA3	1.96	0.66
12:f:3135:GLN:HA	12:f:3136:PRO:C	2.19	0.66
12:f:3828:SER:O	12:f:3832:PHE:N	2.19	0.66
12:f:1903:SER:HA	12:f:2017:THR:HA	1.78	0.66
12:f:3700:ASN:C	12:f:3702:THR:H	2.02	0.66
12:e:4334:THR:O	12:e:4338:ASP:N	2.20	0.66
12:f:117:ALA:N	12:f:138:LEU:O	2.17	0.66
12:f:2268:LEU:HA	12:f:2275:TRP:HA	1.77	0.66
12:f:2862:ASP:O	12:f:2866:ALA:N	2.28	0.66
12:f:4562:GLY:O	12:f:4644:CYS:HA	1.95	0.66
12:m:3767:ILE:O	12:m:3771:GLU:N	2.29	0.66
12:f:1937:ASP:O	12:f:1941:MET:N	2.23	0.66
12:f:2324:LEU:HA	12:f:2334:SER:HA	1.78	0.66
12:f:3637:ASP:H	12:f:3681:THR:HA	1.59	0.66
14:i:155:VAL:O	14:i:159:HIS:N	2.24	0.66
12:n:3767:ILE:O	12:n:3771:GLU:N	2.29	0.66
14:i:133:VAL:N	14:i:226:PRO:O	2.30	0.65
12:f:1854:LEU:HA	12:f:1869:GLY:HA2	1.78	0.65
12:e:2370:SER:O	12:e:2374:ILE:N	2.21	0.65
12:f:1546:TYR:O	12:f:1549:GLY:N	2.29	0.65
12:f:3105:VAL:O	12:f:3109:PHE:N	2.29	0.65
12:e:866:THR:HA	12:e:946:SER:HA	1.78	0.65
12:e:1882:THR:O	12:e:1885:THR:N	2.30	0.65
12:e:1905:PHE:N	12:e:2039:LEU:O	2.22	0.65
12:f:1313:SER:O	12:f:1315:SER:N	2.29	0.65
12:f:3104:GLN:O	12:f:3108:GLU:N	2.18	0.65
14:j:173:LEU:C	14:j:224:GLY:HA3	2.21	0.65
12:e:3537:GLN:HA	12:e:3543:PHE:H	1.61	0.65
12:f:3939:SER:CA	12:f:3945:LYS:HA	2.25	0.65
12:f:4502:LYS:O	12:f:4506:ASN:N	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:g:366:LYS:CA	15:l:3:GLU:HA	2.25	0.65
12:e:810:LYS:CA	14:i:357:GLU:H	2.09	0.65
12:e:1015:GLU:HA	12:e:1018:PHE:O	1.97	0.65
12:f:1911:GLY:O	12:f:1915:SER:N	2.28	0.65
12:f:3086:PHE:C	12:f:3089:CYS:H	2.05	0.65
14:i:137:ALA:N	14:i:230:VAL:O	2.23	0.65
12:f:4044:CYS:N	12:f:4145:PHE:O	2.30	0.64
12:f:2219:GLY:HA2	12:f:2341:ILE:O	1.97	0.64
12:f:3837:HIS:C	12:f:3839:VAL:H	2.03	0.64
2:H:42:GLY:HA3	3:J:387:TRP:HA	1.79	0.64
12:e:4246:LEU:O	12:e:4251:ILE:N	2.31	0.64
14:r:37:SER:C	14:r:39:ILE:N	2.55	0.64
12:e:270:THR:O	12:e:274:GLU:N	2.24	0.64
12:e:283:ARG:HA	12:f:175:GLY:HA3	1.78	0.64
12:e:2936:ILE:O	12:e:3094:PHE:N	2.31	0.64
12:f:948:LYS:O	12:f:951:GLY:N	2.30	0.64
12:f:2242:GLU:HA	12:f:2249:GLY:H	1.63	0.64
12:f:2518:ILE:O	12:f:2522:THR:N	2.27	0.64
12:f:3107:LYS:O	12:f:3111:SER:N	2.25	0.64
12:f:3498:ASN:O	12:f:3500:MET:N	2.31	0.64
12:f:3760:ILE:O	12:f:3764:ASP:HA	1.97	0.64
12:f:3773:LEU:O	12:f:3776:GLU:N	2.30	0.64
12:f:4535:SER:O	12:f:4538:GLU:N	2.30	0.64
14:j:234:CYS:C	14:j:236:ALA:N	2.53	0.64
12:f:3681:THR:O	12:f:3683:ASP:N	2.31	0.64
12:e:1860:GLN:HA	12:e:1864:ALA:O	1.98	0.64
12:f:829:LEU:O	12:f:833:VAL:N	2.30	0.64
12:f:2188:GLU:C	12:f:2190:TYR:H	2.04	0.64
12:f:2423:LEU:O	12:f:2427:PHE:N	2.30	0.64
12:f:3591:ASP:O	12:f:3683:ASP:N	2.32	0.63
12:f:1932:CYS:N	12:f:1958:ASP:O	2.27	0.63
14:j:62:GLU:O	14:j:64:GLY:N	2.31	0.63
4:K:186:ALA:N	4:K:216:VAL:O	2.30	0.63
12:f:2983:SER:O	12:f:2987:ASN:HA	1.99	0.63
14:j:288:VAL:O	14:j:293:GLY:N	2.31	0.63
12:e:2264:LEU:O	12:e:2279:LEU:N	2.28	0.63
12:e:2600:GLY:O	12:e:2604:THR:N	2.27	0.63
12:e:2932:HIS:O	12:e:3090:VAL:N	2.28	0.63
12:f:2638:TYR:O	12:f:2653:VAL:N	2.32	0.63
12:e:2690:GLY:O	12:e:2703:LEU:N	2.32	0.63
12:f:885:VAL:O	12:f:889:ASN:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:e:2691:GLY:HA2	12:e:2703:LEU:H	1.64	0.62
12:f:2062:ALA:O	12:f:2066:ALA:N	2.28	0.62
12:f:2618:VAL:O	12:f:2662:PHE:N	2.32	0.62
12:f:4138:LEU:O	12:f:4141:ALA:N	2.32	0.62
12:f:2039:LEU:HA	12:f:4255:ARG:HA	1.80	0.62
12:f:2635:PHE:O	12:f:2639:CYS:N	2.25	0.62
12:e:4317:THR:C	12:e:4319:SER:H	2.07	0.62
1:C:51:ALA:HB2	1:E:173:GLY:HA3	1.80	0.62
12:e:4249:GLN:O	12:e:4254:GLY:N	2.32	0.62
12:f:1405:SER:HA	12:f:3658:GLY:HA2	1.80	0.62
12:f:2771:ALA:O	12:f:2775:GLU:N	2.22	0.62
12:f:1902:GLY:H	12:f:2015:PHE:HA	1.65	0.62
12:f:2260:SER:O	12:f:2264:LEU:N	2.32	0.62
12:f:2645:PRO:C	14:q:220:THR:O	2.39	0.62
14:i:149:LEU:O	14:i:153:ALA:N	2.18	0.62
8:U:25:GLY:HA3	8:U:43:ALA:HB3	1.81	0.62
12:f:2254:ILE:O	12:f:2304:ASP:N	2.32	0.62
12:f:3006:GLU:O	12:f:3010:THR:N	2.26	0.62
12:e:2163:ASP:HA	12:e:4529:ALA:C	2.25	0.62
12:f:121:ARG:H	12:f:135:LEU:HA	1.64	0.62
14:i:69:THR:HA	14:i:79:HIS:HA	1.80	0.62
14:j:257:HIS:N	14:j:332:PRO:HA	2.14	0.62
9:V:38:GLY:HA3	9:V:59:ARG:HA	1.82	0.61
12:f:1417:MET:O	12:f:1421:HIS:N	2.33	0.61
12:f:2301:ILE:O	12:f:2342:MET:N	2.33	0.61
12:f:1920:GLY:O	12:f:1924:GLY:N	2.34	0.61
7:O:47:ILE:O	7:O:51:ARG:N	2.33	0.61
12:f:2992:PHE:O	12:f:3064:VAL:HA	2.00	0.61
12:e:1022:ALA:O	12:e:1026:MET:N	2.32	0.61
14:i:262:CYS:O	14:i:267:ALA:N	2.33	0.61
12:f:806:ALA:HB2	14:j:354:LEU:O	2.00	0.61
12:f:961:GLU:HA	12:f:1108:ASP:O	2.01	0.61
12:f:4538:GLU:O	12:f:4595:GLN:N	2.29	0.61
12:e:4002:LEU:O	12:e:4006:HIS:N	2.18	0.61
12:f:2557:VAL:O	12:f:2754:ALA:HA	1.99	0.61
12:e:4235:PRO:HA	12:e:4238:ILE:H	1.65	0.61
12:f:1667:SER:N	12:f:1672:VAL:O	2.24	0.61
12:f:2762:LEU:O	12:f:2766:ALA:N	2.34	0.61
12:e:403:HIS:HA	12:e:532:GLU:HA	1.83	0.61
13:p:551:LEU:O	13:p:562:THR:N	2.33	0.61
12:e:2039:LEU:HA	12:e:4255:ARG:HA	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:2663:CYS:O	12:f:2711:ALA:N	2.33	0.60
12:f:4001:LEU:O	12:f:4005:ALA:N	2.21	0.60
12:f:4139:LEU:HA	12:f:4142:GLY:O	2.01	0.60
12:f:1930:PHE:N	12:f:1956:CYS:O	2.35	0.60
14:j:182:GLN:HA	14:j:214:LEU:N	2.16	0.60
15:k:58:ARG:HA	15:k:61:ASP:O	2.00	0.60
13:o:508:LEU:O	13:o:517:LEU:N	2.35	0.60
12:e:2162:SER:O	12:e:4530:GLN:HA	2.02	0.60
12:f:923:THR:HA	12:f:1036:SER:CA	2.28	0.60
12:f:4284:LEU:N	12:f:4294:ILE:O	2.32	0.60
12:f:4323:LEU:HA	12:f:4637:GLU:O	2.01	0.60
13:p:508:LEU:O	13:p:517:LEU:N	2.35	0.60
12:e:2901:TYR:O	12:e:2906:ASP:HA	2.00	0.60
12:f:2040:ALA:N	12:f:4254:GLY:O	2.34	0.60
15:k:27:GLY:HA3	15:k:43:ALA:C	2.27	0.60
12:f:2795:SER:O	12:f:2798:GLU:N	2.30	0.60
14:i:137:ALA:O	14:i:232:THR:N	2.32	0.60
13:o:551:LEU:O	13:o:562:THR:N	2.33	0.60
1:I:41:ARG:O	1:I:70:SER:N	2.34	0.60
12:e:3822:HIS:O	12:e:3824:LEU:N	2.33	0.60
12:f:2598:GLY:O	12:f:2797:ARG:N	2.35	0.60
12:e:152:PHE:O	12:e:157:VAL:N	2.35	0.60
12:f:1370:LEU:O	12:f:1373:PHE:N	2.35	0.60
12:f:1655:LYS:C	12:f:1657:MET:H	2.09	0.60
12:f:1983:ARG:C	12:f:1985:HIS:N	2.59	0.59
12:e:947:HIS:O	12:e:948:LYS:C	2.45	0.59
12:f:2659:LEU:N	12:f:2705:ARG:O	2.36	0.59
13:h:409:SER:N	13:h:420:ASP:O	2.25	0.59
12:f:1956:CYS:O	12:f:1958:ASP:N	2.35	0.59
12:f:2302:VAL:O	12:f:2304:ASP:N	2.35	0.59
12:f:2989:LYS:HA	12:f:3061:ASN:O	2.02	0.59
14:j:149:LEU:O	14:j:153:ALA:N	2.27	0.59
12:f:2245:GLU:C	12:f:2247:VAL:H	2.10	0.59
12:e:3518:GLY:HA3	12:e:3699:VAL:HA	1.84	0.59
12:f:1355:GLN:O	12:f:1359:LEU:N	2.27	0.59
12:f:2297:LYS:O	12:f:2299:GLN:N	2.36	0.59
12:f:4002:LEU:O	12:f:4006:HIS:N	2.31	0.59
11:Y:45:GLU:N	11:Y:281:SER:O	2.35	0.59
12:f:733:LEU:CB	14:j:364:MET:HA	2.33	0.59
12:f:1983:ARG:O	12:f:1986:SER:N	2.33	0.59
12:m:152:PHE:O	12:m:157:VAL:N	2.27	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:ASP:HA	6:P:93:GLU:H	1.68	0.59
12:f:3106:GLY:O	12:f:3110:THR:N	2.24	0.59
14:j:234:CYS:C	14:j:236:ALA:H	2.11	0.59
12:f:4329:ARG:O	12:f:4333:THR:N	2.32	0.59
12:e:2266:GLY:HA2	12:e:2276:THR:O	2.02	0.58
12:f:1731:THR:HA	12:f:1784:ASN:HA	1.83	0.58
12:f:2760:PRO:HA	12:f:2763:ARG:H	1.67	0.58
12:e:3874:GLY:HA2	12:e:4146:VAL:N	2.18	0.58
12:f:156:ALA:O	12:f:160:PHE:N	2.26	0.58
12:f:2566:ASP:O	12:f:2603:MET:HA	2.03	0.58
12:f:2873:TYR:HA	12:f:2882:ILE:O	2.02	0.58
14:i:363:LEU:C	14:i:365:LYS:N	2.61	0.58
14:j:53:SER:O	14:j:55:LYS:N	2.36	0.58
14:j:181:PHE:CA	14:j:313:GLY:HA2	2.34	0.58
12:m:153:ILE:O	12:m:158:ALA:N	2.34	0.58
12:m:1057:TYR:C	12:m:1059:CYS:N	2.60	0.58
12:e:1554:SER:HA	12:e:1642:GLY:HA3	1.86	0.58
12:e:2951:ALA:O	12:e:2956:LEU:N	2.22	0.58
12:e:2639:CYS:HA	12:e:2652:PRO:HA	1.85	0.58
12:f:2933:LEU:N	12:f:3064:VAL:O	2.37	0.58
12:f:3873:ARG:N	12:f:4021:MET:O	2.36	0.58
14:i:37:SER:O	14:i:41:SER:N	2.29	0.58
12:e:2167:GLY:N	12:e:4533:SER:HA	2.18	0.58
12:e:4039:THR:HA	12:e:4141:ALA:O	2.04	0.58
12:f:888:LEU:C	12:f:891:HIS:H	2.11	0.58
14:i:59:VAL:O	14:i:109:LEU:N	2.29	0.58
14:r:273:SER:O	14:r:277:GLU:N	2.36	0.58
12:e:2166:PRO:C	12:e:4533:SER:HA	2.28	0.58
12:e:3874:GLY:HA2	12:e:4146:VAL:H	1.68	0.58
12:f:220:CYS:O	12:f:225:GLU:N	2.37	0.58
12:f:1015:GLU:HA	12:f:1018:PHE:O	2.04	0.58
12:f:1398:MET:HA	12:f:2903:GLU:HA	1.85	0.58
12:e:733:LEU:O	14:i:364:MET:N	2.36	0.58
12:f:868:VAL:O	12:f:870:ASP:N	2.37	0.58
12:f:2213:ILE:O	12:f:2217:ASN:N	2.35	0.58
12:f:915:LEU:C	12:f:918:GLY:H	2.12	0.58
12:e:3993:ILE:O	12:e:3997:ARG:N	2.37	0.57
12:f:1513:TYR:O	12:f:1517:GLU:N	2.36	0.57
15:l:80:VAL:HA	15:l:88:LEU:O	2.04	0.57
12:e:1554:SER:HA	12:e:1642:GLY:CA	2.33	0.57
12:f:963:ARG:O	12:f:969:ILE:CA	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:4040:PRO:HA	12:f:4124:LEU:O	2.04	0.57
12:f:4041:VAL:N	12:f:4124:LEU:O	2.37	0.57
15:l:57:VAL:O	15:l:61:ASP:N	2.32	0.57
12:f:4249:GLN:HA	12:f:4253:GLY:HA3	1.85	0.57
12:f:4322:GLY:O	12:f:4637:GLU:HA	2.03	0.57
14:r:56:ASN:O	14:r:132:LEU:N	2.27	0.57
12:e:80:GLU:HA	12:e:115:SER:HA	1.87	0.57
12:f:2538:GLU:H	12:f:2547:PRO:HA	1.68	0.57
12:f:3562:TRP:O	12:f:3566:SER:N	2.29	0.57
14:i:73:LYS:HA	14:i:77:ALA:O	2.04	0.57
13:o:391:GLY:HA3	13:o:396:HIS:HA	1.86	0.57
12:e:4192:GLU:C	12:e:4194:LEU:H	2.12	0.57
12:f:1309:THR:C	12:f:1311:LEU:H	2.13	0.57
12:f:1983:ARG:C	12:f:1985:HIS:H	2.13	0.57
14:j:218:VAL:HA	14:j:263:LEU:C	2.29	0.57
12:n:803:LEU:O	12:n:894:SER:CA	2.52	0.57
12:e:4036:LYS:O	12:e:4038:ASN:N	2.33	0.57
12:f:2162:SER:O	12:f:2167:GLY:N	2.23	0.57
14:j:233:LYS:H	14:j:273:SER:HA	1.70	0.57
14:j:355:ALA:O	14:j:356:ALA:C	2.46	0.57
12:e:2590:PRO:O	12:e:2731:VAL:HA	2.04	0.57
12:f:918:GLY:N	12:f:950:GLY:HA3	2.20	0.57
12:f:2728:LEU:O	12:f:2731:VAL:N	2.31	0.57
12:f:3890:ILE:O	12:f:3894:GLY:HA3	2.05	0.57
12:f:3517:ALA:HA	12:f:3525:ARG:HA	1.86	0.56
12:e:165:ILE:O	12:e:171:ALA:N	2.38	0.56
12:e:1019:TYR:C	12:e:1021:ASN:H	2.12	0.56
12:e:2934:LEU:O	12:e:3092:ASN:N	2.35	0.56
12:f:948:LYS:O	12:f:949:PRO:C	2.47	0.56
12:f:962:LEU:HA	12:f:970:TYR:O	2.05	0.56
