



Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 07:42 AM EST

PDB ID : 3J68
EMDB ID : EMD-5758
Title : Structural mechanism of the dynein powerstroke (pre-powerstroke state)
Authors : Lin, J.; Okada, K.; Raytchev, M.; Smith, M.C.; Nicastro, D.
Deposited on : 2013-12-23
Resolution : 30.00 Å(reported)
Based on initial model : 4AKI

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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

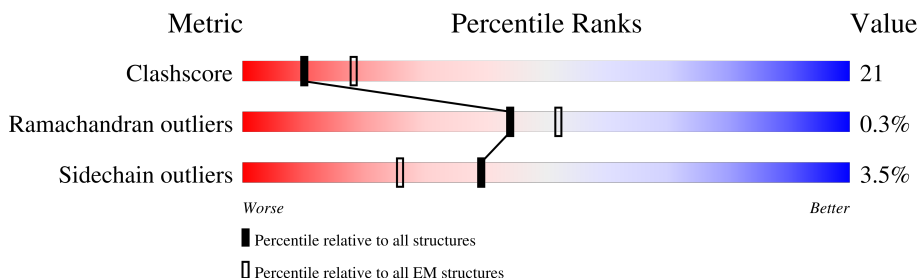
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 30.00 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2286	

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 18105 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.

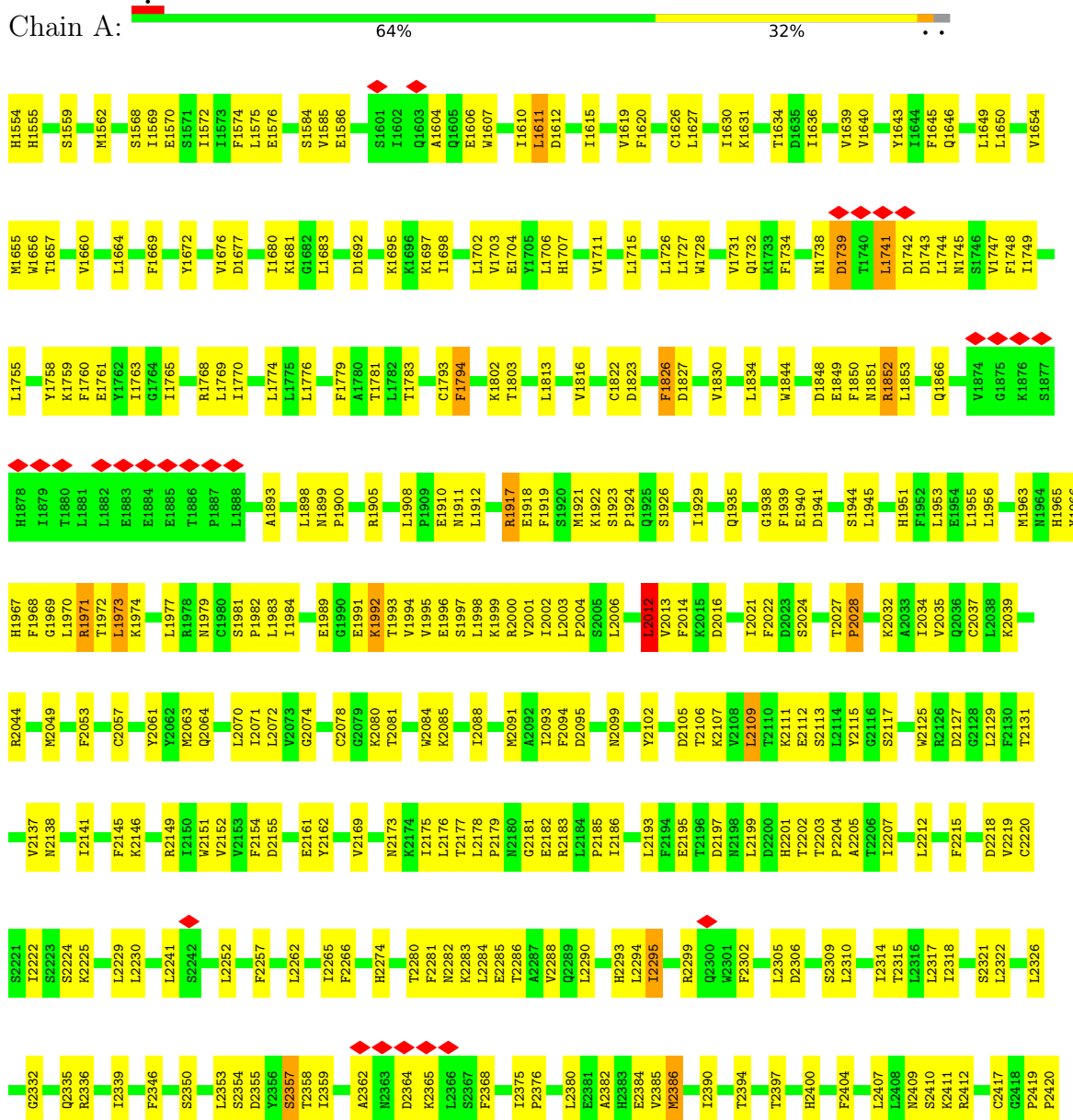
- Molecule 1 is a protein called Dynein motor domain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2245	18105	11610	3004	3403	88	0	0

3 Residue-property plots

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

• Molecule 1: Dynein motor domain



L4063	L4064	L4065	L4070	L4071	L4072	L4073	L4074	Q4077	A4078	A4079	S4084	T4085	L4088	L4092	Y3967	A3973	S3976	N3978	N3979	I3980	P3981	W3982	Q3984	A3983	Q3984	V3985	Y3993	Y3994	G3995	I3998	K4002	D4003	L4004	L4010	L4014	F4015	C4016	G4017	S4018	D4019	N4020	L4021	Q4022	S3926	Y3927	W3934	F3935	I3939	T3943	R3944	V3946	P3947	G3949	F3950	S3951	Y3955	D3960	F3963	A3964	L4045	I4048	L4059	W4062																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
F3874	K3875	T3876	C3877	H3878	L3884	F3885	A3886	P3887	L3888	L3889	Q3890	R3894	F3895	E3898	T3906	W3911	G3912	F3915	F3916	T3917	G3918	K3919	L3920	S3921	V3922	G3923	K3924	S3925	Y3926	Y3927	W3934	F3935	I3939	T3943	R3944	V3946	P3947	G3949	F3950	S3951	Y3955	D3960	F3963	A3964	L4045	I4048	L4059	W4062																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
R3792	K3799	L3803	A3804	K3805	A3806	S3807	K3808	S3809	S3810	L3811	L3816	G3817	S3818	I3819	E3820	N3821	L3822	N3823	Y3824	A3825	K3831	S3832	K3833	I3834	E3835	G3836	G3837	W3838	I3839	Q3845	M3846	S3847	L3848	F3849	W3850	Y3851	K3852	T3853	Y3854	L3855	H3858	Q3859	T3862	A3865	E3869	K3870	F3871	K3872	M3873																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
L3887	L3890	D3891	K3892	K3893	F3894	K3895	M3896	L3897	M3898	L3901	E3906	F3907	Q3910	D3912	N3913	L3914	V3915	Y3918	G3922	I3928	M3931	F3941	S3945	I3946	V3956	I3958	L3959	Y3965	K3966	Y3967	Y3968	Y3969	Y3970	Y3971	Y3972	Y3973	Y3974	Y3975	Y3976	Y3977	Y3978	Y3979	Y3980	Y3981	Y3982	Y3983	Y3984	Y3985	Y3986	Y3987	Y3988	Y3989	Y3990	Y3991	Y3992	Y3993	Y3994	Y3995	Y3996	Y3997	Y3998	Y3999	Y4000	Y4001	Y4002	Y4003	Y4004	Y4005	Y4006	Y4007	Y4008	Y4009	Y4010	Y4011	Y4012	Y4013	Y4014	Y4015	Y4016	Y4017	Y4018	Y4019	Y4020	Y4021	Y4022	Y4023	Y4024	Y4025	Y4026	Y4027	Y4028	Y4029	Y4030	Y4031	Y4032	Y4033	Y4034	Y4035	Y4036	Y4037	Y4038	Y4039	Y4040	Y4041	Y4042	Y4043	Y4044	Y4045	Y4046	Y4047	Y4048	Y4049	Y4050	Y4051	Y4052	Y4053	Y4054	Y4055	Y4056	Y4057	Y4058	Y4059	Y4060	Y4061	Y4062	Y4063	Y4064	Y4065	Y4066	Y4067	Y4068	Y4069	Y4070	Y4071	Y4072	Y4073	Y4074	Y4075	Y4076	Y4077	Y4078	Y4079	Y4080	Y4081	Y4082	Y4083	Y4084	Y4085	Y4086	Y4087	Y4088	Y4089	Y4090	Y4091	Y4092	Y4093	Y4094	Y4095	Y4096	Y4097	Y4098	Y4099	Y4100	Y4101	Y4102	Y4103	Y4104	Y4105	Y4106	Y4107	Y4108	Y4109	Y4110	Y4111	Y4112	Y4113	Y4114	Y4115	Y4116	Y4117	Y4118	Y4119	Y4120	Y4121	Y4122	Y4123	Y4124	Y4125	Y4126	Y4127	Y4128	Y4129	Y4130	Y4131	Y4132	Y4133	Y4134	Y4135	Y4136	Y4137	Y4138	Y4139	Y4140	Y4141	Y4142	Y4143	Y4144	Y4145	Y4146	Y4147	Y4148	Y4149	Y4150	Y4151	Y4152	Y4153	Y4154	Y4155	Y4156	Y4157	Y4158	Y4159	Y4160	Y4161	Y4162	Y4163	Y4164	Y4165	Y4166	Y4167	Y4168	Y4169	Y4170	Y4171	Y4172	Y4173	Y4174	Y4175	Y4176	Y4177	Y4178	Y4179	Y4180	Y4181	Y4182	Y4183	Y4184	Y4185	Y4186	Y4187	Y4188	Y4189	Y4190	Y4191	Y4192	Y4193	Y4194	Y4195	Y4196	Y4197	Y4198	Y4199	Y4200	Y4201	Y4202	Y4203	Y4204	Y4205	Y4206	Y4207	Y4208	Y4209	Y4210	Y4211	Y4212	Y4213	Y4214	Y4215	Y4216	Y4217	Y4218	Y4219	Y4220	Y4221	Y4222	Y4223	Y4224	Y4225	Y4226	Y4227	Y4228	Y4229	Y4230	Y4231	Y4232	Y4233	Y4234	Y4235	Y4236	Y4237	Y4238	Y4239	Y4240	Y4241	Y4242	Y4243	Y4244	Y4245	Y4246	Y4247	Y4248	Y4249	Y4250	Y4251	Y4252	Y4253	Y4254	Y4255	Y4256	Y4257	Y4258	Y4259	Y4260	Y4261	Y4262	Y4263	Y4264	Y4265	Y4266	Y4267	Y4268	Y4269	Y4270	Y4271	Y4272	Y4273	Y4274	Y4275	Y4276	Y4277	Y4278	Y4279	Y4280	Y4281	Y4282	Y4283	Y4284	Y4285	Y4286	Y4287	Y4288	Y4289	Y4290	Y4291	Y4292	Y4293	Y4294	Y4295	Y4296	Y4297	Y4298	Y4299	Y4300	Y4301	Y4302	Y4303	Y4304	Y4305	Y4306	Y4307	Y4308	Y4309	Y4310	Y4311	Y4312	Y4313	Y4314	Y4315	Y4316	Y4317	Y4318	Y4319	Y4320	Y4321	Y4322	Y4323	Y4324	Y4325	Y4326	Y4327	Y4328	Y4329	Y4330	Y4331	Y4332	Y4333	Y4334	Y4335	Y4336	Y4337	Y4338	Y4339	Y4340	Y4341	Y4342	Y4343	Y4344	Y4345	Y4346	Y4347	Y4348	Y4349	Y4350	Y4351	Y4352	Y4353	Y4354	Y4355	Y4356	Y4357	Y4358	Y4359	Y4360	Y4361	Y4362	Y4363	Y4364	Y4365	Y4366	Y4367	Y4368	Y4369	Y4370	Y4371	Y4372	Y4373	Y4374	Y4375	Y4376	Y4377	Y4378	Y4379	Y4380	Y4381	Y4382	Y4383	Y4384	Y4385	Y4386	Y4387	Y4388	Y4389	Y4390	Y4391	Y4392	Y4393	Y4394	Y4395	Y4396	Y4397	Y4398	Y4399	Y4400	Y4401	Y4402	Y4403	Y4404	Y4405	Y4406	Y4407	Y4408	Y4409	Y4410	Y4411	Y4412	Y4413	Y4414	Y4415	Y4416	Y4417	Y4418	Y4419	Y4420	Y4421	Y4422	Y4423	Y4424	Y4425	Y4426	Y4427	Y4428	Y4429	Y4430	Y4431	Y4432	Y4433	Y4434	Y4435	Y4436	Y4437	Y4438	Y4439	Y4440	Y4441	Y4442	Y4443	Y4444	Y4445	Y4446	Y4447	Y4448	Y4449	Y4450	Y4451	Y4452	Y4453	Y4454	Y4455	Y4456	Y4457	Y4458	Y4459	Y4460	Y4461	Y4462	Y4463	Y4464	Y4465	Y4466	Y4467	Y4468	Y4469	Y4470	Y4471	Y4472	Y4473	Y4474	Y4475	Y4476	Y4477	Y4478	Y4479	Y4480	Y4481	Y4482	Y4483	Y4484	Y4485	Y4486	Y4487	Y4488	Y4489	Y4490	Y4491	Y4492	Y4493	Y4494	Y4495	Y4496	Y4497	Y4498	Y4499	Y4500	Y4501	Y4502	Y4503	Y4504	Y4505	Y4506	Y4507	Y4508	Y4509	Y4510	Y4511	Y4512	Y4513	Y4514	Y4515	Y4516	Y4517	Y4518	Y4519	Y4520	Y4521	Y4522	Y4523	Y4524	Y4525	Y4526	Y4527	Y4528	Y4529	Y4530	Y4531	Y4532	Y4533	Y4534	Y4535	Y4536	Y4537	Y4538	Y4539	Y4540	Y4541	Y4542	Y4543	Y4544	Y4545	Y4546	Y4547	Y4548	Y4549	Y4550	Y4551	Y4552	Y4553	Y4554	Y4555	Y4556	Y4557	Y4558	Y4559	Y4560	Y4561	Y4562	Y4563	Y4564	Y4565	Y4566	Y4567	Y4568	Y4569	Y4570	Y4571	Y4572	Y4573	Y4574	Y4575	Y4576	Y4577	Y4578	Y4579	Y4580	Y4581	Y4582	Y4583	Y4584	Y4585	Y4586	Y4587	Y4588	Y4589	Y4590	Y4591	Y4592	Y4593	Y4594	Y4595	Y4596	Y4597	Y4598	Y4599	Y4600	Y4601	Y4602	Y4603	Y4604	Y4605	Y4606	Y4607	Y4608	Y4609	Y4610	Y4611	Y4612	Y4613	Y4614	Y4615	Y4616	Y4617	Y4618	Y4619	Y4620	Y4621	Y4622	Y4623	Y4624	Y4625	Y4626	Y4627	Y4628	Y4629	Y4630	Y4631	Y4632	Y4633	Y4634	Y4635	Y4636	Y4637	Y4638	Y4639	Y4640	Y4641	Y4642	Y4643	Y4644	Y4645	Y4646	Y4647	Y4648	Y4649	Y4650	Y4651	Y4652	Y4653	Y4654	Y4655	Y4656	Y4657	Y4658	Y4659	Y4660	Y4661	Y4662	Y4663	Y4664	Y4665	Y4666	Y4667	Y4668	Y4669	Y4670	Y4671	Y4672	Y4673	Y4674	Y4675	Y4676	Y4677	Y4678	Y4679	Y4680	Y4681	Y4682	Y4683	Y4684	Y4685	Y4686	Y4687	Y4688	Y4689	Y4690	Y4691	Y4692	Y4693	Y4694	Y4695	Y4696	Y4697	Y4698	Y4699	Y4700	Y4701	Y4702	Y4703	Y4704	Y4705	Y4706	Y4707	Y4708	Y4709	Y4710	Y4711	Y4712	Y4713	Y4714	Y4715	Y4716	Y4717	Y4718	Y4719	Y4720	Y4721	Y4722	Y4723	Y4724	Y4725	Y4726	Y4727	Y4728	Y4729	Y4730	Y4731	Y4732	Y4733	Y4734	Y4735	Y4736	Y4737	Y4738	Y4739	Y4740	Y4741	Y4742	Y4743	Y4744	Y4745	Y4746	Y4747	Y4748	Y4749	Y4750	Y4751	Y4752	Y4753	Y4754	Y4755	Y4756	Y4757	Y4758	Y4759	Y4760	Y4761	Y4762	Y4763	Y4764	Y4765	Y4766	Y4767	Y4768	Y4769	Y4770	Y4771	Y4772	Y4773	Y4774	Y4775	Y4776	Y4777	Y4778	Y4779	Y4780	Y4781	Y4782	Y4783	Y4784	Y4785	Y4786	Y4787	Y4788	Y4789	Y4790	Y4791	Y4792	Y4793	Y4794	Y4795	Y4796	Y4797	Y4798	Y4799	Y4800	Y4801	Y4802	Y4803	Y4804	Y4805	Y4806	Y4807	Y4808	Y4809	Y4810	Y4811	Y4812	Y4813	Y4814	Y4815	Y4816	Y4817	Y4818	Y4819	Y4820	Y4821	Y4822	Y4823	Y4824	Y4825	Y4826	Y4827	Y4828	Y4829	Y4830	Y4831	Y4832	Y4833	Y4834	Y4835	Y4836	Y4837	Y4838	Y4839	Y4840	Y4841	Y4842	Y4843	Y4844	Y4845	Y4846	Y4847	Y4848	Y4849	Y4850	Y4851	Y4852	Y4853	Y4854	Y4855	Y4856	Y4857	Y4858	Y4859	Y4860	Y4861	Y4862	Y4863	Y4864	Y4865	Y4866	Y4867	Y4868	Y4869	Y4870	Y4871	Y4872	Y4873	Y4874	Y4875	Y4876	Y4877	Y4878	Y4879	Y4880	Y4881	Y4882	Y4883	Y4884	Y4885	Y4886	Y4887	Y4888	Y4889	Y4890	Y4891	Y4892	Y4893	Y4894	Y4895	Y4896	Y4897	Y4898	Y4899	Y4900	Y4901	Y4902	Y4903	Y4904	Y4905	Y4906	Y4907	Y4908	Y4909	Y4910	Y4911	Y4912	Y4913	Y4914	Y4915	Y4916	Y4917	Y4918	Y4919	Y4920	Y4921	Y4922	Y4923	Y4924	Y4925	Y4926	Y4927	Y4928	Y4929	Y4930	Y4931	Y4932	Y4933	Y4934	Y4935	Y4936	Y4937	Y4938	Y4939	Y4940	Y4941	Y4942	Y4943	Y4944	Y4945	Y4946	Y4947	Y4948	Y4949	Y4950	Y4951	Y4952	Y4953	Y4954	Y4955	Y4956	Y4957	Y4958	Y4959	Y4960	Y4961	Y4962	Y4963	Y4964	Y4965	Y4966	Y4967	Y4968	Y4969	Y4970	Y4971	Y4972	Y4973	Y4974	Y4975	Y4976	Y4977	Y4978	Y4979	Y4980	Y4981	Y4982	Y4983	Y4984	Y4985	Y4986	Y4987	Y4988	Y4989	Y4990	Y4991	Y4992	Y4993	Y4994	Y4995	Y4996	Y4997	Y4998	Y4999	Y5000	Y5001	Y5002	Y5003	Y5004	Y5005	Y5006	Y5007	Y5008	Y5009	Y5010	Y5011	Y5012	Y5013

4 Experimental information

Property	Value	Source
EM reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of tilted images used	Not provided	
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	Not provided	
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	100	Depositor
Minimum defocus (nm)	6000	Depositor
Maximum defocus (nm)	8000	Depositor
Magnification	13500	Depositor