12:m:39:PRO:O	12:m:46:GLY:N	2.37	0.56
12:e:283:ARG:HA	12:f:176:ASP:H	1.71	0.56
12:e:869:TYR:H	12:e:951:GLY:HA2	1.70	0.56
12:e:918:GLY:N	12:e:950:GLY:HA2	2.20	0.56
12:e:3409:VAL:O	12:e:3413:ARG:N	2.34	0.56
12:f:1261:TRP:O	12:f:1265:LYS:N	2.38	0.56
12:f:1725:GLU:O	12:f:1729:LYS:N	2.38	0.56
12:f:2381:ARG:O	12:f:2385:ILE:N	2.38	0.56
12:f:2618:VAL:N	12:f:2660:VAL:O	2.33	0.56
12:f:2961:ILE:O	12:f:2963:VAL:N	2.38	0.56
12:f:4287:LYS:HA	12:f:4291:HIS:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:i:56:ASN:HA	14:i:105:ASN:O	2.05	0.56
12:f:962:LEU:HA	12:f:971:LEU:HA	1.87	0.56
12:f:4443:LYS:O	12:f:4445:THR:N	2.37	0.56
5:L:181:LYS:O	5:L:185:GLY:N	2.32	0.56
14:i:229:VAL:O	14:i:269:LEU:HA	2.05	0.56
14:j:53:SER:C	14:j:55:LYS:H	2.14	0.56
12:e:2163:ASP:O	12:e:4536:LEU:N	2.38	0.56
12:f:1348:GLU:HA	12:f:1432:GLY:CA	2.36	0.56
12:f:2324:LEU:HA	12:f:2335:LEU:H	1.71	0.56
12:f:2439:HIS:O	12:f:2443:LEU:N	2.29	0.56
12:e:4179:LEU:O	12:e:4183:LEU:N	2.35	0.56
12:f:884:ALA:O	12:f:888:LEU:N	2.38	0.56
12:f:1516:PHE:O	12:f:1520:ALA:N	2.27	0.56
13:p:391:GLY:HA3	13:p:396:HIS:HA	1.86	0.56
12:f:2503:SER:C	12:f:2505:ASP:H	2.13	0.56
12:f:3514:ILE:O	12:f:3518:GLY:HA3	2.06	0.56
12:f:3847:LYS:C	12:f:3849:VAL:H	2.12	0.56
12:f:4043:MET:N	12:f:4126:LEU:O	2.39	0.56
14:j:62:GLU:O	14:j:65:SER:N	2.32	0.56
12:n:776:PRO:CA	13:p:375:LEU:O	2.53	0.56
12:f:924:GLN:O	12:f:929:GLN:N	2.31	0.56
12:f:1902:GLY:HA2	12:f:2037:ARG:O	2.05	0.56
12:f:2220:LEU:N	12:f:2341:ILE:O	2.39	0.56
12:f:3928:THR:O	12:f:3931:GLN:N	2.38	0.56
13:p:573:LEU:HA	13:p:589:ASP:HA	1.88	0.56
12:f:80:GLU:N	12:f:102:ASN:O	2.27	0.55
12:f:912:GLY:O	12:f:1026:MET:HA	2.06	0.55
12:f:2559:THR:HA	12:f:2754:ALA:C	2.31	0.55
12:f:2594:CYS:HA	12:f:2712:CYS:O	2.05	0.55
12:f:2504:GLY:O	12:f:2734:VAL:HA	2.07	0.55
13:h:394:ASN:O	12:m:599:GLY:HA3	2.06	0.55
12:f:2600:GLY:O	12:f:2603:MET:N	2.39	0.55
12:e:2789:GLN:C	12:e:2791:HIS:H	2.13	0.55
12:f:3513:PHE:O	12:f:3518:GLY:N	2.39	0.55
14:i:91:LEU:O	14:i:103:ARG:HA	2.06	0.55
14:i:227:VAL:O	14:i:268:ALA:N	2.39	0.55
3:J:137:MET:O	3:J:304:VAL:N	2.39	0.55
12:f:803:LEU:HA	14:j:355:ALA:HA	1.88	0.55
12:f:2250:VAL:O	12:f:2300:TRP:N	2.39	0.55
13:o:573:LEU:HA	13:o:589:ASP:HA	1.88	0.55
12:e:1861:MET:C	12:e:1863:ASN:H	2.12	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:2952:TRP:O	12:f:2955:GLY:N	2.32	0.55
12:f:4327:ALA:O	12:f:4331:LEU:N	2.34	0.55
12:f:2189:MET:C	12:f:2191:LEU:H	2.15	0.55
14:i:301:LEU:O	14:i:309:PHE:N	2.23	0.55
12:f:917:ALA:O	12:f:950:GLY:HA3	2.06	0.55
12:f:1880:VAL:O	12:f:1882:THR:N	2.39	0.55
12:e:3997:ARG:C	12:e:3999:ASP:H	2.14	0.55
12:f:1026:MET:C	12:f:1028:ASP:H	2.15	0.55
12:f:4167:SER:O	12:f:4171:LYS:N	2.25	0.55
15:k:37:PRO:O	15:k:42:TYR:N	2.34	0.55
12:e:2255:ASP:O	12:e:2257:LYS:N	2.40	0.54
12:f:1906:GLY:HA3	12:f:2042:THR:CA	2.38	0.54
12:f:3944:PHE:HA	12:f:3975:SER:O	2.07	0.54
12:e:2308:ASP:O	12:e:2310:GLU:N	2.36	0.54
12:f:1474:GLU:CA	12:f:1587:LEU:HA	2.28	0.54
12:f:2499:LEU:O	12:f:2502:LEU:N	2.34	0.54
12:f:4326:ASN:O	12:f:4330:VAL:N	2.27	0.54
14:j:75:GLN:HA	14:j:91:LEU:CA	2.38	0.54
12:f:2597:PRO:O	12:f:2599:SER:N	2.41	0.54
12:f:995:SER:HA	12:f:1020:ARG:CA	2.25	0.54
12:f:4543:VAL:HA	12:f:4589:GLN:O	2.08	0.54
13:g:409:SER:O	13:g:419:GLN:N	2.40	0.54
14:i:363:LEU:O	14:i:365:LYS:N	2.40	0.54
12:e:2985:CYS:HA	12:e:3033:CYS:HA	1.88	0.54
12:f:2639:CYS:HA	12:f:2653:VAL:H	1.73	0.54
12:f:4604:VAL:HA	12:f:4625:GLU:HA	1.88	0.54
12:e:435:ARG:HA	12:e:447:LYS:HA	1.90	0.54
12:f:1959:GLU:N	12:f:2017:THR:O	2.41	0.54
12:f:4248:ALA:O	12:f:4253:GLY:N	2.41	0.54
12:m:119:ILE:O	12:m:136:ARG:N	2.40	0.54
1:C:48:MET:CB	1:E:173:GLY:HA2	2.38	0.54
12:e:483:VAL:O	12:e:512:PHE:N	2.40	0.54
12:f:1093:PHE:C	12:f:1095:ASN:H	2.16	0.54
13:h:551:LEU:O	13:h:562:THR:N	2.41	0.54
14:i:181:PHE:O	14:i:313:GLY:HA3	2.07	0.54
14:j:56:ASN:O	14:j:131:THR:HA	2.05	0.54
4:K:94:ILE:HA	4:K:110:PRO:HA	1.90	0.54
12:f:2536:ASP:O	12:f:2548:TRP:N	2.21	0.54
12:f:4167:SER:O	12:f:4169:ILE:N	2.41	0.54
1:B:42:PRO:HA	1:B:69:LEU:HA	1.89	0.54
12:e:753:LEU:O	12:e:757:GLY:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:912:GLY:C	12:f:1026:MET:HA	2.33	0.54
12:f:2227:GLY:C	12:f:2229:GLY:H	2.15	0.54
12:f:2937:GLY:C	12:f:3069:ASN:HA	2.32	0.54
12:e:2162:SER:C	12:e:4530:GLN:HA	2.32	0.54
12:e:2789:GLN:O	12:e:2791:HIS:N	2.39	0.54
12:f:4485:ARG:HA	12:f:4513:GLY:O	2.07	0.54
14:j:257:HIS:CA	14:j:332:PRO:HA	2.38	0.54
12:f:2242:GLU:CA	12:f:2249:GLY:H	2.20	0.53
12:f:2365:SER:O	12:f:2368:VAL:N	2.41	0.53
12:f:3690:PRO:O	12:f:3694:SER:N	2.39	0.53
12:f:4010:SER:O	12:f:4014:GLY:HA2	2.07	0.53
12:f:4378:ARG:HA	12:f:4438:CYS:O	2.08	0.53
13:p:384:VAL:HA	13:p:402:SER:HA	1.90	0.53
12:f:2548:TRP:O	12:f:2552:VAL:N	2.42	0.53
12:f:2740:GLY:O	12:f:2743:SER:N	2.41	0.53
12:e:960:HIS:O	12:e:1107:ILE:HA	2.09	0.53
12:e:4167:SER:O	12:e:4171:LYS:N	2.40	0.53
12:f:2229:GLY:O	12:f:2232:MET:N	2.42	0.53
12:f:4283:LYS:HA	12:f:4295:GLN:HA	1.89	0.53
15:l:16:GLY:HA3	15:l:93:ASN:H	1.74	0.53
12:m:132:SER:H	12:n:41:LEU:C	2.17	0.53
12:n:3891:LYS:O	12:n:3895:THR:N	2.42	0.53
13:o:384:VAL:HA	13:o:402:SER:HA	1.89	0.53
12:f:948:LYS:O	12:f:950:GLY:N	2.41	0.53
12:f:4174:ASN:N	12:f:4232:ASN:HA	2.24	0.53
15:k:65:ASP:O	15:l:74:LYS:N	2.41	0.53
12:e:720:ILE:CB	12:e:735:LEU:HA	2.39	0.53
12:e:3685:THR:O	12:e:4446:ASN:HA	2.09	0.53
12:e:734:LYS:HA	14:i:363:LEU:CA	2.39	0.53
12:f:1210:TYR:C	12:f:1212:ASP:N	2.66	0.53
12:f:1639:GLU:O	12:f:1643:ASN:N	2.36	0.53
12:f:2599:SER:O	12:f:2738:TYR:HA	2.08	0.53
12:f:2926:PHE:O	12:f:3061:ASN:HA	2.08	0.53
12:f:4174:ASN:H	12:f:4232:ASN:HA	1.72	0.53
14:i:43:VAL:O	14:i:46:ARG:N	2.35	0.53
12:f:2227:GLY:C	12:f:2229:GLY:N	2.65	0.53
12:f:4185:TRP:O	12:f:4189:ILE:N	2.30	0.53
12:e:818:GLU:O	12:e:819:GLY:C	2.50	0.53
5:L:145:LYS:O	5:L:178:GLN:N	2.38	0.53
12:e:4631:ASP:O	12:e:4633:ARG:N	2.41	0.53
12:f:2147:PRO:O	12:f:2362:VAL:HA	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:j:239:VAL:O	14:j:243:GLU:N	2.31	0.53
12:f:1313:SER:C	12:f:1315:SER:N	2.67	0.53
12:f:1731:THR:O	12:f:1784:ASN:HA	2.09	0.53
14:j:56:ASN:N	14:j:130:GLU:O	2.42	0.53
14:j:140:SER:HA	14:j:236:ALA:HA	1.91	0.53
14:j:274:VAL:HA	14:j:277:GLU:HA	1.91	0.53
12:f:1344:ASP:O	12:f:1348:GLU:N	2.41	0.52
12:f:1793:ALA:HA	12:f:2058:GLY:HA2	1.91	0.52
12:f:2365:SER:C	12:f:2367:ASP:H	2.17	0.52
12:m:3891:LYS:O	12:m:3895:THR:N	2.41	0.52
12:f:539:SER:O	12:f:543:THR:N	2.37	0.52
12:f:2898:LYS:O	12:f:2902:GLU:N	2.25	0.52
12:e:3926:GLY:HA3	12:e:3958:SER:CB	2.39	0.52
12:n:4087:ALA:O	12:n:4091:GLY:N	2.43	0.52
12:e:2592:VAL:O	12:e:2733:VAL:HA	2.10	0.52
12:f:38:VAL:O	12:f:42:LEU:N	2.35	0.52
12:f:1272:ARG:O	12:f:1275:GLU:N	2.42	0.52
12:f:2302:VAL:HA	12:f:2342:MET:O	2.08	0.52
14:j:289:HIS:HA	14:j:294:PHE:N	2.24	0.52
6:P:312:LYS:O	6:P:315:GLN:N	2.42	0.52
12:f:4631:ASP:O	12:f:4634:SER:N	2.43	0.52
15:k:12:GLN:O	15:k:17:VAL:N	2.42	0.52
12:f:2162:SER:HA	12:f:2168:VAL:H	1.74	0.52
12:f:3133:LEU:O	12:f:3135:GLN:N	2.37	0.52
4:K:163:PHE:HA	4:K:170:ASN:HA	1.91	0.52
12:f:929:GLN:O	12:f:931:GLU:N	2.42	0.52
12:f:2785:THR:C	12:f:2787:ASP:H	2.18	0.52
12:f:3058:VAL:O	12:f:3062:LEU:N	2.43	0.52
12:e:806:ALA:HA	14:i:356:ALA:CA	2.32	0.52
12:f:1405:SER:CA	12:f:3658:GLY:HA2	2.40	0.52
12:f:2301:ILE:O	12:f:2341:ILE:HA	2.09	0.52
12:f:2623:SER:C	12:f:2625:ALA:N	2.67	0.52
12:e:810:LYS:N	14:i:357:GLU:N	2.57	0.52
12:e:3073:GLU:O	12:e:3080:ALA:N	2.43	0.52
12:e:4604:VAL:HA	12:e:4624:PHE:O	2.10	0.52
12:f:1650:LEU:C	12:f:1652:LYS:H	2.17	0.52
12:f:2931:GLY:O	12:f:3063:HIS:HA	2.10	0.52
12:f:3941:LEU:O	12:f:3944:PHE:N	2.43	0.52
12:f:3943:ALA:HA	12:f:3976:GLU:O	2.09	0.52
13:g:359:LEU:N	13:g:371:GLN:O	2.42	0.52
12:m:4087:ALA:O	12:m:4091:GLY:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:e:806:ALA:CB	14:i:355:ALA:HA	2.19	0.52
12:e:2255:ASP:C	12:e:2257:LYS:H	2.17	0.52
12:f:1406:GLU:H	12:f:3658:GLY:CA	2.23	0.52
12:f:3489:TRP:O	12:f:3492:THR:N	2.42	0.52
12:f:3656:THR:O	12:f:3658:GLY:N	2.43	0.52
12:m:975:ILE:C	12:m:977:GLU:N	2.68	0.52
12:f:2145:MET:O	12:f:2149:LEU:N	2.43	0.51
12:f:3517:ALA:CA	12:f:3525:ARG:HA	2.41	0.51
14:j:53:SER:C	14:j:55:LYS:N	2.68	0.51
12:e:806:ALA:HB1	14:i:355:ALA:CA	2.33	0.51
12:f:1112:VAL:O	12:f:1113:GLN:C	2.52	0.51
12:f:2253:ILE:HA	12:f:2302:VAL:O	2.10	0.51
12:f:3555:ASN:O	12:f:3558:GLU:N	2.43	0.51
14:j:320:ILE:O	14:j:323:LEU:N	2.44	0.51
12:e:4248:ALA:O	12:e:4253:GLY:HA3	2.11	0.51
12:f:2778:THR:O	12:f:2782:GLU:N	2.44	0.51
12:f:3516:TYR:O	12:f:3519:TYR:N	2.39	0.51
1:B:325:ASP:HA	6:P:93:GLU:N	2.25	0.51
12:f:891:HIS:C	12:m:688:SER:CB	2.83	0.51
12:f:1908:ALA:O	12:f:1910:THR:N	2.40	0.51
12:f:2128:ALA:O	12:f:2131:LEU:N	2.42	0.51
12:f:2319:LEU:O	12:f:2359:CYS:HA	2.11	0.51
12:f:2548:TRP:O	12:f:2551:LYS:N	2.44	0.51
12:f:2766:ALA:O	12:f:2770:THR:N	2.30	0.51
12:f:3757:LYS:H	12:f:3759:ARG:H	1.59	0.51
12:f:3901:TYR:O	12:f:3904:GLU:N	2.43	0.51
14:q:55:LYS:O	14:q:105:ASN:N	2.42	0.51
12:e:2301:ILE:O	12:e:2342:MET:N	2.34	0.51
12:e:4234:SER:O	12:e:4238:ILE:N	2.44	0.51
12:f:3613:SER:HA	12:f:3636:GLN:O	2.11	0.51
12:f:3670:ASP:O	12:f:3672:SER:N	2.43	0.51
12:f:3692:LEU:O	12:f:3695:ARG:N	2.44	0.51
9:V:60:HIS:O	9:V:90:HIS:HA	2.10	0.51
12:e:3587:PRO:HA	12:e:3697:THR:O	2.11	0.51
12:f:1109:TYR:O	12:f:1113:GLN:N	2.41	0.51
12:f:1363:LEU:O	12:f:1366:LEU:N	2.44	0.51
12:f:4530:GLN:C	12:f:4533:SER:H	2.19	0.51
15:k:18:GLN:H	15:k:92:GLN:HA	1.75	0.51
12:f:1905:PHE:O	12:f:2042:THR:HA	2.10	0.51
12:f:4308:TRP:O	12:f:4312:LEU:N	2.38	0.51
14:j:269:LEU:N	14:j:310:ILE:O	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:155:GLY:N	1:D:170:ILE:O	2.36	0.51
12:f:3217:GLU:O	12:f:3220:ARG:N	2.44	0.51
14:j:216:ASP:C	14:j:218:VAL:H	2.19	0.51
12:e:1098:THR:HA	12:e:1110:GLY:HA2	1.94	0.50
12:f:948:LYS:C	12:f:950:GLY:N	2.65	0.50
12:f:1135:LEU:O	12:f:1138:ASN:N	2.44	0.50
12:f:2533:PRO:O	12:f:2536:ASP:N	2.44	0.50
12:m:806:ALA:CB	14:q:356:ALA:N	2.43	0.50
12:f:2500:TRP:O	12:f:2504:GLY:HA3	2.11	0.50
12:f:3891:LYS:O	12:f:3895:THR:N	2.44	0.50
12:f:4445:THR:O	12:f:4449:ARG:N	2.36	0.50
12:f:2004:LYS:O	12:f:2006:VAL:N	2.44	0.50
12:f:2620:LEU:HA	12:f:3019:GLY:HA2	1.94	0.50
12:f:2714:PRO:C	12:f:2716:THR:H	2.19	0.50
12:f:4238:ILE:O	12:f:4240:TRP:N	2.44	0.50
14:j:181:PHE:C	14:j:313:GLY:HA2	2.36	0.50
12:m:1029:GLY:C	12:m:1031:VAL:H	2.20	0.50
12:e:2255:ASP:HA	12:e:2304:ASP:O	2.11	0.50
12:f:1351:TRP:H	12:f:1430:THR:HA	1.73	0.50
12:f:2768:PRO:O	12:f:2772:ALA:N	2.39	0.50
12:f:3901:TYR:O	12:f:3905:PHE:N	2.34	0.50
12:f:2667:ASN:O	12:f:2720:ARG:HA	2.12	0.50
12:f:3024:ASP:O	12:f:3027:ALA:N	2.45	0.50
12:f:4176:ARG:O	12:f:4180:TYR:N	2.22	0.50
14:j:356:ALA:O	14:j:357:GLU:C	2.54	0.50
12:f:2686:MET:HA	12:f:2691:GLY:C	2.36	0.50
12:f:3627:LEU:O	12:f:3671:LEU:HA	2.12	0.50
12:f:3637:ASP:N	12:f:3681:THR:HA	2.25	0.50
13:o:315:VAL:O	13:o:326:GLU:N	2.45	0.50
10:Z:1141:LEU:O	10:Z:1145:GLU:N	2.45	0.50
12:e:2759:VAL:HA	12:e:2814:GLU:O	2.12	0.50
12:f:1895:ALA:O	12:f:1900:LEU:N	2.45	0.50
12:f:3198:GLN:HA	12:f:3493:SER:HA	1.92	0.50
12:f:4093:TRP:HA	12:f:4123:ARG:H	1.77	0.50
14:j:37:SER:O	14:j:40:LEU:N	2.45	0.50
1:E:41:ARG:O	1:E:70:SER:N	2.33	0.50
12:e:818:GLU:O	12:e:820:ILE:N	2.45	0.50
12:e:4538:GLU:O	12:e:4595:GLN:N	2.37	0.50
12:f:4462:ARG:C	12:f:4464:TRP:N	2.70	0.50
14:i:137:ALA:O	14:i:231:CYS:HA	2.12	0.50
15:k:25:THR:C	15:k:27:GLY:H	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:98:GLN:O	1:G:100:GLN:N	2.45	0.50
12:f:2597:PRO:C	12:f:2599:SER:N	2.70	0.50
12:f:2686:MET:O	12:f:2691:GLY:N	2.44	0.50
12:f:3837:HIS:C	12:f:3839:VAL:N	2.66	0.50
12:m:437:ILE:O	12:m:441:LYS:N	2.42	0.50
14:j:257:HIS:HA	14:j:332:PRO:HA	1.94	0.49
14:j:369:LEU:O	14:j:373:GLN:N	2.19	0.49
12:f:3489:TRP:O	12:f:3490:GLU:C	2.55	0.49
14:i:57:ILE:O	14:i:59:VAL:N	2.45	0.49
6:M:155:HIS:O	6:M:160:LEU:N	2.33	0.49
12:f:1590:ASP:O	12:f:1594:ILE:N	2.44	0.49
12:f:2983:SER:C	12:f:2987:ASN:HA	2.38	0.49
12:f:3506:ASP:N	12:f:3543:PHE:HA	2.28	0.49
12:f:4560:VAL:O	12:f:4587:LEU:HA	2.12	0.49
1:E:20:VAL:HA	1:E:36:PRO:HA	1.94	0.49
12:f:33:HIS:O	12:f:37:LEU:N	2.36	0.49
12:f:957:ASN:HA	12:f:1104:PRO:O	2.12	0.49
12:f:1758:TRP:O	12:f:1761:ASN:N	2.45	0.49
12:f:3751:GLN:C	12:f:3753:LEU:H	2.21	0.49
12:f:4169:ILE:O	12:f:4177:ALA:N	2.45	0.49
14:i:119:LEU:C	14:i:122:ALA:H	2.20	0.49
15:k:17:VAL:HA	15:k:92:GLN:HA	1.93	0.49
12:f:1479:ASN:HA	12:f:1484:CYS:O	2.12	0.49
12:f:2306:ASP:O	12:f:2308:ASP:N	2.45	0.49
12:m:195:HIS:O	12:m:199:ASN:N	2.45	0.49
5:L:167:TYR:N	5:L:199:LYS:O	2.31	0.49
12:e:995:SER:HA	12:e:1018:PHE:CA	2.38	0.49
12:f:1726:ILE:C	12:f:1733:ILE:HA	2.37	0.49
14:j:232:THR:O	14:j:233:LYS:C	2.55	0.49
12:n:1054:TRP:C	12:n:1056:GLN:H	2.20	0.49
12:e:2774:VAL:O	12:e:2778:THR:N	2.38	0.49
12:f:925:VAL:HA	12:f:930:ALA:N	2.28	0.49
12:f:1380:TYR:C	12:f:1382:SER:N	2.71	0.49
12:f:2981:ARG:O	12:f:2986:LYS:N	2.34	0.49
12:n:315:SER:O	12:n:319:ASP:N	2.45	0.49
13:p:315:VAL:O	13:p:326:GLU:N	2.45	0.49
12:e:2635:PHE:O	12:e:2639:CYS:N	2.45	0.49
12:e:2995:ASP:O	12:e:2999:VAL:N	2.46	0.49
12:f:888:LEU:O	12:f:893:TYR:N	2.28	0.49
12:f:2300:TRP:HA	12:f:2340:ARG:O	2.12	0.49
13:h:266:SER:O	13:h:598:ASP:N	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:h:436:SER:O	13:h:450:GLY:N	2.40	0.49
12:f:1420:LEU:C	12:f:1422:VAL:H	2.21	0.49
12:f:2163:ASP:O	12:f:4535:SER:HA	2.12	0.49
12:f:3626:ALA:O	12:f:3630:GLY:N	2.46	0.49
12:f:3700:ASN:C	12:f:3702:THR:N	2.70	0.49
1:E:42:PRO:HA	1:E:69:LEU:HA	1.95	0.49
12:f:4462:ARG:C	12:f:4464:TRP:H	2.21	0.49
12:n:776:PRO:C	13:p:375:LEU:O	2.56	0.49
12:f:1846:PHE:HA	12:f:1857:LEU:HA	1.95	0.48
12:f:4634:SER:O	12:f:4638:ARG:N	2.44	0.48
12:e:3999:ASP:C	12:e:4001:LEU:H	2.21	0.48
12:e:4335:GLN:O	12:e:4338:ASP:C	2.56	0.48
12:f:4060:ALA:C	12:f:4063:ASN:H	2.21	0.48
14:j:231:CYS:O	14:j:272:THR:O	2.31	0.48
12:n:840:VAL:O	12:n:844:GLN:N	2.37	0.48
12:f:1655:LYS:C	12:f:1657:MET:N	2.71	0.48
12:f:2089:GLY:O	12:f:2092:ALA:N	2.47	0.48
3:J:248:TYR:O	3:J:256:LEU:N	2.40	0.48
12:f:1542:ARG:O	12:f:1545:VAL:N	2.45	0.48
12:f:4252:TYR:O	12:f:4256:VAL:N	2.39	0.48
8:U:82:MET:HA	8:U:99:MET:O	2.14	0.48
12:e:4234:SER:O	12:e:4237:LYS:N	2.46	0.48
12:f:846:LYS:O	12:f:850:LEU:N	2.26	0.48
12:f:1964:GLU:O	12:f:1967:MET:N	2.46	0.48
12:f:4375:ALA:O	12:f:4378:ARG:N	2.46	0.48
12:f:4570:CYS:HA	12:f:4574:LYS:O	2.13	0.48
13:g:551:LEU:O	13:g:562:THR:N	2.47	0.48
12:f:2245:GLU:C	12:f:2247:VAL:N	2.72	0.48
12:f:4044:CYS:O	12:f:4147:PHE:N	2.40	0.48
14:j:289:HIS:HA	14:j:294:PHE:O	2.14	0.48
1:G:41:ARG:O	1:G:70:SER:N	2.38	0.48
12:f:892:SER:O	12:f:893:TYR:C	2.56	0.48
12:f:1758:TRP:O	12:f:1760:GLU:N	2.47	0.48
12:f:2958:VAL:HA	12:f:2991:ALA:O	2.14	0.48
14:i:186:GLU:HA	14:i:297:THR:HA	1.96	0.48
14:j:257:HIS:HA	14:j:332:PRO:O	2.13	0.48
12:m:585:PHE:O	12:m:589:ASN:N	2.47	0.48
12:m:747:SER:HA	12:m:768:ALA:HB1	1.95	0.48
12:e:539:SER:O	12:e:543:THR:N	2.43	0.48
12:e:2160:LEU:O	12:e:2161:LEU:C	2.56	0.48
12:f:209:ILE:O	12:f:210:HIS:C	2.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:2365:SER:O	12:f:2367:ASP:N	2.47	0.48
14:i:289:HIS:HA	14:i:294:PHE:N	2.29	0.48
12:f:918:GLY:HA2	12:f:950:GLY:CA	2.44	0.48
12:f:2936:ILE:O	12:f:3095:GLY:N	2.37	0.48
12:f:3907:HIS:O	12:f:3911:GLY:N	2.47	0.48
13:h:435:THR:H	13:h:451:SER:HA	1.77	0.48
14:j:273:SER:O	14:j:276:GLU:N	2.47	0.48
12:e:2585:LEU:C	12:e:2588:HIS:H	2.22	0.47
12:f:1028:ASP:O	12:f:1031:VAL:N	2.47	0.47
12:f:2085:HIS:HA	12:f:2357:SER:HA	1.96	0.47
12:f:2426:TYR:HA	12:f:2431:GLY:HA3	1.95	0.47
12:f:4510:CYS:HA	12:f:4561:THR:O	2.13	0.47
14:i:59:VAL:N	14:i:107:TRP:O	2.47	0.47
14:j:159:HIS:O	14:j:163:MET:N	2.29	0.47
12:e:3588:LEU:O	12:e:3698:PHE:HA	2.13	0.47
12:e:4458:GLY:C	12:e:4474:THR:HA	2.38	0.47
12:f:1057:TYR:C	12:f:1059:CYS:N	2.72	0.47
12:f:2772:ALA:O	12:f:2776:PHE:N	2.40	0.47
12:f:3759:ARG:C	12:f:3762:ASP:H	2.22	0.47
1:A:98:GLN:O	1:A:100:GLN:N	2.48	0.47
12:f:2199:VAL:C	12:f:2201:GLY:H	2.22	0.47
12:f:2482:GLN:O	12:f:2485:GLN:N	2.47	0.47
12:f:3891:LYS:C	12:f:3894:GLY:H	2.22	0.47
12:e:4182:LEU:O	12:e:4186:PHE:N	2.31	0.47
12:e:4192:GLU:C	12:e:4194:LEU:N	2.71	0.47
12:f:887:ASP:O	12:f:891:HIS:N	2.47	0.47
12:f:2356:VAL:O	12:f:2359:CYS:N	2.48	0.47
12:f:2397:ARG:HA	12:f:2403:ASP:H	1.79	0.47
12:f:3699:VAL:O	12:f:3701:PHE:N	2.42	0.47
12:f:4030:ILE:O	12:f:4035:VAL:N	2.46	0.47
14:j:323:LEU:O	14:j:326:ASN:N	2.47	0.47
12:n:2694:ARG:O	12:n:2698:GLN:N	2.48	0.47
1:A:200:LYS:O	1:B:117:PRO:HA	2.15	0.47
1:D:156:VAL:HA	1:D:169:PRO:HA	1.97	0.47
12:e:4529:ALA:O	12:e:4534:TRP:O	2.31	0.47
12:f:2644:THR:C	12:f:2646:ASN:N	2.72	0.47
12:e:1902:GLY:HA2	12:e:2037:ARG:O	2.14	0.47
12:e:4150:PRO:O	12:e:4152:GLY:N	2.47	0.47
12:e:4152:GLY:N	12:e:4314:ASP:O	2.46	0.47
12:f:479:VAL:O	12:f:483:VAL:N	2.42	0.47
12:f:2930:GLN:O	12:f:2932:HIS:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:j:64:GLY:C	14:j:66:GLY:H	2.22	0.47
12:m:2694:ARG:O	12:m:2698:GLN:N	2.47	0.47
12:n:86:GLU:O	12:n:96:LYS:N	2.42	0.47
1:F:145:LEU:O	1:F:343:GLY:HA3	2.14	0.47
1:I:161:GLY:O	1:I:186:ALA:HB1	2.15	0.47
11:Y:427:LYS:HA	11:Y:457:HIS:HA	1.96	0.47
12:e:900:VAL:O	12:e:904:ASP:N	2.36	0.47
12:e:2663:CYS:O	12:e:2711:ALA:N	2.45	0.47
12:e:3601:MET:O	12:e:3605:LYS:N	2.48	0.47
12:f:1995:ALA:C	12:f:1997:ILE:H	2.23	0.47
12:f:2191:LEU:O	12:f:2192:THR:C	2.57	0.47
12:f:3482:LEU:O	12:f:3483:SER:C	2.57	0.47
12:f:3773:LEU:O	12:f:3775:ARG:N	2.47	0.47
12:f:4542:GLU:O	12:f:4590:LEU:HA	2.13	0.47
14:i:43:VAL:C	14:i:46:ARG:H	2.23	0.47
14:j:66:GLY:O	14:j:69:THR:N	2.48	0.47
14:j:137:ALA:O	14:j:139:MET:N	2.48	0.47
14:j:272:THR:HA	14:j:278:LYS:O	2.14	0.47
15:l:58:ARG:HA	15:l:62:PRO:CA	2.30	0.47
1:A:20:VAL:HA	1:A:36:PRO:HA	1.97	0.47
12:f:1527:LEU:O	12:f:1528:ASN:C	2.56	0.47
12:f:2677:GLN:O	12:f:2680:ILE:N	2.48	0.47
12:f:4068:SER:HA	12:f:4095:MET:O	2.15	0.47
12:f:4567:GLY:O	12:f:4578:SER:N	2.30	0.47
14:j:218:VAL:HA	14:j:263:LEU:O	2.14	0.47
12:e:535:GLY:HA2	12:e:546:TRP:HA	1.97	0.47
12:e:4606:THR:HA	12:e:4622:VAL:O	2.14	0.47
12:f:1486:LEU:O	12:f:1488:ARG:N	2.48	0.47
12:f:1902:GLY:N	12:f:2015:PHE:HA	2.29	0.47
15:k:27:GLY:HA3	15:k:44:ASN:N	2.30	0.47
12:m:4549:GLN:O	12:m:4550:SER:CB	2.63	0.47
4:K:160:SER:O	4:K:173:TRP:N	2.35	0.47
12:e:435:ARG:O	12:e:447:LYS:N	2.48	0.47
12:e:1018:PHE:O	12:e:1020:ARG:N	2.47	0.47
12:f:1731:THR:CA	12:f:1784:ASN:HA	2.45	0.47
12:f:2499:LEU:C	12:f:2502:LEU:H	2.18	0.47
12:f:2777:TYR:O	12:f:2781:GLN:N	2.32	0.47
12:f:3869:ASN:C	12:f:3871:VAL:N	2.71	0.47
14:i:119:LEU:O	14:i:122:ALA:N	2.47	0.47
14:i:232:THR:HA	14:i:272:THR:O	2.15	0.47
12:n:1054:TRP:C	12:n:1056:GLN:N	2.73	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:e:819:GLY:O	12:e:820:ILE:C	2.57	0.46
12:e:1351:TRP:H	12:e:1430:THR:HA	1.79	0.46
12:f:2257:LYS:O	12:f:2678:ARG:HA	2.15	0.46
12:f:888:LEU:O	12:f:892:SER:N	2.48	0.46
12:e:120:LYS:HA	12:e:135:LEU:HA	1.96	0.46
12:e:810:LYS:HA	14:i:357:GLU:H	1.80	0.46
12:e:4249:GLN:HA	12:e:4253:GLY:HA3	1.97	0.46
12:f:4387:TRP:O	12:f:4388:LEU:C	2.59	0.46
14:i:64:GLY:C	14:i:66:GLY:H	2.24	0.46
12:f:1380:TYR:O	12:f:1382:SER:N	2.48	0.46
12:f:4015:GLU:HA	12:f:4018:MET:H	1.81	0.46
14:i:367:GLN:C	14:i:369:LEU:H	2.22	0.46
1:C:145:LEU:O	1:C:343:GLY:HA3	2.15	0.46
12:e:1098:THR:O	12:e:1109:TYR:N	2.44	0.46
12:f:1475:LEU:H	12:f:1586:PRO:C	2.24	0.46
12:f:2660:VAL:HA	12:f:2707:GLN:O	2.16	0.46
12:f:3588:LEU:HA	12:f:3679:LEU:O	2.16	0.46
14:j:269:LEU:O	14:j:309:PHE:HA	2.15	0.46
12:f:960:HIS:N	12:f:1106:VAL:O	2.48	0.46
12:f:2754:ALA:C	12:f:2756:LEU:H	2.24	0.46
13:g:315:VAL:O	13:g:326:GLU:N	2.48	0.46
1:D:51:ALA:HB2	1:F:173:GLY:HA3	1.98	0.46
1:E:145:LEU:O	1:E:343:GLY:HA3	2.15	0.46
11:Y:50:TYR:HA	11:Y:56:GLU:O	2.16	0.46
12:e:119:ILE:O	12:e:136:ARG:N	2.49	0.46
12:f:1309:THR:C	12:f:1311:LEU:N	2.74	0.46