Image detector	GENERIC GATAN (2k x 2k)	Depositor
Maximum voxel value	160.067	Depositor
Minimum voxel value	96.788	Depositor
Average voxel value	123.910	Depositor
Voxel value standard deviation	7.732	Depositor
Recommended contour level	127.0	Depositor
Tomogram size (\AA)	492.8, 354.816, 492.8	wwPDB
Tomogram dimensions	50, 36, 50	wwPDB
Tomogram angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Grid spacing (\AA)	9.856, 9.856, 9.856	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.59	1/18472 (0.0%)	0.82	12/24968 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2872	GLU	CG-CD	7.56	1.63	1.51

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1741	LEU	CB-CG-CD1	8.47	125.39	111.00
1	A	1973	LEU	CB-CG-CD1	-7.39	98.44	111.00
1	A	2872	GLU	OE1-CD-OE2	-7.26	114.59	123.30
1	A	2866	LEU	CA-CB-CG	6.12	129.38	115.30
1	A	1769	LEU	CA-CB-CG	6.08	129.28	115.30
1	A	2866	LEU	CB-CG-CD1	6.06	121.30	111.00
1	A	2012	LEU	CA-CB-CG	5.82	128.67	115.30
1	A	3577	MET	CG-SD-CE	5.72	109.35	100.20
1	A	1611	LEU	CB-CG-CD2	-5.42	101.79	111.00
1	A	1769	LEU	CB-CG-CD1	5.27	119.96	111.00
1	A	1776	LEU	CB-CG-CD1	-5.25	102.08	111.00
1	A	1917	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1739	ASP	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	18105	0	18146	779	0
All	All	18105	0	18146	779	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 21.

All (779) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1620:PHE:HD1	1:A:1760:PHE:CZ	1.58	1.22
1:A:4033:LEU:CD1	1:A:4035:GLN:HB2	1.76	1.16
1:A:3534:LEU:CD1	1:A:3618:TYR:HE2	1.59	1.15
1:A:3777:VAL:HG11	1:A:3895:PHE:HE1	1.06	1.15
1:A:2111:LYS:HD3	1:A:2161:GLU:HG3	1.18	1.14
1:A:3525:ILE:HD11	1:A:3646:ILE:HG22	1.25	1.12
1:A:3024:LEU:HD11	1:A:3303:LYS:HG3	1.31	1.12
1:A:1645:PHE:HB3	1:A:1765:ILE:HG22	1.34	1.09
1:A:2107:LYS:HE3	1:A:2495:ASP:OD2	1.51	1.09
1:A:2141:ILE:HD12	1:A:2146:LYS:HE2	1.20	1.09
1:A:2488:GLU:HB3	1:A:2491:LEU:HD12	1.36	1.08
1:A:2707:VAL:HB	1:A:2712:LEU:HD11	1.19	1.07
1:A:1992:LYS:HG3	1:A:2024:SER:HB2	1.17	1.07
1:A:2380:LEU:HD13	1:A:2390:ILE:HD11	1.34	1.06
1:A:3303:LYS:HA	1:A:3306:TRP:CD1	1.89	1.06
1:A:3530:PHE:CD1	1:A:3618:TYR:HD2	1.71	1.06
1:A:2380:LEU:HD22	1:A:2384:GLU:OE1	1.55	1.06
1:A:1645:PHE:HB3	1:A:1765:ILE:CG2	1.87	1.05
1:A:2494:LEU:CD1	1:A:2498:GLY:HA2	1.86	1.05
1:A:2494:LEU:HD13	1:A:2498:GLY:CA	1.85	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1823:ASP:HB2	1:A:1852:ARG:O	1.56	1.04
1:A:2988:SER:HB3	1:A:2989:PRO:HD2	1.04	1.04
1:A:1983:LEU:HD22	1:A:1997:SER:OG	1.58	1.03
1:A:2707:VAL:CB	1:A:2712:LEU:HD11	1.89	1.03
1:A:1992:LYS:CG	1:A:2024:SER:HB2	1.86	1.03
1:A:2920:TRP:HB2	1:A:2989:PRO:HG3	1.06	1.02
1:A:2988:SER:HB3	1:A:2989:PRO:CD	1.90	1.02
1:A:3777:VAL:CG1	1:A:3895:PHE:HE1	1.74	1.01
1:A:2448:ASP:HB2	1:A:2829:GLU:OE2	1.59	1.01
1:A:2386:MET:HB2	1:A:2627:ARG:HD3	1.42	1.00
1:A:3534:LEU:HD12	1:A:3618:TYR:HE2	1.24	1.00
1:A:1620:PHE:CD1	1:A:1760:PHE:CZ	2.50	1.00
1:A:1822:CYS:HB2	1:A:1853:LEU:HD21	1.43	0.99
1:A:3303:LYS:O	1:A:3306:TRP:HD1	1.43	0.99
1:A:3534:LEU:CD1	1:A:3618:TYR:CE2	2.45	0.99
1:A:2745:ILE:HG23	1:A:2756:MET:HE1	1.45	0.98
1:A:2380:LEU:CD1	1:A:2390:ILE:HD11	1.93	0.98
1:A:1970:LEU:HD13	1:A:1974:LYS:HE3	1.45	0.98
1:A:3777:VAL:HG11	1:A:3895:PHE:CE1	1.97	0.98
1:A:2476:LYS:H	1:A:2476:LYS:HD3	1.26	0.97
1:A:2476:LYS:H	1:A:2476:LYS:CD	1.74	0.97
1:A:4033:LEU:HD11	1:A:4035:GLN:HB2	1.47	0.97
1:A:2386:MET:CB	1:A:2627:ARG:HD3	1.95	0.96
1:A:3534:LEU:HD12	1:A:3618:TYR:CE2	2.01	0.96
1:A:3406:PHE:HB2	1:A:3513:VAL:CG1	1.94	0.96
1:A:2988:SER:CB	1:A:2989:PRO:HD2	1.97	0.95
1:A:4065:LEU:HD11	1:A:4070:ILE:HD11	1.48	0.95
1:A:1645:PHE:CB	1:A:1765:ILE:HG22	1.96	0.95
1:A:3024:LEU:CD1	1:A:3303:LYS:HG3	1.96	0.95
1:A:1802:LYS:HG2	1:A:1921:MET:HG3	1.47	0.94
1:A:3509:LEU:CD1	1:A:3513:VAL:HG21	1.98	0.94
1:A:2787:HIS:HA	1:A:3460:PRO:HD2	1.49	0.94
1:A:2137:VAL:O	1:A:2141:ILE:HG23	1.69	0.93
1:A:3530:PHE:CD1	1:A:3618:TYR:CD2	2.56	0.93
1:A:3460:PRO:O	1:A:3463:SER:HB2	1.67	0.92
1:A:2563:SER:HB3	1:A:2566:SER:H	1.35	0.92
1:A:3737:THR:HB	1:A:3740:THR:OG1	1.70	0.92
1:A:1992:LYS:HE2	1:A:2024:SER:O	1.71	0.91
1:A:2494:LEU:HD13	1:A:2498:GLY:HA2	0.94	0.91
1:A:1620:PHE:HD1	1:A:1760:PHE:HZ	1.07	0.91
1:A:2400:HIS:NE2	1:A:2559:LEU:HD13	1.86	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2111:LYS:HD3	1:A:2161:GLU:CG	2.00	0.90
1:A:2920:TRP:HB2	1:A:2989:PRO:CG	1.99	0.90
1:A:2400:HIS:CD2	1:A:2559:LEU:HD13	2.06	0.90
1:A:3946:VAL:HG12	1:A:3950:PHE:O	1.72	0.90
1:A:2787:HIS:HA	1:A:3460:PRO:CG	2.02	0.89
1:A:2064:GLN:OE1	1:A:2091:MET:HE1	1.71	0.89
1:A:1939:PHE:CD2	1:A:1940:GLU:O	2.26	0.89
1:A:1823:ASP:CB	1:A:1852:ARG:O	2.20	0.89
1:A:4033:LEU:HD13	1:A:4035:GLN:HB2	1.54	0.89
1:A:1726:LEU:HD12	1:A:3984:GLN:HB3	1.55	0.88
1:A:2787:HIS:HA	1:A:3460:PRO:CD	2.03	0.88
1:A:2064:GLN:NE2	1:A:2091:MET:SD	2.47	0.88
1:A:3534:LEU:HD13	1:A:3618:TYR:HE2	1.38	0.88
1:A:1866:GLN:OE1	1:A:1911:ASN:HB2	1.74	0.87
1:A:2787:HIS:HA	1:A:3460:PRO:HG2	1.56	0.87
1:A:2112:GLU:HB3	1:A:2117:SER:HB2	1.57	0.87
1:A:1924:PRO:HB2	1:A:1929:ILE:HD11	1.55	0.87
1:A:3303:LYS:O	1:A:3306:TRP:CD1	2.28	0.87
1:A:1562:MET:HB3	1:A:1569:ILE:HD11	1.55	0.86
1:A:1649:LEU:HD11	1:A:1704:GLU:HG3	1.56	0.86
1:A:2446:SER:H	1:A:2449:THR:CG2	1.86	0.86
1:A:2766:LYS:HE2	1:A:2890:THR:HB	1.58	0.85
1:A:2446:SER:H	1:A:2449:THR:HG23	1.39	0.85
1:A:2920:TRP:CB	1:A:2989:PRO:HG3	2.01	0.85
1:A:1649:LEU:CD1	1:A:1704:GLU:HG3	2.07	0.84
1:A:2336:ARG:HD3	1:A:2355:ASP:OD2	1.77	0.84
1:A:3024:LEU:HD11	1:A:3303:LYS:CG	2.07	0.84
1:A:2141:ILE:CD1	1:A:2146:LYS:HE2	2.06	0.84
1:A:1940:GLU:HB2	1:A:1989:GLU:O	1.77	0.84
1:A:3656:VAL:HG13	1:A:3677:LEU:HB3	1.59	0.83
1:A:2755:HIS:HB2	1:A:2911:ARG:O	1.79	0.83
1:A:2274:HIS:HE1	1:A:2326:LEU:O	1.61	0.83
1:A:2106:THR:OG1	1:A:2154:PHE:HB3	1.78	0.83
1:A:2131:THR:HG22	1:A:2176:LEU:HD21	1.59	0.83
1:A:2488:GLU:HB3	1:A:2491:LEU:CD1	2.08	0.82
1:A:2488:GLU:CB	1:A:2491:LEU:HD12	2.09	0.82
1:A:3923:VAL:HG23	1:A:4038:GLU:HA	1.62	0.82
1:A:1849:GLU:HG2	1:A:1899:ASN:ND2	1.95	0.81
1:A:3303:LYS:HA	1:A:3306:TRP:NE1	1.95	0.81
1:A:3645:SER:HB3	1:A:3890:GLN:HE21	1.45	0.81
1:A:2332:GLY:HA2	1:A:2335:GLN:HB2	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2111:LYS:NZ	1:A:2161:GLU:HG2	1.94	0.81
1:A:1620:PHE:CD1	1:A:1760:PHE:HZ	1.96	0.80
1:A:1604:ALA:HA	1:A:1607:TRP:NE1	1.95	0.80
1:A:3303:LYS:C	1:A:3306:TRP:HD1	1.84	0.80
1:A:1630:ILE:HG22	1:A:1655:MET:SD	2.21	0.80
1:A:2362:ALA:HB3	1:A:2365:LYS:O	1.81	0.80
1:A:2476:LYS:NZ	1:A:2528:ARG:HD2	1.97	0.80
1:A:4033:LEU:CD1	1:A:4035:GLN:CB	2.60	0.80
1:A:3799:LYS:O	1:A:3803:LEU:HG	1.82	0.79
1:A:1970:LEU:HD12	1:A:1971:ARG:N	1.98	0.79
1:A:2064:GLN:OE1	1:A:2091:MET:CE	2.29	0.78
1:A:1604:ALA:HA	1:A:1607:TRP:CD1	2.18	0.78
1:A:2181:GLY:O	1:A:2182:GLU:HG3	1.83	0.78
1:A:3509:LEU:HD12	1:A:3513:VAL:CG2	2.13	0.78
1:A:1956:LEU:HB3	1:A:1968:PHE:CE2	2.18	0.78
1:A:2707:VAL:HB	1:A:2712:LEU:CD1	2.09	0.78
1:A:2707:VAL:CG1	1:A:2712:LEU:CD1	2.61	0.78
1:A:2476:LYS:HG2	1:A:2478:ASP:O	1.84	0.77
1:A:3303:LYS:CA	1:A:3306:TRP:CD1	2.66	0.77
1:A:1645:PHE:CB	1:A:1765:ILE:CG2	2.61	0.77
1:A:3534:LEU:HD11	1:A:3614:LEU:HD23	1.67	0.77
1:A:1939:PHE:HD2	1:A:1940:GLU:O	1.67	0.76
1:A:2032:LYS:O	1:A:2035:VAL:HG12	1.85	0.76
1:A:3460:PRO:O	1:A:3463:SER:CB	2.32	0.76
1:A:2563:SER:HB2	1:A:2566:SER:OG	1.86	0.75
1:A:3406:PHE:HB2	1:A:3513:VAL:HG12	1.69	0.75
1:A:3816:LEU:HD23	1:A:3847:SER:OG	1.86	0.75
1:A:3946:VAL:CG1	1:A:3950:PHE:O	2.34	0.75
1:A:2064:GLN:OE1	1:A:2151:TRP:HH2	1.67	0.75
1:A:3406:PHE:HB2	1:A:3513:VAL:HG11	1.69	0.75
1:A:3777:VAL:CG1	1:A:3895:PHE:CE1	2.63	0.75
1:A:1983:LEU:HD21	1:A:2000:ARG:HD2	1.69	0.74
1:A:3618:TYR:N	1:A:3618:TYR:CD1	2.54	0.74
1:A:3871:PHE:CZ	1:A:3873:MET:HB2	2.22	0.74
1:A:3939:ILE:HG13	1:A:4010:LEU:CD2	2.16	0.74
1:A:3530:PHE:HD1	1:A:3618:TYR:HD2	1.31	0.74
1:A:2411:LYS:HG2	1:A:2530:HIS:HE1	1.51	0.74
1:A:2176:LEU:O	1:A:2183:ARG:HA	1.88	0.74
1:A:2107:LYS:HE2	1:A:2499:SER:HB3	1.67	0.74
1:A:1744:LEU:HA	1:A:1760:PHE:CE2	2.23	0.74
1:A:2745:ILE:HG23	1:A:2756:MET:CE	2.17	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1569:ILE:HA	1:A:1584:SER:HA	1.70	0.73
1:A:1940:GLU:HG3	1:A:1941:ASP:H	1.52	0.73
1:A:3303:LYS:CA	1:A:3306:TRP:HD1	2.02	0.73
1:A:3566:LEU:HA	1:A:3583:LEU:CD2	2.18	0.73
1:A:3303:LYS:HA	1:A:3306:TRP:HD1	1.53	0.73
1:A:2707:VAL:CG1	1:A:2712:LEU:HD11	2.18	0.73
1:A:3525:ILE:CD1	1:A:3646:ILE:HG22	2.13	0.73
1:A:3534:LEU:HD13	1:A:3618:TYR:CE2	2.19	0.73
1:A:2201:HIS:CE1	1:A:2497:TYR:HA	2.24	0.72
1:A:1822:CYS:SG	1:A:1850:PHE:HA	2.29	0.72
1:A:2112:GLU:HB3	1:A:2117:SER:CB	2.19	0.72
1:A:3509:LEU:CD1	1:A:3513:VAL:CG2	2.68	0.72
1:A:2787:HIS:CA	1:A:3460:PRO:HD2	2.20	0.71
1:A:1849:GLU:HG2	1:A:1899:ASN:HD22	1.53	0.71
1:A:1970:LEU:HD13	1:A:1974:LYS:CE	2.20	0.71
1:A:1612:ASP:HA	1:A:1615:ILE:CD1	2.21	0.71
1:A:3792:ARG:HB2	1:A:3955:TYR:CD1	2.26	0.71
1:A:1956:LEU:HB3	1:A:1968:PHE:HE2	1.53	0.71
1:A:2960:THR:HB	1:A:2963:ASP:HB2	1.73	0.71
1:A:1774:LEU:HD21	1:A:1922:LYS:O	1.91	0.70
1:A:2141:ILE:HD12	1:A:2146:LYS:CE	2.11	0.70
1:A:3305:ARG:O	1:A:3307:LEU:N	2.24	0.70
1:A:2003:LEU:HA	1:A:2006:LEU:HD12	1.74	0.70
1:A:3530:PHE:HD1	1:A:3618:TYR:CD2	2.04	0.70
1:A:3774:ILE:O	1:A:3778:VAL:HG23	1.91	0.70
1:A:3645:SER:HB3	1:A:3890:GLN:NE2	2.06	0.70
1:A:1995:VAL:HG21	1:A:2024:SER:HB3	1.74	0.70
1:A:4033:LEU:HD13	1:A:4035:GLN:CB	2.21	0.70