12:f:1896:LEU:C	12:f:1899:ARG:H	2.24	0.46
12:f:2597:PRO:O	12:f:2598:GLY:C	2.58	0.46
12:f:2937:GLY:HA3	12:f:3095:GLY:C	2.41	0.46
12:f:3945:LYS:C	12:f:3947:LEU:H	2.23	0.46
12:m:716:ARG:HA	12:m:823:VAL:HA	1.97	0.46
12:m:3407:LYS:O	12:m:3408:ARG:C	2.58	0.46
12:e:1675:GLY:HA3	12:e:1684:VAL:O	2.16	0.46
12:e:3997:ARG:C	12:e:3999:ASP:N	2.73	0.46
12:f:1371:LYS:C	12:f:1373:PHE:H	2.24	0.46
1:G:200:LYS:O	2:H:112:PRO:HA	2.16	0.46
12:f:1926:PHE:O	12:f:1953:ALA:HA	2.16	0.46
14:j:186:GLU:HA	14:j:297:THR:O	2.16	0.46
13:o:268:ASN:N	13:o:596:ILE:O	2.49	0.46
12:f:333:ASN:O	12:f:336:MET:N	2.49	0.46
12:f:972:ASN:HA	12:f:973:PRO:C	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:4026:ASP:O	12:f:4029:HIS:N	2.48	0.46
12:m:715:GLY:O	12:m:824:TRP:N	2.46	0.46
12:n:1057:TYR:C	12:n:1059:CYS:H	2.23	0.46
12:e:1136:GLY:HA3	12:e:1208:TRP:HA	1.98	0.45
12:f:1585:SER:O	12:f:1587:LEU:N	2.50	0.45
15:l:26:GLU:C	15:l:28:ILE:H	2.25	0.45
12:e:1351:TRP:N	12:e:1430:THR:HA	2.31	0.45
12:e:4537:GLU:C	12:e:4539:LEU:H	2.23	0.45
12:f:113:SER:O	12:f:141:SER:HA	2.17	0.45
12:f:116:LEU:HA	12:f:139:THR:HA	1.98	0.45
12:f:1758:TRP:O	12:f:1759:SER:C	2.57	0.45
12:f:4387:TRP:O	12:f:4390:LEU:N	2.48	0.45
14:j:182:GLN:HA	14:j:214:LEU:H	1.79	0.45
12:e:4184:ALA:O	12:e:4188:ALA:N	2.49	0.45
12:f:3577:ALA:O	12:f:3580:LEU:N	2.45	0.45
12:m:654:ILE:O	12:m:657:GLN:N	2.50	0.45
12:n:4549:GLN:O	12:n:4550:SER:CB	2.63	0.45
12:e:4402:VAL:C	12:e:4404:ASN:H	2.25	0.45
12:f:2255:ASP:HA	12:f:2304:ASP:O	2.16	0.45
12:f:2667:ASN:C	12:f:2720:ARG:HA	2.41	0.45
12:f:4545:VAL:HA	12:f:4587:LEU:O	2.16	0.45
13:p:268:ASN:N	13:p:596:ILE:O	2.49	0.45
12:f:929:GLN:O	12:f:930:ALA:C	2.58	0.45
12:f:2365:SER:C	12:f:2367:ASP:N	2.75	0.45
12:f:3773:LEU:C	12:f:3775:ARG:N	2.74	0.45
14:j:185:ILE:O	14:j:297:THR:HA	2.16	0.45
12:e:2066:ALA:C	12:e:2068:LYS:N	2.74	0.45
12:f:1841:GLN:O	12:f:1843:ARG:N	2.50	0.45
1:A:145:LEU:O	1:A:343:GLY:HA3	2.17	0.45
12:f:1283:TYR:O	12:f:1284:GLU:C	2.60	0.45
12:f:2489:TYR:CA	12:f:2543:GLY:HA2	2.46	0.45
12:f:2503:SER:C	12:f:2505:ASP:N	2.72	0.45
12:f:3130:TYR:C	12:f:3132:LYS:H	2.24	0.45
12:n:3407:LYS:O	12:n:3408:ARG:C	2.59	0.45
1:D:161:GLY:O	1:D:186:ALA:HB1	2.17	0.45
1:G:161:GLY:O	1:G:186:ALA:HB1	2.16	0.45
12:e:3612:THR:O	12:e:3635:VAL:HA	2.16	0.45
12:f:82:SER:O	12:f:84:LEU:N	2.50	0.45
12:f:948:LYS:C	12:f:951:GLY:H	2.23	0.45
12:f:1395:LYS:C	12:f:1397:ASN:N	2.73	0.45
12:f:2968:THR:O	12:f:2972:PHE:N	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:3869:ASN:HA	12:f:4020:ILE:O	2.17	0.45
12:f:4224:ASP:O	12:f:4228:LYS:N	2.33	0.45
14:j:117:GLY:C	14:j:119:LEU:H	2.24	0.45
12:n:776:PRO:CB	13:p:375:LEU:C	2.80	0.45
12:e:2162:SER:O	12:e:2165:PHE:O	2.35	0.45
12:e:2644:THR:C	12:e:2646:ASN:H	2.25	0.45
12:e:4527:TYR:O	12:e:4530:GLN:N	2.46	0.45
12:f:995:SER:C	12:f:1019:TYR:O	2.60	0.45
12:f:1272:ARG:C	12:f:1274:GLU:N	2.75	0.45
12:f:2593:LEU:O	12:f:2712:CYS:O	2.35	0.45
12:f:3645:LEU:O	12:f:3649:LEU:N	2.34	0.45
12:f:4060:ALA:HA	12:f:4063:ASN:HA	1.98	0.45
12:f:4208:GLY:O	12:f:4211:ASP:N	2.50	0.45
12:m:802:SER:O	12:m:806:ALA:HB2	2.17	0.45
12:n:803:LEU:CA	12:n:894:SER:O	2.63	0.45
12:e:2596:PRO:O	12:e:2598:GLY:N	2.49	0.45
12:f:1983:ARG:O	12:f:1985:HIS:N	2.50	0.45
12:f:2162:SER:HA	12:f:2168:VAL:N	2.31	0.45
12:f:2189:MET:C	12:f:2191:LEU:N	2.74	0.45
15:l:67:THR:O	15:l:81:ALA:HA	2.17	0.45
12:n:839:THR:O	12:n:843:PHE:N	2.38	0.45
12:e:1070:ASN:O	12:e:1073:GLY:N	2.51	0.44
12:e:1747:ALA:O	12:e:1750:VAL:N	2.50	0.44
12:f:1475:LEU:H	12:f:1587:LEU:HA	1.82	0.44
15:k:25:THR:O	15:k:27:GLY:N	2.50	0.44
4:K:62:PHE:HA	4:K:76:ILE:O	2.17	0.44
12:f:2406:GLU:O	12:f:2410:SER:N	2.51	0.44
12:f:3637:ASP:HA	12:f:3681:THR:HA	2.00	0.44
14:i:367:GLN:C	14:i:369:LEU:N	2.74	0.44
12:e:2051:GLN:HA	12:e:2062:ALA:O	2.17	0.44
12:e:2056:SER:C	12:e:2058:GLY:H	2.24	0.44
12:f:1030:PRO:O	12:f:1034:GLU:N	2.49	0.44
12:f:2621:ASN:H	12:f:3019:GLY:N	2.16	0.44
15:l:69:LEU:C	15:l:71:ILE:H	2.25	0.44
1:B:332:ALA:H	6:P:86:GLY:HA3	1.82	0.44
12:e:720:ILE:HA	12:e:735:LEU:CA	2.34	0.44
12:e:912:GLY:CA	12:e:1026:MET:HA	2.48	0.44
12:f:1348:GLU:HA	12:f:1432:GLY:N	2.32	0.44
12:f:2388:ASP:O	12:f:2390:GLY:N	2.50	0.44
12:f:3505:GLY:N	12:f:3542:GLN:O	2.40	0.44
12:f:4279:ASP:C	12:f:4281:GLU:H	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:h:527:VAL:HA	13:h:544:ASP:HA	1.99	0.44
12:e:2772:ALA:O	12:e:2776:PHE:N	2.39	0.44
12:f:1313:SER:O	12:f:1316:GLU:N	2.47	0.44
12:f:1692:ILE:C	12:f:1695:HIS:H	2.24	0.44
12:f:2855:LEU:O	12:f:2859:PRO:HA	2.17	0.44
12:f:3069:ASN:O	12:f:3070:PRO:C	2.61	0.44
12:f:3700:ASN:O	12:f:3702:THR:N	2.49	0.44
12:f:4508:HIS:HA	12:f:4559:GLY:O	2.18	0.44
14:i:311:PRO:O	14:i:315:ASP:N	2.51	0.44
14:j:151:LYS:O	14:j:155:VAL:N	2.35	0.44
12:f:961:GLU:HA	12:f:1108:ASP:C	2.43	0.44
12:f:2249:GLY:HA2	12:f:2298:ARG:O	2.17	0.44
12:f:3602:ASN:C	12:f:3605:LYS:H	2.26	0.44
12:f:4129:GLU:O	12:f:4131:ASN:N	2.50	0.44
14:j:94:HIS:HA	14:j:101:HIS:HA	1.99	0.44
11:Y:426:PHE:O	11:Y:458:VAL:N	2.50	0.44
12:e:2390:GLY:O	12:e:2394:ALA:N	2.51	0.44
12:e:2963:VAL:O	12:e:3665:GLY:HA2	2.18	0.44
6:P:258:GLY:O	6:P:260:CYS:N	2.48	0.44
12:e:283:ARG:CA	12:f:176:ASP:H	2.29	0.44
12:e:4511:LEU:C	12:e:4513:GLY:H	2.26	0.44
12:f:513:ASP:O	12:f:517:ALA:N	2.37	0.44
12:f:2186:CYS:O	12:f:2191:LEU:N	2.50	0.44
12:f:4554:ASP:C	12:f:4556:CYS:N	2.75	0.44
13:h:480:THR:H	13:h:501:SER:HA	1.82	0.44
1:B:153:THR:O	1:B:173:GLY:N	2.45	0.44
1:D:145:LEU:O	1:D:343:GLY:HA3	2.18	0.44
12:e:804:LEU:HA	12:e:894:SER:O	2.18	0.44
12:e:3950:LYS:O	12:e:3954:ASP:N	2.51	0.44
12:e:4336:GLY:C	12:e:4339:MET:H	2.26	0.44
12:f:1731:THR:C	12:f:1784:ASN:HA	2.43	0.44
12:f:3555:ASN:O	12:f:3556:ALA:C	2.61	0.44
12:f:4307:GLN:O	12:f:4311:LEU:N	2.45	0.44
12:f:4510:CYS:O	12:f:4511:LEU:C	2.61	0.44
12:m:539:SER:O	12:m:543:THR:N	2.40	0.44
12:m:975:ILE:O	12:m:978:CYS:N	2.50	0.44
12:e:286:TYR:CB	12:f:175:GLY:HA2	2.48	0.43
12:e:993:VAL:C	12:e:995:SER:H	2.26	0.43
12:f:1197:LEU:C	12:f:1199:LYS:N	2.76	0.43
12:f:2754:ALA:C	12:f:2756:LEU:N	2.75	0.43
12:f:4239:PRO:O	12:f:4242:ALA:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:g:359:LEU:O	13:g:370:VAL:N	2.51	0.43
14:i:109:LEU:O	14:i:110:ASP:C	2.61	0.43
14:j:216:ASP:C	14:j:218:VAL:N	2.75	0.43
1:A:19:GLY:O	1:A:37:ASN:N	2.41	0.43
12:e:3085:LEU:O	12:e:3089:CYS:N	2.52	0.43
12:f:974:PRO:O	12:f:977:GLU:N	2.51	0.43
12:f:1109:TYR:O	12:f:1112:VAL:N	2.50	0.43
12:f:2379:LEU:C	12:f:2381:ARG:N	2.74	0.43
12:f:2912:PHE:O	12:f:2916:LEU:N	2.51	0.43
12:f:4043:MET:H	12:f:4126:LEU:C	2.25	0.43
12:f:4280:SER:O	12:f:4297:PRO:HA	2.19	0.43
12:f:863:SER:O	12:f:867:CYS:N	2.40	0.43
12:f:2569:VAL:O	12:f:2570:PRO:C	2.61	0.43
13:h:436:SER:N	13:h:450:GLY:O	2.39	0.43
12:e:37:LEU:O	12:e:41:LEU:N	2.39	0.43
12:e:994:LEU:HA	12:e:1019:TYR:O	2.18	0.43
12:e:2162:SER:HA	12:e:2165:PHE:O	2.17	0.43
12:e:4192:GLU:O	12:e:4194:LEU:N	2.51	0.43
12:f:2226:SER:C	12:f:2228:SER:H	2.27	0.43
12:f:2598:GLY:C	12:f:2600:GLY:H	2.26	0.43
12:f:4173:PRO:O	12:f:4176:ARG:N	2.51	0.43
1:C:161:GLY:O	1:C:186:ALA:HB1	2.19	0.43
10:Z:1186:ALA:O	10:Z:1188:SER:N	2.51	0.43
12:e:4459:ILE:HA	12:e:4473:MET:O	2.18	0.43
12:f:1301:LYS:O	12:f:1305:GLU:N	2.51	0.43
12:f:1390:LEU:O	12:f:1393:TYR:N	2.52	0.43
12:f:1680:GLU:C	12:f:1682:GLU:H	2.26	0.43
12:f:1987:SER:O	12:f:1989:ASN:N	2.48	0.43
12:f:4297:PRO:O	12:f:4299:GLY:N	2.51	0.43
14:i:115:HIS:O	14:i:118:LEU:C	2.62	0.43
14:j:82:LYS:O	14:j:83:GLY:C	2.60	0.43
14:j:180:ASP:O	14:j:181:PHE:C	2.62	0.43
15:k:28:ILE:HA	15:k:40:THR:HA	2.00	0.43
12:e:996:LEU:N	12:e:1019:TYR:H	2.15	0.43
12:e:4339:MET:O	12:e:4343:MET:N	2.49	0.43
12:f:3528:LEU:O	12:f:3529:PHE:C	2.62	0.43
12:f:3822:HIS:C	12:f:3824:LEU:H	2.27	0.43
1:F:158:LEU:O	1:F:301:SER:N	2.51	0.43
1:I:200:LYS:O	3:J:98:PRO:HA	2.19	0.43
4:K:154:ILE:N	4:K:179:PHE:O	2.42	0.43
12:e:832:TYR:O	12:e:836:LEU:N	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:e:2593:LEU:O	12:e:2711:ALA:HA	2.19	0.43
12:e:2795:SER:O	12:e:2798:GLU:N	2.51	0.43
12:e:4562:GLY:O	12:e:4645:THR:HA	2.18	0.43
12:f:3626:ALA:HA	12:f:3630:GLY:C	2.43	0.43
14:j:273:SER:O	14:j:276:GLU:C	2.60	0.43
1:D:238:LYS:HA	1:D:252:GLY:HA2	2.00	0.43
6:Q:26:PRO:O	6:Q:28:ASP:N	2.51	0.43
7:R:18:GLU:O	7:R:22:TYR:N	2.52	0.43
12:e:1070:ASN:C	12:e:1073:GLY:H	2.27	0.43
12:e:1838:TRP:O	12:e:1841:GLN:N	2.46	0.43
12:f:2219:GLY:O	12:f:2360:GLY:N	2.44	0.43
14:i:138:ASP:HA	14:i:232:THR:O	2.18	0.43
12:m:25:ALA:N	12:m:125:ILE:O	2.52	0.43
12:e:1554:SER:HA	12:e:1642:GLY:HA2	2.01	0.43
12:e:4288:VAL:HA	12:e:4322:GLY:HA2	2.00	0.43
12:f:1860:GLN:HA	12:f:1865:LYS:HA	2.00	0.43
1:B:51:ALA:HB2	1:D:173:GLY:HA3	2.01	0.42
12:e:2161:LEU:O	12:e:2165:PHE:N	2.49	0.42
12:e:2264:LEU:C	12:e:2279:LEU:H	2.25	0.42
12:e:3538:GLN:C	12:e:3540:ASN:H	2.26	0.42
12:e:3672:SER:C	12:e:3674:SER:H	2.26	0.42
12:e:4274:THR:C	12:e:4277:SER:H	2.27	0.42
12:f:2773:MET:O	12:f:2774:VAL:C	2.61	0.42
12:f:4564:LYS:O	12:f:4642:VAL:CA	2.48	0.42
12:f:4574:LYS:HA	12:f:4625:GLU:O	2.19	0.42
12:e:946:SER:O	12:e:947:HIS:C	2.61	0.42
12:e:1059:CYS:O	12:e:1061:TRP:N	2.52	0.42
12:f:891:HIS:O	12:f:892:SER:C	2.62	0.42
12:f:1368:ASN:O	12:f:1369:GLN:C	2.62	0.42
12:f:2304:ASP:HA	12:f:2344:GLU:O	2.19	0.42
12:f:2759:VAL:C	12:f:2761:SER:H	2.28	0.42
12:f:2770:THR:O	12:f:2771:ALA:C	2.62	0.42
12:e:869:TYR:H	12:e:951:GLY:CA	2.29	0.42
12:e:4219:VAL:O	12:e:4220:ASP:C	2.61	0.42
12:f:945:VAL:O	12:f:946:SER:C	2.62	0.42
12:f:4036:LYS:C	12:f:4038:ASN:H	2.27	0.42
12:f:4182:LEU:O	12:f:4183:LEU:C	2.59	0.42
13:g:480:THR:N	13:g:500:SER:O	2.52	0.42
12:e:993:VAL:C	12:e:995:SER:N	2.77	0.42
12:e:2789:GLN:C	12:e:2791:HIS:N	2.77	0.42
12:e:3637:ASP:HA	12:e:3680:SER:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:2055:TYR:HA	12:f:2059:PHE:O	2.18	0.42
12:f:2600:GLY:O	12:f:2601:LYS:C	2.63	0.42
12:f:2714:PRO:C	12:f:2716:THR:N	2.78	0.42