1:A:2175:ILE:HG12	1:A:2183:ARG:HB3	1.74	0.69
1:A:2294:LEU:HB3	1:A:2317:LEU:HD22	1.74	0.69
1:A:3979:ASN:O	1:A:3981:PRO:HD2	1.92	0.69
1:A:2514:GLY:O	1:A:2523:TRP:CH2	2.45	0.69
1:A:3871:PHE:HZ	1:A:3873:MET:HB2	1.56	0.69
1:A:2203:THR:HG22	1:A:2205:ALA:H	1.56	0.69
1:A:3330:TYR:OH	1:A:3346:LEU:HD22	1.92	0.69
1:A:2125:TRP:CZ2	1:A:2178:LEU:HD13	2.27	0.69
1:A:1646:GLN:NE2	1:A:1758:TYR:OH	2.26	0.68
1:A:1983:LEU:HB3	1:A:1993:THR:HG23	1.75	0.68
1:A:3935:PHE:HB2	1:A:4014:VAL:HG11	1.75	0.68
1:A:1630:ILE:HA	1:A:1634:THR:HG22	1.75	0.68
1:A:3850:TRP:NE1	1:A:3854:TYR:HB3	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2419:PRO:O	1:A:2424:LYS:HE3	1.93	0.68
1:A:1967:HIS:C	1:A:1968:PHE:HD1	1.97	0.68
1:A:2305:LEU:HD11	1:A:2368:PHE:CG	2.29	0.68
1:A:2293:HIS:CE1	1:A:2409:ASN:HB3	2.29	0.68
1:A:3509:LEU:HD12	1:A:3513:VAL:HG21	1.75	0.68
1:A:3785:TYR:HE2	1:A:3859:VAL:HG22	1.57	0.68
1:A:2285:GLU:HB2	1:A:2412:ARG:NH2	2.08	0.68
1:A:2252:LEU:HD21	1:A:2310:LEU:HD23	1.76	0.67
1:A:2111:LYS:HZ2	1:A:2161:GLU:HG2	1.58	0.67
1:A:1744:LEU:HA	1:A:1760:PHE:CD2	2.29	0.67
1:A:3566:LEU:HA	1:A:3583:LEU:HD21	1.76	0.67
1:A:2293:HIS:NE2	1:A:2409:ASN:HB3	2.09	0.67
1:A:1698:ILE:O	1:A:1702:LEU:HG	1.94	0.67
1:A:2386:MET:HB3	1:A:2627:ARG:HD3	1.75	0.67
1:A:3848:LEU:HD21	1:A:3852:LYS:HE3	1.75	0.67
1:A:1626:CYS:SG	1:A:1639:VAL:HG11	2.35	0.67
1:A:2476:LYS:HZ1	1:A:2528:ARG:HD2	1.59	0.67
1:A:3837:GLY:O	1:A:3871:PHE:HD1	1.77	0.67
1:A:3979:ASN:C	1:A:3981:PRO:HD2	2.16	0.66
1:A:1822:CYS:SG	1:A:1849:GLU:O	2.53	0.66
1:A:2493:LYS:HG3	1:A:2494:LEU:H	1.60	0.66
1:A:3473:ALA:HB3	1:A:3476:ARG:O	1.96	0.66
1:A:2707:VAL:CG1	1:A:2712:LEU:HD12	2.26	0.66
1:A:2107:LYS:CE	1:A:2495:ASP:OD2	2.37	0.66
1:A:2220:CYS:SG	1:A:2224:SER:HB2	2.36	0.66
1:A:2631:THR:O	1:A:2635:THR:HG22	1.96	0.66
1:A:2080:LYS:HG2	1:A:2215:PHE:CE1	2.30	0.66
1:A:1992:LYS:HG3	1:A:2024:SER:CB	2.11	0.65
1:A:2514:GLY:HA3	1:A:2523:TRP:CZ2	2.32	0.65
1:A:3566:LEU:CD1	1:A:3570:LEU:HD11	2.26	0.65
1:A:3566:LEU:O	1:A:3570:LEU:HG	1.97	0.65
1:A:3566:LEU:HD13	1:A:3570:LEU:CD1	2.27	0.65
1:A:3998:ILE:HG21	1:A:4004:LEU:HG	1.77	0.65
1:A:1706:LEU:CD2	1:A:1935:GLN:HG2	2.27	0.65
1:A:2382:ALA:O	1:A:2385:VAL:HG12	1.96	0.65
1:A:2448:ASP:HB2	1:A:2829:GLU:CD	2.17	0.65
1:A:3819:ILE:O	1:A:3823:ASN:HB2	1.97	0.65
1:A:1703:VAL:HG13	1:A:1770:ILE:HD13	1.78	0.64
1:A:1953:LEU:CD1	1:A:1973:LEU:HB3	2.27	0.64
1:A:3459:ASP:OD2	1:A:3461:ILE:HG12	1.97	0.64
1:A:3998:ILE:CG2	1:A:4004:LEU:HG	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2495:ASP:O	1:A:2498:GLY:N	2.30	0.64
1:A:2095:ASP:CG	1:A:2149:ARG:NH2	2.50	0.64
1:A:2728:LEU:HD12	1:A:2771:ARG:CZ	2.27	0.64
1:A:3010:LEU:HD21	1:A:3317:SER:HB3	1.79	0.64
1:A:2222:ILE:HG23	1:A:2284:LEU:HD11	1.80	0.64
1:A:3303:LYS:HD2	1:A:3306:TRP:CD1	2.33	0.64
1:A:1826:PHE:HE1	1:A:1853:LEU:HD22	1.62	0.64
1:A:2779:LEU:HD23	1:A:2812:ARG:O	1.97	0.64
1:A:1970:LEU:CD1	1:A:1974:LYS:HE3	2.24	0.64
1:A:3509:LEU:HD11	1:A:3513:VAL:HG21	1.76	0.64
1:A:2290:LEU:HD13	1:A:2407:LEU:HD23	1.79	0.64
1:A:3737:THR:OG1	1:A:3740:THR:HB	1.98	0.63
1:A:1562:MET:CB	1:A:1569:ILE:HD11	2.29	0.63
1:A:3618:TYR:N	1:A:3618:TYR:HD1	1.94	0.63
1:A:1645:PHE:CG	1:A:1765:ILE:HG22	2.32	0.63
1:A:1827:ASP:HB3	1:A:1830:VAL:HG12	1.81	0.63
1:A:1938:GLY:O	1:A:1989:GLU:HB3	1.98	0.63
1:A:1612:ASP:HA	1:A:1615:ILE:HD11	1.78	0.63
1:A:3792:ARG:HB2	1:A:3955:TYR:CE1	2.33	0.63
1:A:1967:HIS:O	1:A:1968:PHE:HD1	1.82	0.63
1:A:2285:GLU:HB2	1:A:2412:ARG:HH22	1.63	0.63
1:A:2842:ASP:O	1:A:2845:GLN:HG2	1.97	0.63
1:A:2536:ASN:HB2	1:A:2543:ARG:HE	1.64	0.63
1:A:1748:PHE:CD2	1:A:1755:LEU:HD22	2.34	0.62
1:A:2512:LYS:O	1:A:2513:GLN:HB2	1.97	0.62
1:A:3409:ASP:HB3	1:A:3518:PHE:HB2	1.81	0.62
1:A:1738:ASN:O	1:A:1739:ASP:OD1	2.16	0.62
1:A:1995:VAL:HG22	1:A:2022:PHE:CE2	2.33	0.62
1:A:1991:GLU:O	1:A:1995:VAL:HG23	1.99	0.62
1:A:2315:THR:HG21	1:A:2350:SER:HB3	1.80	0.62
1:A:2151:TRP:HE3	1:A:2193:LEU:HD11	1.64	0.62
1:A:2632:ALA:HB3	1:A:2647:LEU:HD21	1.80	0.62
1:A:3525:ILE:HD11	1:A:3646:ILE:CG2	2.15	0.62
1:A:1996:GLU:O	1:A:2000:ARG:HG3	2.00	0.62
1:A:3785:TYR:CE2	1:A:3859:VAL:HG22	2.33	0.62
1:A:3912:GLY:O	1:A:3915:PHE:CE2	2.53	0.62
1:A:2282:ASN:HB3	1:A:2552:ARG:HG3	1.82	0.61
1:A:3641:PHE:HA	1:A:3889:LEU:HD21	1.81	0.61
1:A:1983:LEU:HD21	1:A:2000:ARG:CD	2.31	0.61
1:A:3307:LEU:HA	1:A:3310:THR:HB	1.81	0.61
1:A:3330:TYR:CE2	1:A:3346:LEU:HD13	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1969:GLY:O	1:A:1972:THR:HB	2.01	0.61
1:A:3530:PHE:CE1	1:A:3618:TYR:CD2	2.88	0.61
1:A:3700:MET:HB3	1:A:4085:THR:HG21	1.81	0.61
1:A:1826:PHE:CE1	1:A:1853:LEU:HD22	2.35	0.61
1:A:1692:ASP:O	1:A:1695:LYS:HB3	2.00	0.61
1:A:3583:LEU:O	1:A:3587:LEU:HG	2.00	0.61