12:f:2855:LEU:HA	12:f:2858:PHE:O	2.20	0.42
12:f:3498:ASN:C	12:f:3500:MET:N	2.76	0.42
14:i:54:GLY:O	14:i:56:ASN:N	2.53	0.42
14:i:166:PRO:O	14:i:169:GLU:N	2.52	0.42
14:i:268:ALA:HA	14:i:312:ALA:N	2.34	0.42
15:k:25:THR:C	15:k:27:GLY:N	2.77	0.42
12:e:3079:ALA:O	12:e:3080:ALA:C	2.62	0.42
12:e:3537:GLN:CA	12:e:3543:PHE:H	2.30	0.42
12:e:4531:ALA:C	12:e:4533:SER:H	2.27	0.42
12:f:2069:ILE:O	12:f:2073:PHE:N	2.24	0.42
12:f:2555:ILE:O	12:f:2750:THR:HA	2.18	0.42
12:f:4610:TYR:O	12:f:4644:CYS:N	2.52	0.42
12:m:627:TYR:O	12:m:628:PRO:C	2.62	0.42
12:e:809:LYS:C	14:i:357:GLU:N	2.77	0.42
12:e:1136:GLY:HA3	12:e:1207:SER:O	2.19	0.42
12:f:3092:ASN:O	12:f:3094:PHE:N	2.53	0.42
12:f:3626:ALA:HA	12:f:3631:ASN:N	2.33	0.42
12:n:3378:ASN:C	12:n:3380:GLU:H	2.27	0.42
14:r:37:SER:O	14:r:38:SER:C	2.62	0.42
12:e:1029:GLY:C	12:e:1031:VAL:H	2.27	0.42
12:e:2937:GLY:CA	12:e:3095:GLY:H	2.32	0.42
12:f:2593:LEU:HA	12:f:2734:VAL:O	2.20	0.42
12:f:4041:VAL:O	12:f:4125:PHE:HA	2.19	0.42
13:h:455:SER:HA	13:h:472:PHE:O	2.19	0.42
1:F:98:GLN:O	1:F:100:GLN:N	2.53	0.42
12:f:1547:LEU:O	12:f:1551:PHE:N	2.50	0.42
12:f:1626:PHE:O	12:f:1629:PHE:N	2.52	0.42
12:f:3877:HIS:O	12:f:3881:ILE:N	2.53	0.42
12:f:4186:PHE:C	12:f:4188:ALA:N	2.77	0.42
14:i:162:LYS:C	14:i:164:LYS:N	2.77	0.42
14:j:181:PHE:HA	14:j:313:GLY:CA	2.42	0.42
14:j:264:GLN:C	14:j:266:GLY:H	2.28	0.42
15:k:71:ILE:HA	15:l:68:PHE:O	2.20	0.42
12:f:717:ILE:O	12:f:737:VAL:HA	2.19	0.42
12:f:1296:LYS:O	12:f:1297:CYS:C	2.62	0.42
12:f:2188:GLU:C	12:f:2190:TYR:N	2.72	0.42
12:f:2898:LYS:C	12:f:2901:TYR:H	2.28	0.42
12:f:3735:GLN:O	12:f:3738:PHE:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:4112:LYS:O	12:f:4115:SER:C	2.63	0.42
14:i:241:GLU:HA	14:i:246:TYR:O	2.20	0.42
14:j:236:ALA:O	14:j:237:VAL:C	2.62	0.42
12:n:666:GLU:HA	12:n:673:TRP:CB	2.50	0.42
2:H:264:PRO:O	2:H:268:GLY:N	2.53	0.42
12:e:784:SER:CB	12:e:837:ALA:HA	2.49	0.42
12:e:1057:TYR:C	12:e:1059:CYS:N	2.78	0.42
12:e:4172:SER:HA	12:e:4173:PRO:HA	1.88	0.42
12:f:1521:LEU:C	12:f:1523:TRP:N	2.74	0.42
12:f:2943:LYS:C	12:f:2945:THR:N	2.77	0.42
12:f:3482:LEU:O	12:f:3484:ALA:N	2.52	0.42
13:g:313:ALA:O	13:g:329:PHE:N	2.52	0.42
14:i:230:VAL:HA	14:i:270:ILE:O	2.20	0.42
14:i:244:HIS:C	14:i:246:TYR:N	2.77	0.42
14:j:64:GLY:C	14:j:66:GLY:N	2.78	0.42
14:j:113:LEU:C	14:j:115:HIS:N	2.78	0.42
15:k:69:LEU:HA	15:l:72:ARG:H	1.85	0.42
15:l:23:VAL:CA	15:l:29:PRO:HA	2.35	0.42
12:m:137:VAL:O	12:n:139:THR:N	2.53	0.42
5:L:179:THR:N	5:L:187:MET:O	2.31	0.41
12:e:3600:ILE:O	12:e:3604:TYR:N	2.52	0.41
12:f:3945:LYS:C	12:f:3947:LEU:N	2.78	0.41
14:j:241:GLU:HA	14:j:246:TYR:H	1.83	0.41
1:F:20:VAL:HA	1:F:36:PRO:HA	2.02	0.41
10:Z:1150:GLU:HA	10:Z:1153:ALA:HB3	2.02	0.41
12:f:2591:LEU:O	12:f:2709:VAL:HA	2.19	0.41
12:f:2986:LYS:O	12:f:2987:ASN:C	2.63	0.41
12:f:4167:SER:C	12:f:4169:ILE:N	2.77	0.41
12:f:4180:TYR:O	12:f:4181:PHE:C	2.61	0.41
15:l:69:LEU:C	15:l:71:ILE:N	2.77	0.41
12:n:3410:GLU:O	12:n:3411:PRO:C	2.62	0.41
12:f:994:LEU:HA	12:f:1022:ALA:N	2.27	0.41
12:f:3199:MET:C	12:f:3201:LEU:N	2.75	0.41
14:i:132:LEU:O	14:i:134:ILE:N	2.53	0.41
12:m:165:ILE:CA	12:m:171:ALA:H	2.33	0.41
12:m:654:ILE:O	12:m:655:ASP:C	2.63	0.41
12:e:1091:GLY:C	12:e:1093:PHE:H	2.27	0.41
12:e:2055:TYR:HA	12:e:2059:PHE:O	2.21	0.41
12:e:2793:ILE:O	12:e:3087:ASN:N	2.54	0.41
12:e:2836:ARG:HA	12:e:3093:TRP:N	2.33	0.41
12:f:2931:GLY:N	12:f:3059:ILE:O	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:4192:GLU:C	12:f:4195:ARG:H	2.29	0.41
13:h:406:LYS:HA	13:h:423:GLU:HA	2.02	0.41
12:e:3617:ASP:C	12:e:3619:PHE:H	2.28	0.41
12:f:441:LYS:O	12:f:445:ASN:N	2.33	0.41
12:f:1879:LEU:O	12:f:1880:VAL:C	2.62	0.41
12:f:2875:ASN:HA	12:f:2878:SER:O	2.20	0.41
12:f:3576:ASN:O	12:f:3577:ALA:C	2.64	0.41
12:f:3626:ALA:HA	12:f:3630:GLY:CA	2.50	0.41
1:A:156:VAL:HA	1:A:169:PRO:HA	2.02	0.41
12:e:3966:PRO:O	12:e:3968:GLN:N	2.43	0.41
12:f:2667:ASN:O	12:f:2669:PRO:O	2.39	0.41
12:f:2836:ARG:HA	12:f:3091:LEU:O	2.21	0.41
12:f:3757:LYS:C	12:f:3759:ARG:H	2.27	0.41
12:f:4510:CYS:HA	12:f:4561:THR:C	2.45	0.41
14:j:43:VAL:O	14:j:46:ARG:N	2.47	0.41
14:j:218:VAL:C	14:j:220:THR:H	2.28	0.41
12:m:112:LYS:H	12:m:142:GLU:C	2.29	0.41
12:n:803:LEU:CB	12:n:895:ASN:CA	2.98	0.41
1:D:330:ILE:N	6:P:20:TYR:O	2.43	0.41
12:e:349:GLU:O	12:e:353:ILE:N	2.49	0.41
12:f:1026:MET:O	12:f:1028:ASP:N	2.51	0.41
12:f:1818:GLN:O	12:f:1819:ARG:C	2.63	0.41
12:f:3591:ASP:N	12:f:3683:ASP:O	2.53	0.41
14:i:161:ASP:C	14:i:164:LYS:H	2.29	0.41
14:j:117:GLY:C	14:j:119:LEU:N	2.78	0.41
1:A:41:ARG:O	1:A:70:SER:N	2.38	0.41
12:e:720:ILE:HA	12:e:736:LYS:H	1.85	0.41
12:e:2943:LYS:C	12:e:2945:THR:H	2.29	0.41
12:f:914:ARG:HA	12:f:949:PRO:C	2.46	0.41
12:f:3642:ASP:O	12:f:3645:LEU:N	2.53	0.41
12:f:4269:LEU:C	12:f:4273:PHE:H	2.24	0.41
12:e:863:SER:O	12:e:867:CYS:N	2.54	0.41
12:e:964:ILE:HA	12:e:969:ILE:HA	2.03	0.41
12:e:4560:VAL:O	12:e:4587:LEU:HA	2.20	0.41
12:e:4602:ALA:O	12:e:4630:GLU:N	2.46	0.41
12:f:918:GLY:HA2	12:f:950:GLY:HA3	2.03	0.41
12:f:1162:SER:O	12:f:1166:ALA:N	2.35	0.41
12:f:1348:GLU:HA	12:f:1432:GLY:HA2	2.03	0.41
12:f:2225:PRO:O	12:f:2228:SER:N	2.54	0.41
12:f:2242:GLU:HA	12:f:2247:VAL:O	2.21	0.41
12:f:2356:VAL:C	12:f:2359:CYS:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:2983:SER:HA	12:f:2988:GLU:N	2.10	0.41
12:f:3011:LEU:HA	12:f:3016:GLU:O	2.21	0.41
12:f:3498:ASN:C	12:f:3500:MET:H	2.29	0.41
12:f:3993:ILE:C	12:f:3996:PHE:H	2.29	0.41
12:f:4299:GLY:HA2	12:f:4304:GLU:C	2.46	0.41
14:j:66:GLY:O	14:j:67:LYS:C	2.63	0.41
14:j:337:GLU:HA	14:j:340:ILE:O	2.21	0.41
12:n:803:LEU:O	12:n:894:SER:N	2.54	0.41
12:e:21:VAL:HA	12:e:122:ALA:HB1	2.03	0.41
12:e:2066:ALA:C	12:e:2068:LYS:H	2.29	0.41
12:e:4511:LEU:C	12:e:4513:GLY:N	2.79	0.41
12:f:1475:LEU:H	12:f:1587:LEU:CA	2.34	0.41
12:f:2367:ASP:HA	12:f:2370:SER:CA	2.41	0.41
12:f:2677:GLN:C	12:f:2680:ILE:H	2.28	0.41
12:f:4629:LYS:O	12:f:4630:GLU:C	2.63	0.41
14:j:137:ALA:O	14:j:138:ASP:C	2.64	0.41
14:j:311:PRO:O	14:j:313:GLY:N	2.54	0.41
12:n:674:GLU:HA	12:n:679:GLY:HA3	2.03	0.41
12:n:1057:TYR:C	12:n:1059:CYS:N	2.79	0.41
11:Y:343:LEU:HA	11:Y:430:HIS:HA	2.03	0.40
12:e:2299:GLN:O	12:e:2339:VAL:HA	2.21	0.40
12:e:2536:ASP:O	12:e:2548:TRP:N	2.50	0.40
12:f:1908:ALA:HA	12:f:1913:THR:H	1.86	0.40
13:g:364:SER:C	13:g:366:LYS:H	2.29	0.40
13:h:437:MET:HA	13:h:449:VAL:HA	2.03	0.40
14:j:54:GLY:O	14:j:55:LYS:C	2.64	0.40
15:k:66:LEU:HA	15:l:73:SER:HA	2.03	0.40
14:q:46:ARG:O	14:q:47:ALA:C	2.63	0.40
12:f:863:SER:O	12:f:864:LEU:C	2.64	0.40
12:f:1313:SER:O	12:f:1314:GLY:C	2.64	0.40
12:f:2255:ASP:C	12:f:2257:LYS:H	2.27	0.40
12:f:3994:GLN:HA	12:f:3998:PRO:HA	2.03	0.40
12:f:4287:LYS:HA	12:f:4291:HIS:C	2.46	0.40
14:j:110:ASP:C	14:j:112:ASP:N	2.79	0.40
1:F:13:VAL:O	1:F:23:ALA:HA	2.22	0.40
12:e:1938:PHE:O	12:e:1941:MET:N	2.54	0.40
12:e:1980:GLU:O	12:e:1983:ARG:N	2.55	0.40
12:e:2591:LEU:O	12:e:2709:VAL:HA	2.22	0.40
12:e:4537:GLU:O	12:e:4539:LEU:N	2.54	0.40
12:f:1132:GLY:O	12:f:1133:GLN:C	2.64	0.40
12:f:3551:GLU:HA	12:f:3554:SER:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:4601:LYS:N	12:f:4604:VAL:O	2.37	0.40
1:C:200:LYS:O	1:D:117:PRO:HA	2.21	0.40
12:e:1859:ILE:O	12:e:1865:LYS:HA	2.20	0.40
12:e:2983:SER:O	12:e:2987:ASN:HA	2.21	0.40
12:f:2255:ASP:C	12:f:2257:LYS:N	2.79	0.40
12:f:2740:GLY:O	12:f:2741:PRO:C	2.63	0.40
12:f:2845:TRP:O	12:f:2849:ASN:N	2.54	0.40
12:f:4238:ILE:C	12:f:4240:TRP:N	2.80	0.40
4:K:47:ARG:HA	4:K:50:ALA:HB3	2.03	0.40
11:Y:114:CYS:C	11:Y:116:TRP:H	2.28	0.40
12:e:949:PRO:C	12:e:951:GLY:H	2.29	0.40
12:e:2336:PRO:C	12:e:2338:ASN:N	2.79	0.40
12:e:4225:ASP:C	12:e:4227:ALA:N	2.78	0.40
12:f:1892:MET:C	12:f:1894:GLN:N	2.80	0.40
12:f:1908:ALA:C	12:f:1910:THR:H	2.26	0.40
12:f:3509:LEU:O	12:f:3513:PHE:N	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	368/376 (98%)	359 (98%)	9 (2%)	0	100	100
1	B	368/376 (98%)	356 (97%)	12 (3%)	0	100	100
1	C	373/376 (99%)	361 (97%)	12 (3%)	0	100	100
1	D	368/376 (98%)	356 (97%)	12 (3%)	0	100	100
1	E	368/376 (98%)	356 (97%)	12 (3%)	0	100	100
1	F	368/376 (98%)	357 (97%)	11 (3%)	0	100	100
1	G	368/376 (98%)	357 (97%)	11 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	368/376 (98%)	354 (96%)	14 (4%)	0	100	100
2	H	368/375 (98%)	357 (97%)	11 (3%)	0	100	100
3	J	377/417 (90%)	365 (97%)	12 (3%)	0	100	100
4	K	276/286 (96%)	268 (97%)	8 (3%)	0	100	100
5	L	267/272 (98%)	261 (98%)	6 (2%)	0	100	100
6	M	330/405 (82%)	311 (94%)	18 (6%)	1 (0%)	37	73
6	N	270/405 (67%)	262 (97%)	7 (3%)	1 (0%)	30	68
6	P	319/405 (79%)	312 (98%)	7 (2%)	0	100	100
6	Q	335/405 (83%)	318 (95%)	17 (5%)	0	100	100
7	O	177/186 (95%)	165 (93%)	12 (7%)	0	100	100
7	R	168/186 (90%)	160 (95%)	8 (5%)	0	100	100
8	U	165/190 (87%)	157 (95%)	8 (5%)	0	100	100
9	V	177/182 (97%)	172 (97%)	5 (3%)	0	100	100
10	W	144/1281 (11%)	138 (96%)	5 (4%)	1 (1%)	19	57
10	Z	190/1281 (15%)	185 (97%)	5 (3%)	0	100	100
11	Y	404/467 (86%)	377 (93%)	24 (6%)	3 (1%)	19	57
12	e	4559/4646 (98%)	4166 (91%)	378 (8%)	15 (0%)	37	73
12	f	4555/4646 (98%)	3899 (86%)	583 (13%)	73 (2%)	8	38
12	m	4552/4646 (98%)	4431 (97%)	115 (2%)	6 (0%)	48	83
12	n	4514/4646 (97%)	4402 (98%)	110 (2%)	2 (0%)	100	100
13	g	356/612 (58%)	352 (99%)	4 (1%)	0	100	100
13	h	356/612 (58%)	346 (97%)	10 (3%)	0	100	100
13	o	356/612 (58%)	350 (98%)	6 (2%)	0	100	100
13	p	356/612 (58%)	350 (98%)	6 (2%)	0	100	100
14	i	291/492 (59%)	248 (85%)	40 (14%)	3 (1%)	13	49
14	j	306/492 (62%)	233 (76%)	61 (20%)	12 (4%)	2	19
14	q	301/492 (61%)	293 (97%)	8 (3%)	0	100	100
14	r	291/492 (59%)	277 (95%)	14 (5%)	0	100	100
15	k	91/96 (95%)	69 (76%)	22 (24%)	0	100	100
15	l	91/96 (95%)	69 (76%)	21 (23%)	1 (1%)	12	47
15	s	91/96 (95%)	84 (92%)	7 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	t	91/96 (95%)	86 (94%)	5 (6%)	0	100	100
All	All	28073/33135 (85%)	26319 (94%)	1636 (6%)	118 (0%)	32	68