1:A:1574:PHE:HB3	1:A:1576:GLU:H	1.65	0.60
1:A:2677:VAL:HG11	1:A:2686:LEU:HD21	1.83	0.60
1:A:1900:PRO:HB3	1:A:1905:ARG:HA	1.83	0.60
1:A:2293:HIS:CE1	1:A:2409:ASN:CB	2.84	0.60
1:A:2563:SER:CB	1:A:2566:SER:OG	2.47	0.60
1:A:2785:LYS:HD3	1:A:3482:GLY:O	2.01	0.60
1:A:3817:GLY:H	1:A:3821:ASN:HB2	1.66	0.60
1:A:1630:ILE:CG2	1:A:1655:MET:SD	2.89	0.60
1:A:2394:THR:H	1:A:2397:THR:HB	1.64	0.60
1:A:3886:ALA:N	1:A:3887:PRO:HD2	2.17	0.60
1:A:1656:TRP:O	1:A:1660:VAL:HG12	2.01	0.60
1:A:3948:HIS:NE2	1:A:4072:ASN:CG	2.55	0.60
1:A:1851:ASN:HD21	1:A:1899:ASN:HB2	1.66	0.60
1:A:3541:MET:HA	1:A:3544:LYS:HG2	1.83	0.60
1:A:4065:LEU:HD11	1:A:4070:ILE:CD1	2.29	0.60
1:A:1620:PHE:HA	1:A:1760:PHE:CE1	2.37	0.60
1:A:2427:ILE:HD12	1:A:2559:LEU:CD2	2.31	0.60
1:A:2489:ILE:HG22	1:A:2535:CYS:HB3	1.84	0.60
1:A:2640:THR:HG23	1:A:2643:SER:H	1.66	0.60
1:A:1984:ILE:HG21	1:A:1989:GLU:HG3	1.84	0.60
1:A:2155:ASP:OD1	1:A:2549:ARG:NH2	2.35	0.59
1:A:2728:LEU:HD12	1:A:2771:ARG:NH2	2.17	0.59
1:A:3429:LEU:HD21	1:A:3439:ARG:HB3	1.83	0.59
1:A:2339:ILE:HG23	1:A:2353:LEU:HB3	1.83	0.59
1:A:1726:LEU:CD1	1:A:3984:GLN:HB3	2.30	0.59
1:A:2081:THR:O	1:A:2085:LYS:HB2	2.02	0.59
1:A:3851:VAL:HG13	1:A:3855:LEU:HD23	1.85	0.59
1:A:2380:LEU:HD11	1:A:2390:ILE:HD11	1.83	0.59
1:A:2354:SER:OG	1:A:2357:SER:HB2	2.02	0.59
1:A:1940:GLU:HG3	1:A:1941:ASP:N	2.18	0.58
1:A:2064:GLN:OE1	1:A:2151:TRP:CH2	2.55	0.58
1:A:2941:THR:HG22	1:A:2942:ASP:H	1.66	0.58
1:A:3555:TYR:HE1	1:A:3593:GLU:HG2	1.68	0.58
1:A:3592:LYS:O	1:A:3596:ASN:HB2	2.03	0.58
1:A:4021:LEU:HD23	1:A:4023:ILE:HG13	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2784:PRO:HG2	1:A:2817:ILE:HD13	1.84	0.58
1:A:3618:TYR:O	1:A:3622:GLY:N	2.34	0.58
1:A:2034:ILE:HD12	1:A:2061:TYR:CZ	2.38	0.58
1:A:2386:MET:CB	1:A:2627:ARG:CD	2.77	0.58
1:A:2755:HIS:NE2	1:A:2835:LEU:HG	2.17	0.58
1:A:2241:LEU:HD13	1:A:2299:ARG:HH11	1.68	0.58
1:A:2257:PHE:HD1	1:A:2262:LEU:HD11	1.69	0.58
1:A:2336:ARG:CD	1:A:2355:ASP:OD2	2.50	0.58
1:A:3810:SER:O	1:A:3838:TRP:HB2	2.03	0.58
1:A:3537:GLU:OE1	1:A:3618:TYR:OH	2.21	0.58
1:A:3737:THR:HB	1:A:3740:THR:CB	2.33	0.58
1:A:3945:LEU:O	1:A:3948:HIS:O	2.21	0.58
1:A:1559:SER:HB3	1:A:1572:ILE:HG22	1.86	0.58
1:A:3839:ILE:HG23	1:A:3873:MET:HG3	1.86	0.58
1:A:4033:LEU:HD12	1:A:4035:GLN:N	2.18	0.58
1:A:2201:HIS:NE2	1:A:2497:TYR:O	2.37	0.57
1:A:2332:GLY:HA2	1:A:2335:GLN:CB	2.31	0.57
1:A:3519:VAL:HG13	1:A:3521:ASN:ND2	2.19	0.57
1:A:2446:SER:H	1:A:2449:THR:HG21	1.67	0.57
1:A:1706:LEU:HD21	1:A:1935:GLN:HG2	1.86	0.57
1:A:1779:PHE:O	1:A:1783:THR:HG22	2.03	0.57
1:A:1911:ASN:OD1	1:A:1912:LEU:N	2.38	0.57
1:A:2071:ILE:HB	1:A:2212:LEU:HD12	1.85	0.57
1:A:4024:VAL:HG11	1:A:4062:TRP:CD2	2.38	0.57
1:A:2938:MET:SD	1:A:3321:ILE:HG21	2.45	0.57
1:A:1781:THR:HG21	1:A:1919:PHE:CD1	2.39	0.57
1:A:1965:HIS:HD2	1:A:2212:LEU:CD2	2.18	0.57
1:A:2846:GLY:O	1:A:2849:TYR:HB3	2.04	0.57
1:A:2437:LEU:H	1:A:2437:LEU:HD12	1.69	0.57
1:A:4017:GLY:HA3	1:A:4021:LEU:HD12	1.87	0.57
1:A:1704:GLU:OE2	1:A:1768:ARG:NH1	2.37	0.57
1:A:2127:ASP:O	1:A:2131:THR:OG1	2.23	0.57
1:A:2476:LYS:HZ2	1:A:2528:ARG:HD2	1.68	0.57
1:A:3912:GLY:O	1:A:3915:PHE:CZ	2.57	0.57
1:A:1939:PHE:O	1:A:1940:GLU:HB3	2.05	0.57
1:A:2476:LYS:CD	1:A:2476:LYS:N	2.52	0.57
1:A:2808:LEU:HD21	1:A:2856:LEU:HD12	1.86	0.57
1:A:1620:PHE:CZ	1:A:1743:ASP:HB3	2.40	0.56
1:A:1995:VAL:HG22	1:A:2022:PHE:CD2	2.40	0.56
1:A:2419:PRO:O	1:A:2424:LYS:CE	2.52	0.56
1:A:2787:HIS:CA	1:A:3460:PRO:HG2	2.32	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3939:ILE:HG13	1:A:4010:LEU:HD22	1.86	0.56
1:A:1619:VAL:HG12	1:A:1760:PHE:HD1	1.70	0.56
1:A:4023:ILE:HD12	1:A:4029:ILE:HD11	1.87	0.56
1:A:2627:ARG:NH1	1:A:2630:TYR:CE2	2.74	0.56
1:A:1983:LEU:HB3	1:A:1993:THR:CG2	2.36	0.56
1:A:2111:LYS:CD	1:A:2161:GLU:HG3	2.13	0.56
1:A:1940:GLU:CB	1:A:1989:GLU:O	2.51	0.56
1:A:2868:ASP:HB2	1:A:2872:GLU:OE1	2.06	0.56
1:A:4037:SER:HB3	1:A:4040:GLU:HB3	1.87	0.56
1:A:2111:LYS:HZ3	1:A:2161:GLU:HG2	1.69	0.56
1:A:2131:THR:HG22	1:A:2176:LEU:CD2	2.34	0.56
1:A:2410:SER:O	1:A:2411:LYS:HB2	2.06	0.56
1:A:2220:CYS:SG	1:A:2224:SER:CB	2.94	0.55
1:A:2386:MET:HB3	1:A:2627:ARG:CD	2.36	0.55
1:A:2151:TRP:CE3	1:A:2193:LEU:HD11	2.41	0.55
1:A:3538:ASN:HB3	1:A:3541:MET:HG2	1.87	0.55
1:A:1823:ASP:HB2	1:A:1853:LEU:HD23	1.88	0.55
1:A:1852:ARG:O	1:A:1852:ARG:HG3	2.06	0.55
1:A:2064:GLN:CD	1:A:2091:MET:CE	2.75	0.55
1:A:3303:LYS:C	1:A:3306:TRP:CD1	2.74	0.55
1:A:4022:GLN:O	1:A:4022:GLN:HG2	2.05	0.55
1:A:2305:LEU:HD11	1:A:2368:PHE:CD1	2.41	0.55
1:A:2514:GLY:C	1:A:2523:TRP:CH2	2.80	0.55
1:A:3303:LYS:HA	1:A:3306:TRP:HE1	1.67	0.55
1:A:2002:ILE:HG22	1:A:2006:LEU:HD11	1.88	0.55
1:A:3440:LEU:HD23	1:A:3462:ILE:HD12	1.88	0.55