All (118) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	M	217	PRO
10	W	1142	PRO
11	Y	175	PRO
11	Y	441	PRO
12	e	4550	SER
12	f	38	VAL
12	f	203	PRO
12	f	2190	TYR
12	f	2429	PRO
12	f	3925	PRO
14	j	63	ASP
14	j	377	PRO
12	m	870	ASP
12	m	1309	THR
12	e	819	GLY
12	e	928	GLY
12	e	1040	VAL
12	e	1862	ALA
12	e	4193	ARG
12	f	716	ARG
12	f	1198	GLU
12	f	1208	TRP
12	f	1310	GLY
12	f	1314	GLY
12	f	1957	PHE
12	f	1984	GLU
12	f	4168	ARG
14	j	54	GLY
12	n	21	VAL
12	n	1309	THR
12	e	726	ARG
12	e	994	LEU
12	e	4318	PRO
12	f	717	ILE
12	f	930	ALA
12	f	1412	HIS

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Mol	Chain	Res	Type
12	f	1656	LYS
12	f	1758	TRP
12	f	1899	ARG
12	f	1931	ASN
12	f	2172	ARG
12	f	2246	GLY
12	f	2366	GLU
12	f	2598	GLY
12	f	2715	PRO
12	f	2754	ALA
12	f	2900	PHE
12	f	3499	GLN
12	f	3513	PHE
12	f	3619	PHE
12	f	3682	ARG
12	f	3774	LYS
12	f	4377	MET
14	i	364	MET
14	j	217	ASN
12	m	976	GLU
12	f	869	TYR
12	f	1058	GLN
12	f	1119	LYS
12	f	1197	LEU
12	f	1312	LEU
12	f	1682	GLU
12	f	1759	SER
12	f	1799	GLU
12	f	2298	ARG
12	f	2504	GLY
12	f	2755	MET
12	f	3189	GLU
12	f	3482	LEU
12	f	3670	ASP
12	f	3671	LEU
12	f	3701	PHE
12	f	3870	ARG
14	i	181	PHE
14	j	138	ASP
14	j	236	ALA
15	l	54	ARG
12	m	210	HIS