1:A:2181:GLY:C	1:A:2182:GLU:HG3	2.27	0.55
1:A:2400:HIS:NE2	1:A:2559:LEU:CD1	2.67	0.55
1:A:2788:ARG:HG3	1:A:3459:ASP:HA	1.89	0.55
1:A:2707:VAL:CB	1:A:2712:LEU:CD1	2.72	0.55
1:A:2745:ILE:HG12	1:A:2756:MET:HE3	1.88	0.55
1:A:3631:MET:CE	1:A:3698:MET:HG3	2.36	0.55
1:A:2476:LYS:HD3	1:A:2476:LYS:N	2.09	0.54
1:A:3683:TYR:O	1:A:3687:SER:HB2	2.07	0.54
1:A:3817:GLY:H	1:A:3821:ASN:CB	2.21	0.54
1:A:2786:ILE:O	1:A:3460:PRO:HB2	2.07	0.54
1:A:4059:LEU:HA	1:A:4063:LEU:HD13	1.89	0.54
1:A:2002:ILE:HB	1:A:2014:PHE:CE2	2.42	0.54
1:A:2707:VAL:HG12	1:A:2712:LEU:HD12	1.89	0.54
1:A:2141:ILE:HG22	1:A:2145:PHE:HB2	1.90	0.54
1:A:2230:LEU:HD23	1:A:2288:VAL:HG13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3877:CYS:SG	1:A:3884:LEU:CD2	2.96	0.54
1:A:2707:VAL:HG12	1:A:2712:LEU:CD1	2.37	0.54
1:A:2201:HIS:CE1	1:A:2497:TYR:CA	2.91	0.54
1:A:2462:THR:HG22	1:A:2476:LYS:HA	1.90	0.54
1:A:3481:ILE:O	1:A:3483:ASP:N	2.36	0.54
1:A:3509:LEU:HD12	1:A:3513:VAL:HG23	1.88	0.54
1:A:2095:ASP:CG	1:A:2149:ARG:HH22	2.11	0.54
1:A:2173:ASN:HB3	1:A:2175:ILE:HG22	1.90	0.54
1:A:3440:LEU:CD2	1:A:3462:ILE:HD12	2.38	0.54
1:A:2787:HIS:HB3	1:A:3461:ILE:HG23	1.91	0.53
1:A:2488:GLU:CD	1:A:2491:LEU:HD11	2.29	0.53
1:A:2336:ARG:HG2	1:A:2355:ASP:OD1	2.08	0.53
1:A:2450:THR:H	1:A:2453:HIS:CE1	2.27	0.53
1:A:3645:SER:CB	1:A:3890:GLN:HE21	2.19	0.53
1:A:2786:ILE:HG12	1:A:2821:ASN:HA	1.90	0.53
1:A:1645:PHE:CZ	1:A:1649:LEU:HD22	2.43	0.53
1:A:2339:ILE:HG12	1:A:2353:LEU:HD23	1.90	0.53
1:A:2788:ARG:HB2	1:A:3459:ASP:HB3	1.91	0.53
1:A:2305:LEU:CD1	1:A:2368:PHE:CD1	2.91	0.53
1:A:3612:ASP:O	1:A:3615:VAL:HG22	2.09	0.53
1:A:3995:GLY:HA2	1:A:3998:ILE:HD13	1.91	0.53
1:A:1627:LEU:HD11	1:A:1631:LYS:HE3	1.89	0.53
1:A:3566:LEU:CA	1:A:3583:LEU:HD21	2.37	0.53
1:A:3656:VAL:CG1	1:A:3677:LEU:HB3	2.36	0.53
1:A:1981:SER:HB3	1:A:1982:PRO:HD3	1.91	0.53
1:A:2063:MET:HB3	1:A:2070:LEU:HD11	1.90	0.53
1:A:1749:ILE:HD13	1:A:1813:LEU:HD22	1.92	0.52
1:A:1970:LEU:HD12	1:A:1970:LEU:C	2.28	0.52
1:A:2833:THR:HG21	1:A:2841:PRO:HD2	1.91	0.52
1:A:3946:VAL:HB	1:A:3947:PRO:HA	1.91	0.52
1:A:1979:ASN:O	1:A:1983:LEU:HD13	2.09	0.52
1:A:2419:PRO:O	1:A:2424:LYS:NZ	2.42	0.52
1:A:2795:PHE:CE2	1:A:2799:LEU:HD11	2.44	0.52
1:A:3692:LYS:HE3	1:A:3898:GLU:HB3	1.91	0.52
1:A:3703:PHE:CE1	1:A:3766:GLU:HG2	2.43	0.52
1:A:2578:ILE:HG21	1:A:2630:TYR:HB2	1.91	0.52
1:A:3877:CYS:SG	1:A:3884:LEU:HD22	2.50	0.52
1:A:2285:GLU:CB	1:A:2412:ARG:NH2	2.73	0.52
1:A:1620:PHE:HA	1:A:1760:PHE:HE1	1.74	0.52
1:A:1822:CYS:SG	1:A:1849:GLU:C	2.88	0.52
1:A:1939:PHE:HD1	1:A:1939:PHE:H	1.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1926:SER:HA	1:A:1929:ILE:HD13	1.92	0.52
1:A:2177:THR:HG22	1:A:2183:ARG:HG2	1.91	0.52
1:A:2380:LEU:HD13	1:A:2390:ILE:CD1	2.23	0.52
1:A:1645:PHE:HB2	1:A:1697:LYS:HG3	1.91	0.52
1:A:1849:GLU:CG	1:A:1899:ASN:HD22	2.22	0.52
1:A:1963:MET:HB3	1:A:1966:TYR:CD2	2.45	0.52
1:A:2290:LEU:HD23	1:A:2321:SER:HA	1.91	0.52
1:A:4034:LEU:HD23	1:A:4034:LEU:O	2.10	0.52
1:A:1645:PHE:HZ	1:A:1768:ARG:HD2	1.75	0.52
1:A:2012:LEU:HD13	1:A:2016:ASP:OD2	2.10	0.52
1:A:3017:VAL:HG21	1:A:3313:PHE:CE2	2.44	0.52
1:A:4021:LEU:HD23	1:A:4023:ILE:CG1	2.39	0.52
1:A:2302:PHE:HA	1:A:2310:LEU:HD11	1.92	0.51
1:A:3323:ASN:HD21	1:A:3361:ASP:H	1.58	0.51
1:A:3547:ASP:HA	1:A:3550:LYS:HB3	1.91	0.51
1:A:3951:SER:HB2	1:A:4002:LYS:HD2	1.91	0.51
1:A:2494:LEU:HD12	1:A:2494:LEU:O	2.10	0.51
1:A:2780:LYS:HD3	1:A:2813:THR:HG22	1.93	0.51
1:A:3934:TRP:CB	1:A:4023:ILE:HD13	2.41	0.51
1:A:1606:GLU:O	1:A:1610:ILE:HG12	2.11	0.51
1:A:1803:THR:HG21	1:A:1848:ASP:OD1	2.10	0.51
1:A:2645:ILE:CD1	1:A:2686:LEU:HG	2.40	0.51
1:A:3911:TRP:HH2	1:A:3926:VAL:CG1	2.23	0.51
1:A:2637:PRO:O	1:A:2639:GLN:NE2	2.44	0.51
1:A:1650:LEU:HD11	1:A:1747:VAL:HG11	1.92	0.51
1:A:1604:ALA:HA	1:A:1607:TRP:HE1	1.72	0.51
1:A:1706:LEU:HD22	1:A:1935:GLN:HG2	1.93	0.51
1:A:2295:ILE:HG12	1:A:2314:ILE:HD12	1.93	0.51
1:A:2427:ILE:HD12	1:A:2559:LEU:HD22	1.92	0.51
1:A:2476:LYS:HZ2	1:A:2528:ARG:HB2	1.76	0.51
1:A:1677:ASP:HA	1:A:1680:ILE:HD12	1.92	0.51
1:A:1849:GLU:CG	1:A:1899:ASN:ND2	2.70	0.51
1:A:2084:TRP:HE3	1:A:2088:ILE:HD12	1.76	0.51
1:A:1917:ARG:HD2	1:A:3963:PHE:CE2	2.46	0.51
1:A:2106:THR:HG1	1:A:2154:PHE:HB3	1.72	0.51
1:A:3645:SER:CB	1:A:3890:GLN:NE2	2.74	0.51
1:A:3737:THR:OG1	1:A:3740:THR:CB	2.59	0.51
1:A:4065:LEU:HD12	1:A:4065:LEU:O	2.10	0.51
1:A:3848:LEU:HD12	1:A:3884:LEU:HD12	1.93	0.51
1:A:2034:ILE:CD1	1:A:2061:TYR:CZ	2.95	0.50
1:A:2112:GLU:CB	1:A:2117:SER:HB2	2.35	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1707:HIS:O	1:A:1711:VAL:HG23	2.10	0.50
1:A:3566:LEU:HD11	1:A:3570:LEU:HD11	1.92	0.50
1:A:3839:ILE:CG2	1:A:3873:MET:HG3	2.41	0.50