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Mol	Chain	Res	Type
12	e	4632	PRO
12	f	1390	LEU
12	f	2645	PRO
12	f	3217	GLU
12	f	3755	GLU
14	j	68	THR
14	j	114	TYR
14	j	344	PRO
12	m	654	ILE
6	N	163	ASP
12	e	2161	LEU
12	e	4326	ASN
12	f	1842	MET
12	f	2883	PRO
12	f	3848	GLY
14	i	57	ILE
14	j	39	ILE
12	f	1396	ILE
12	f	1487	ILE
12	f	2931	GLY
12	f	1103	GLY
12	f	1206	PRO
12	f	1997	ILE
12	f	2360	GLY
12	f	2613	PRO
12	f	3212	VAL
12	f	4132	PRO
14	j	374	PRO
12	e	732	VAL
12	e	4151	PRO
12	f	805	VAL
12	f	1511	PRO
12	f	2291	VAL
12	f	3981	THR
12	m	627	TYR
11	Y	77	PRO
12	e	3736	GLY
12	f	1211	ILE
14	j	51	LEU
12	f	2570	PRO

5.3.2 Protein sidechains [i](#)

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

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 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

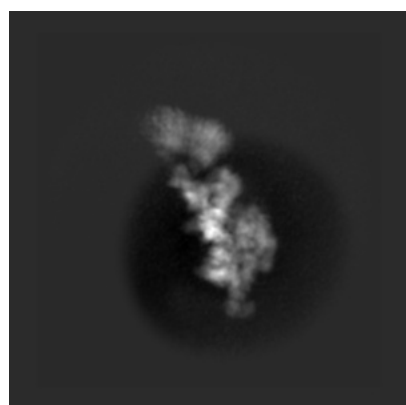
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46845. These allow visual inspection of the internal detail of the map and identification of artifacts.

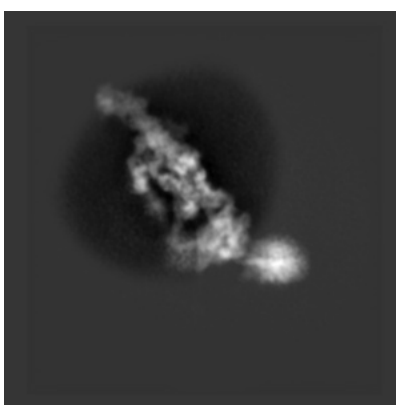
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

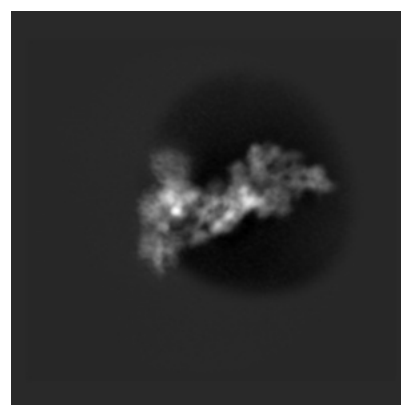
6.1.1 Primary map



X



Y

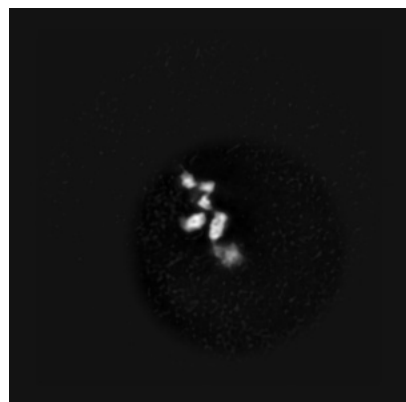


Z

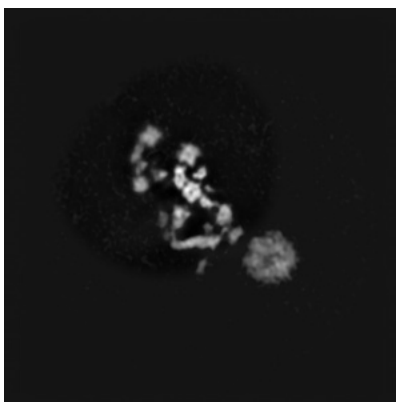
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

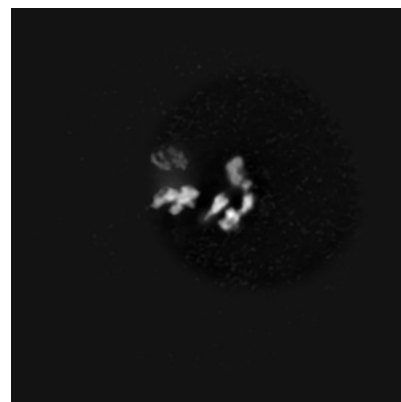
6.2.1 Primary map



X Index: 150



Y Index: 150

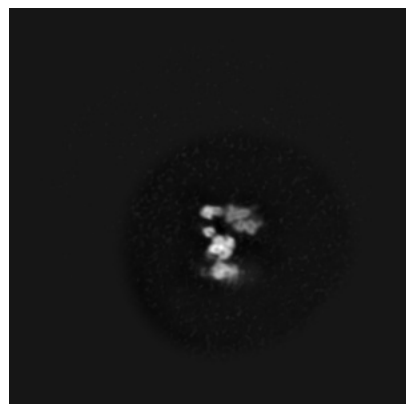


Z Index: 150

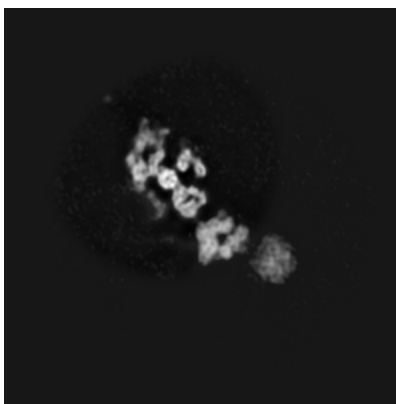
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

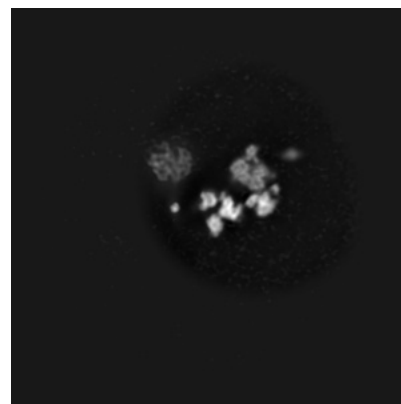
6.3.1 Primary map



X Index: 174



Y Index: 157

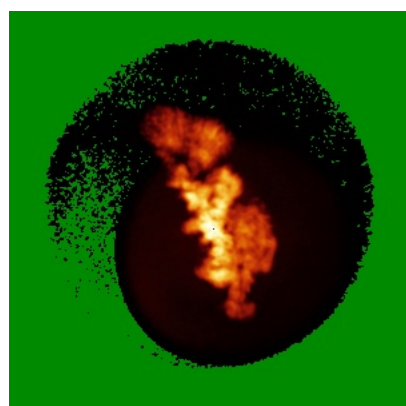


Z Index: 136

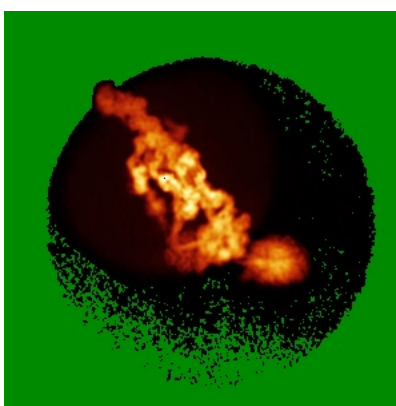
The images above show the largest variance slices of the map in three orthogonal directions.

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

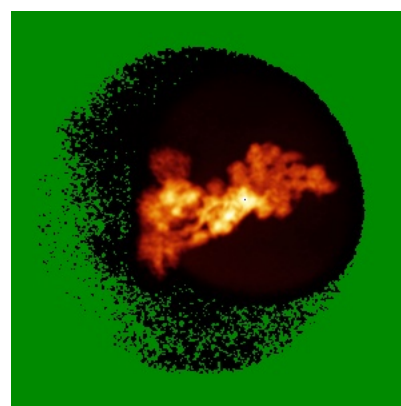
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

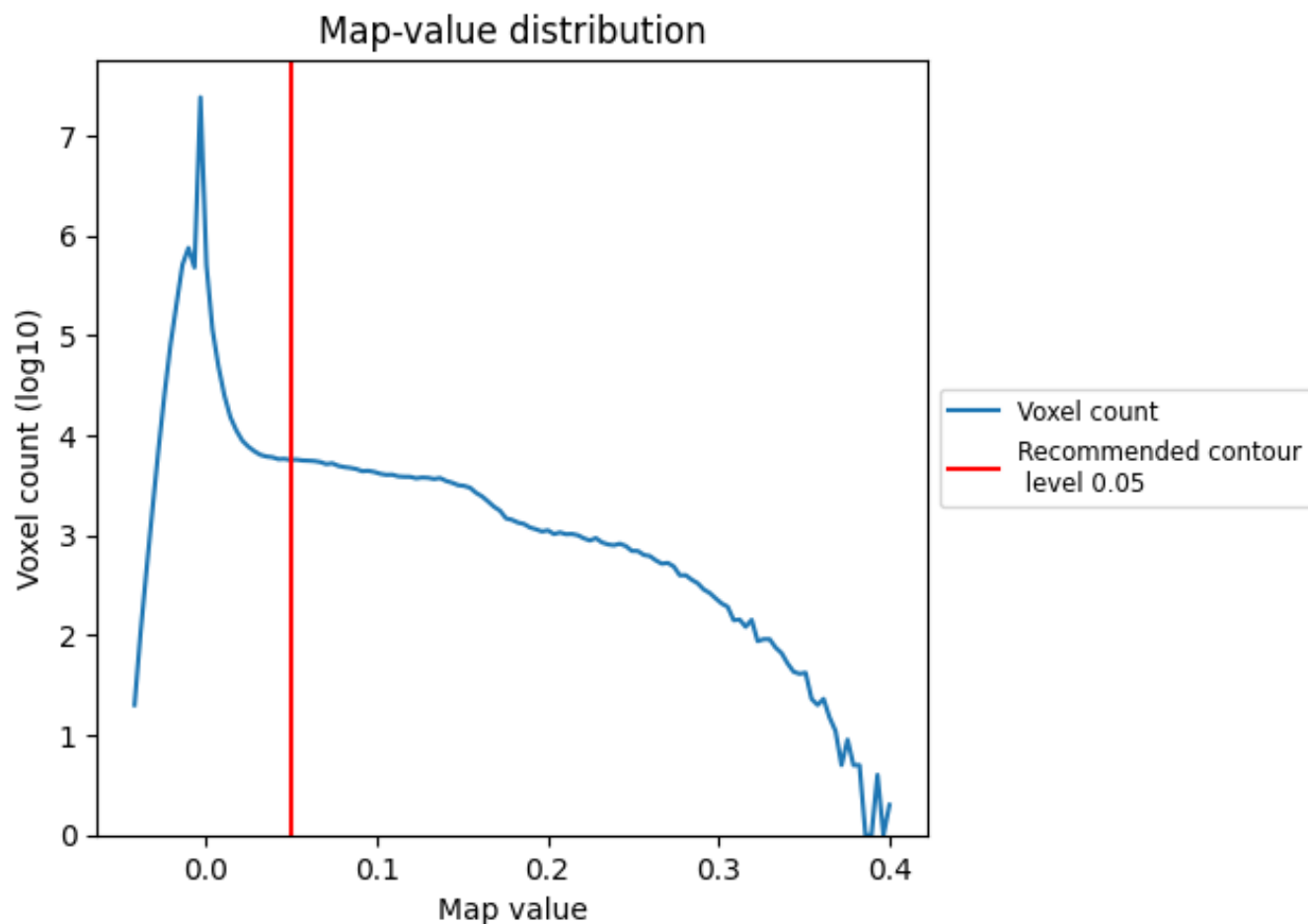
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

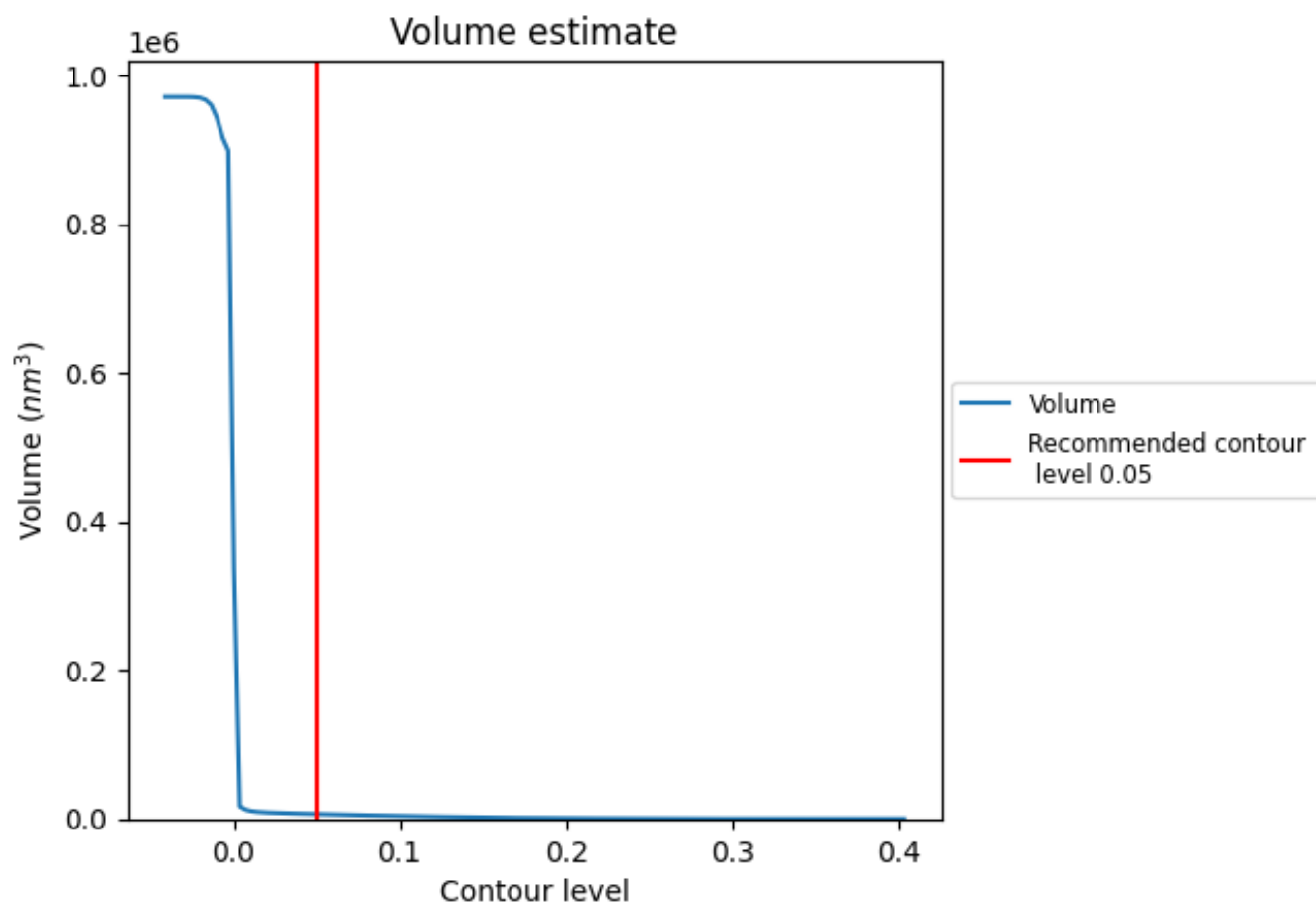
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

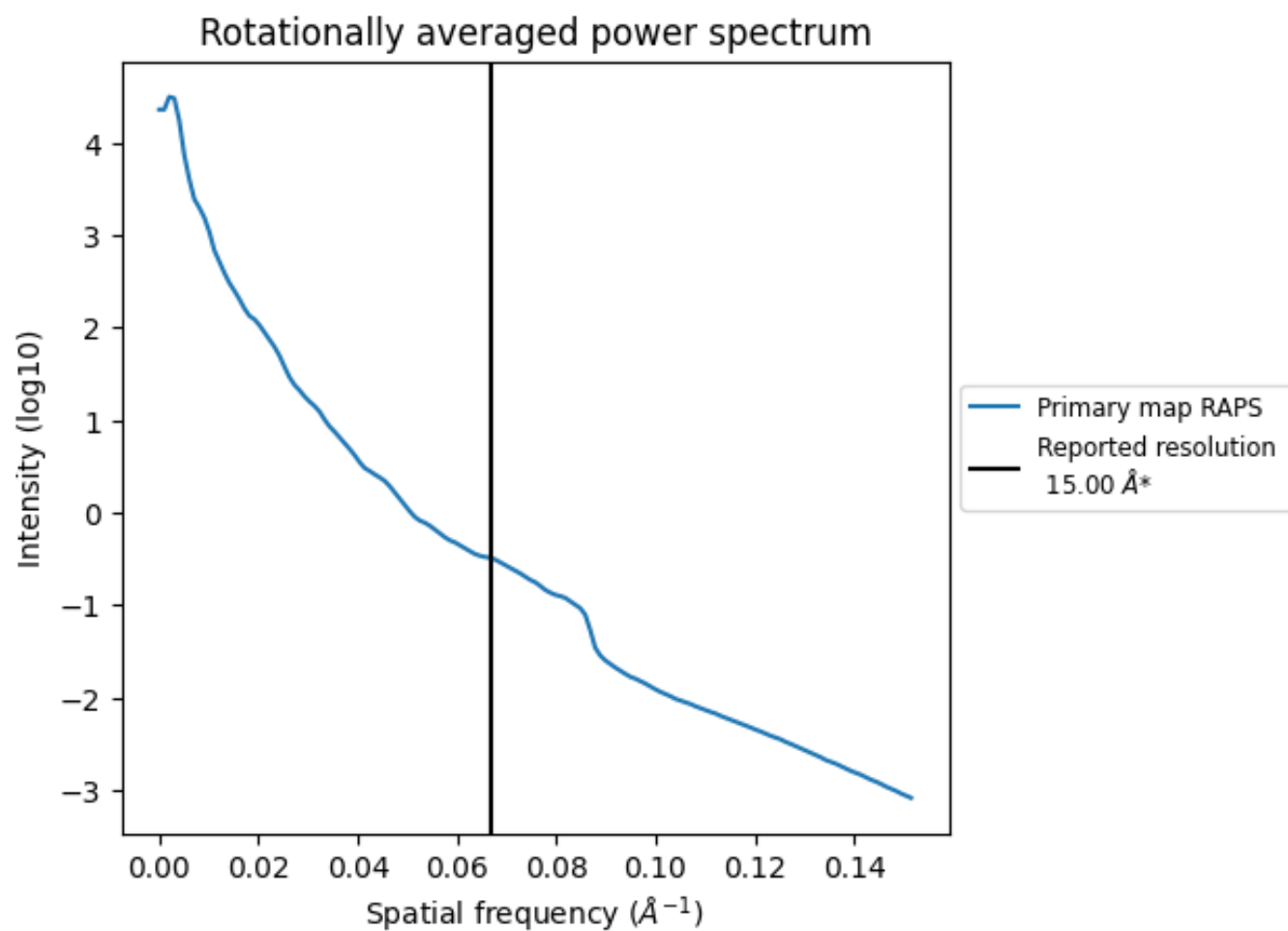
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 6296 nm^3 ; this corresponds to an approximate mass of 5688 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 0.067 Å⁻¹

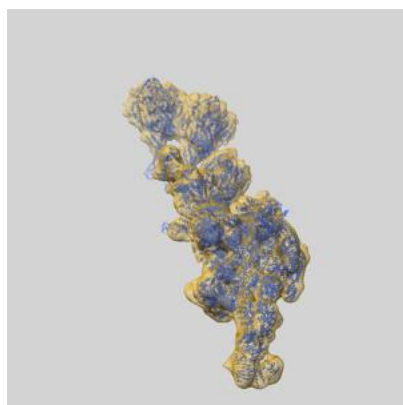
8 Fourier-Shell correlation

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

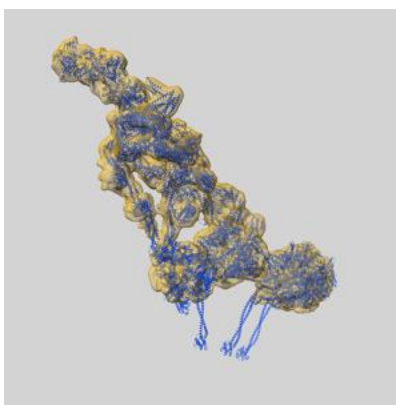
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-46845 and PDB model 9DGR. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

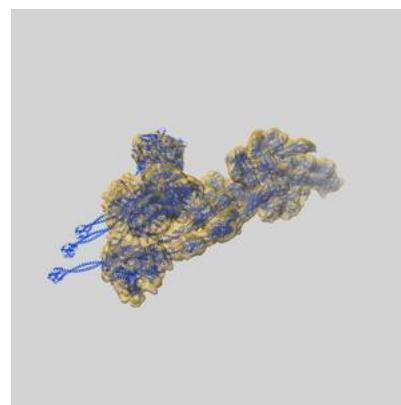
9.1 Map-model overlay [i](#)



X



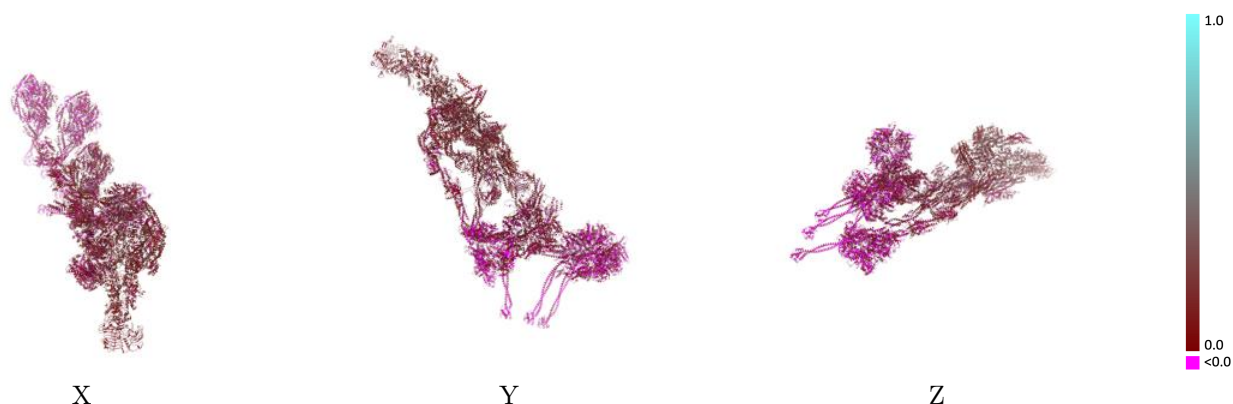
Y



Z

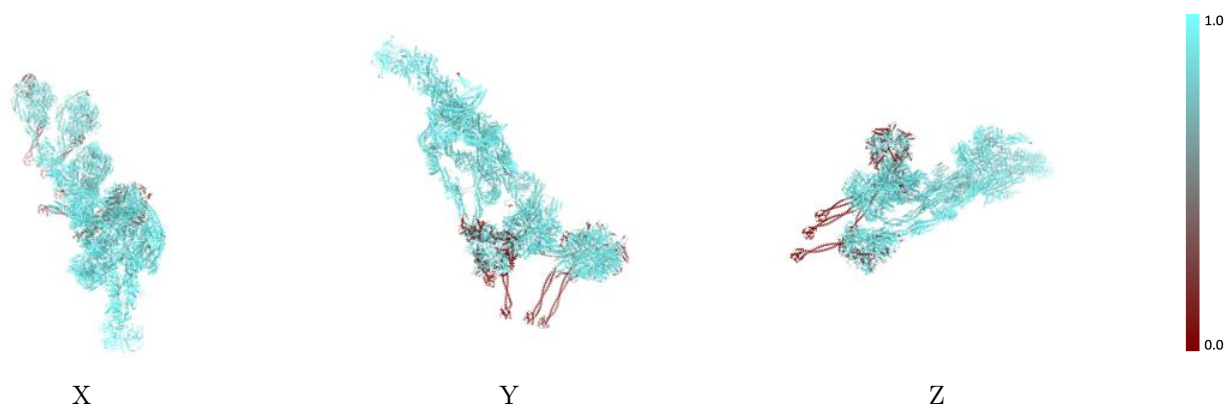
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



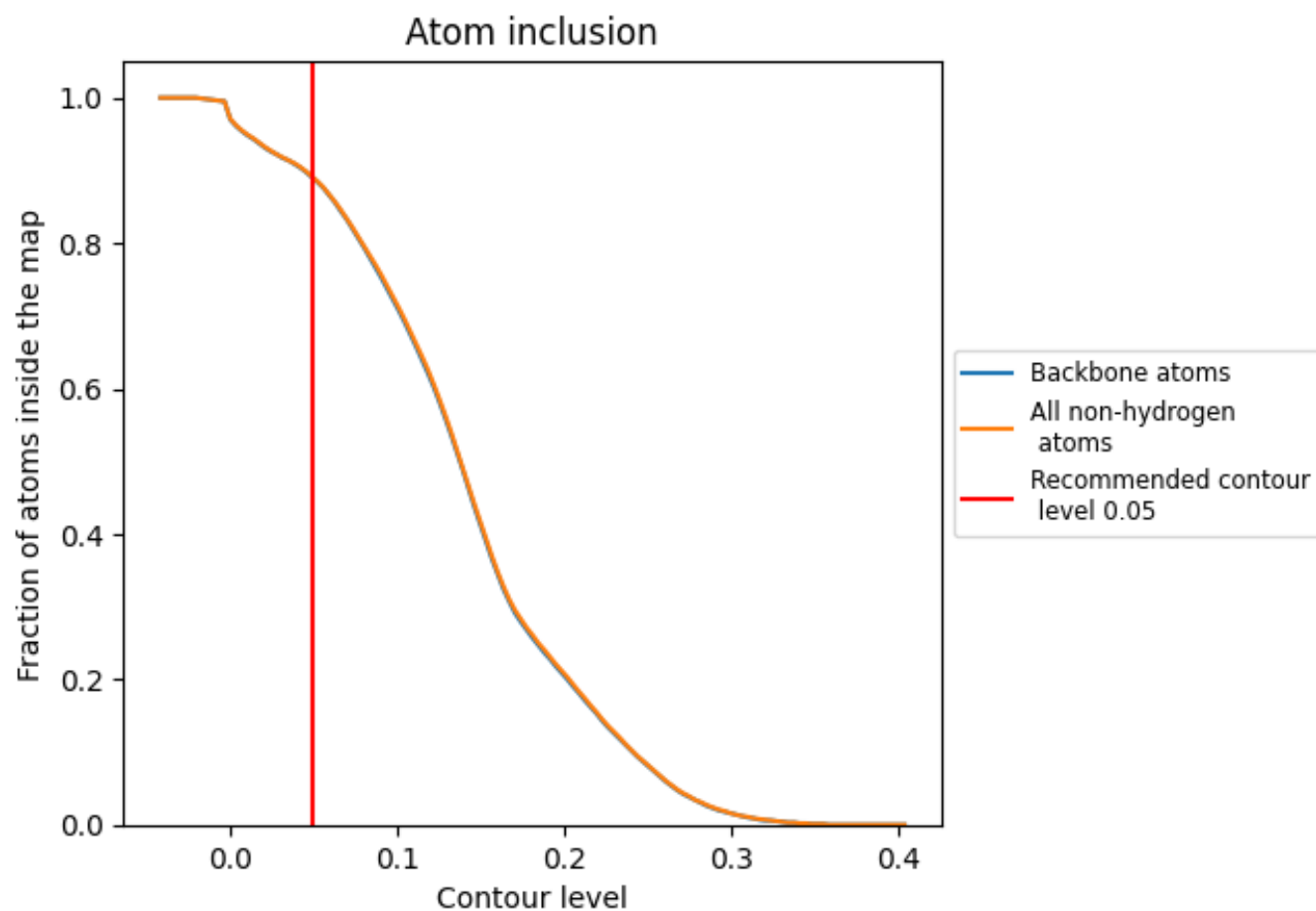
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 89% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8900	 0.0960
A	 1.0000	 0.1630
B	 1.0000	 0.1730
C	 1.0000	 0.1720
D	 1.0000	 0.1690
E	 1.0000	 0.1690
F	 1.0000	 0.1710
G	 1.0000	 0.1720
H	 1.0000	 0.1580
I	 0.9900	 0.1630
J	 0.9970	 0.1600
K	 1.0000	 0.1540
L	 0.9990	 0.1650
M	 0.9950	 0.1500
N	 0.9800	 0.1540
O	 1.0000	 0.1550
P	 0.9960	 0.1750
Q	 0.9780	 0.1660
R	 1.0000	 0.1550
U	 0.9780	 0.1210
V	 1.0000	 0.1350
W	 1.0000	 0.1400
Y	 0.9580	 0.1330
Z	 0.9990	 0.1740
e	 0.6470	 0.0500
f	 0.9470	 0.1060
g	 1.0000	 0.0740
h	 1.0000	 0.0950
i	 0.9600	 0.0840
j	 1.0000	 0.1310
k	 1.0000	 0.1220
l	 1.0000	 0.0990
m	 0.8960	 0.0640
n	 0.8400	 0.0540
o	 1.0000	 0.0970



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Chain	Atom inclusion	Q-score
p	 0.9990	 0.0840
q	 1.0000	 0.1170
r	 0.9970	 0.0810
s	 0.9950	 0.0960
t	 1.0000	 0.1000