1:A:3737:THR:CB	1:A:3740:THR:CB	2.89	0.50
1:A:2385:VAL:HG23	1:A:2574:TYR:HD1	1.77	0.50
1:A:3854:TYR:O	1:A:3858:HIS:HB2	2.10	0.50
1:A:2109:LEU:HD13	1:A:2129:LEU:HD23	1.94	0.50
1:A:2115:TYR:OH	1:A:2162:TYR:O	2.23	0.50
1:A:3979:ASN:C	1:A:3981:PRO:CD	2.80	0.50
1:A:1748:PHE:HD2	1:A:1755:LEU:HD22	1.77	0.50
1:A:2960:THR:HG22	1:A:2961:ILE:N	2.28	0.49
1:A:3845:GLN:OE1	1:A:3878:HIS:HB2	2.11	0.49
1:A:1570:GLU:HB2	1:A:1585:VAL:HA	1.93	0.49
1:A:1657:THR:HG21	1:A:1734:PHE:O	2.12	0.49
1:A:1748:PHE:CE2	1:A:1755:LEU:HD22	2.47	0.49
1:A:2102:TYR:HB2	1:A:2152:VAL:HG22	1.93	0.49
1:A:2064:GLN:NE2	1:A:2091:MET:CE	2.76	0.49
1:A:2448:ASP:CB	1:A:2829:GLU:OE2	2.47	0.49
1:A:3692:LYS:HE3	1:A:3898:GLU:O	2.13	0.49
1:A:3787:THR:HG22	1:A:3875:MET:HB2	1.93	0.49
1:A:3855:LEU:HD12	1:A:3859:VAL:HG23	1.93	0.49
1:A:1664:LEU:HD23	1:A:1669:PHE:HZ	1.77	0.49
1:A:2563:SER:CB	1:A:2566:SER:H	2.15	0.49
1:A:2982:VAL:HG12	1:A:2983:GLY:N	2.27	0.49
1:A:3350:LYS:HA	1:A:3353:LEU:HD12	1.94	0.49
1:A:3725:VAL:HG22	1:A:3731:ASP:HA	1.93	0.49
1:A:2034:ILE:CD1	1:A:2061:TYR:CE2	2.95	0.49
1:A:2074:GLY:O	1:A:2197:ASP:HA	2.13	0.49
1:A:3946:VAL:HA	1:A:3947:PRO:C	2.33	0.49
1:A:2645:ILE:HD11	1:A:2686:LEU:HG	1.94	0.49
1:A:2762:SER:O	1:A:2763:ARG:HB2	2.12	0.49
1:A:4065:LEU:HD12	1:A:4065:LEU:C	2.33	0.49
1:A:1911:ASN:OD1	1:A:1912:LEU:HG	2.13	0.49
1:A:2002:ILE:HB	1:A:2014:PHE:HE2	1.78	0.49
1:A:2514:GLY:CA	1:A:2523:TRP:CZ2	2.96	0.49
1:A:2839:ASP:O	1:A:2841:PRO:HD3	2.12	0.49
1:A:3833:LYS:HZ3	1:A:3862:THR:HG21	1.76	0.49
1:A:3978:ASN:O	1:A:3981:PRO:CD	2.60	0.49
1:A:2364:ASP:O	1:A:2365:LYS:HG2	2.13	0.49
1:A:3671:VAL:O	1:A:3674:ILE:HG22	2.13	0.49
1:A:3373:LEU:O	1:A:3373:LEU:HD23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3889:LEU:HG	1:A:3894:ARG:HD3	1.95	0.48
1:A:1626:CYS:SG	1:A:1639:VAL:CG1	3.01	0.48
1:A:2169:VAL:HG13	1:A:2186:ILE:HG12	1.94	0.48
1:A:2354:SER:OG	1:A:2357:SER:CB	2.61	0.48
1:A:1967:HIS:NE2	1:A:2204:PRO:HB3	2.28	0.48
1:A:1983:LEU:HD21	1:A:2000:ARG:NE	2.28	0.48
1:A:2137:VAL:O	1:A:2141:ILE:CG2	2.50	0.48
1:A:3911:TRP:HH2	1:A:3926:VAL:HG12	1.77	0.48
1:A:1645:PHE:CD2	1:A:1765:ILE:HG22	2.48	0.48
1:A:2654:ARG:HH22	1:A:2691:SER:HB2	1.77	0.48
1:A:3566:LEU:HD13	1:A:3570:LEU:HD12	1.95	0.48
1:A:1626:CYS:HB2	1:A:1643:TYR:CD2	2.48	0.48
1:A:1849:GLU:OE2	1:A:1899:ASN:ND2	2.47	0.48
1:A:3541:MET:HB2	1:A:3607:PHE:HE1	1.78	0.48
1:A:2860:THR:HG22	1:A:2865:LEU:O	2.13	0.48
1:A:3737:THR:CB	1:A:3740:THR:HB	2.44	0.48
1:A:4033:LEU:HD12	1:A:4036:GLN:H	1.78	0.48
1:A:1731:VAL:HG12	1:A:1732:GLN:N	2.28	0.48
1:A:2828:LEU:HD13	1:A:2902:MET:SD	2.53	0.48
1:A:3703:PHE:HE1	1:A:3766:GLU:HG2	1.79	0.48
1:A:1794:PHE:HD1	1:A:1802:LYS:HB3	1.79	0.48
1:A:2084:TRP:CZ3	1:A:2085:LYS:HG3	2.49	0.48
1:A:3353:LEU:HD23	1:A:3358:VAL:HG11	1.95	0.48
1:A:1826:PHE:CE1	1:A:1853:LEU:CD2	2.96	0.48
1:A:2476:LYS:H	1:A:2476:LYS:HD2	1.72	0.48
1:A:2580:LYS:HG2	1:A:2586:ARG:HH22	1.79	0.47
1:A:2358:THR:HG22	1:A:2359:ILE:N	2.29	0.47
1:A:2741:HIS:O	1:A:2745:ILE:HG13	2.15	0.47
1:A:4084:SER:O	1:A:4088:LEU:HG	2.14	0.47
1:A:3721:THR:O	1:A:3725:VAL:HG23	2.14	0.47
1:A:2445:PHE:HA	1:A:2449:THR:HG21	1.96	0.47
1:A:2446:SER:N	1:A:2449:THR:HG23	2.19	0.47
1:A:1844:TRP:CD1	1:A:1893:ALA:HB3	2.50	0.47
1:A:2125:TRP:CZ2	1:A:2178:LEU:CD1	2.97	0.47
1:A:3415:ILE:HD13	1:A:3453:GLN:HG3	1.97	0.47
1:A:3462:ILE:O	1:A:3465:LEU:N	2.45	0.47
1:A:3459:ASP:OD2	1:A:3461:ILE:CG1	2.61	0.47
1:A:3690:LEU:HD23	1:A:3694:PHE:HB3	1.96	0.47
1:A:3924:TRP:O	1:A:3927:TYR:HB3	2.15	0.47
1:A:3612:ASP:O	1:A:3615:VAL:CG2	2.63	0.47
1:A:3592:LYS:O	1:A:3596:ASN:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1554:HIS:O	1:A:1555:HIS:HB2	2.15	0.46
1:A:1636:ILE:O	1:A:1640:VAL:HG23	2.15	0.46
1:A:1683:LEU:HB3	1:A:1702:LEU:HD21	1.96	0.46
1:A:2105:ASP:OD2	1:A:2508:GLN:HB2	2.15	0.46
1:A:2318:ILE:O	1:A:2322:LEU:HB2	2.16	0.46
1:A:3934:TRP:HB3	1:A:4023:ILE:HD13	1.97	0.46
1:A:3877:CYS:SG	1:A:3884:LEU:HD21	2.55	0.46
1:A:1683:LEU:HD22	1:A:1698:ILE:HG23	1.96	0.46
1:A:3967:TYR:HE2	1:A:3985:VAL:HA	1.80	0.46
1:A:1681:LYS:HE2	1:A:1939:PHE:CE1	2.50	0.46
1:A:2878:VAL:HA	1:A:2881:ILE:HD12	1.97	0.46
1:A:2112:GLU:HB3	1:A:2117:SER:OG	2.16	0.46
1:A:2204:PRO:HA	1:A:2207:ILE:HD12	1.97	0.46
1:A:2199:LEU:O	1:A:2201:HIS:N	2.49	0.46
1:A:2424:LYS:H	1:A:2424:LYS:HG3	1.52	0.46
1:A:2627:ARG:NH1	1:A:2630:TYR:CD2	2.84	0.46
1:A:2571:TYR:HA	1:A:2574:TYR:HB2	1.97	0.46
1:A:2654:ARG:NH1	1:A:2658:ASP:OD1	2.49	0.46
1:A:1660:VAL:HG13	1:A:1728:TRP:CH2	2.51	0.46
1:A:3508:PHE:O	1:A:3512:ARG:HG2	2.16	0.46
1:A:3807:SER:O	1:A:3808:LYS:HB2	2.16	0.46
1:A:2286:THR:HA	1:A:2412:ARG:NE	2.31	0.45
1:A:2835:LEU:HD23	1:A:2911:ARG:HB2	1.97	0.45
1:A:3760:LEU:HD21	1:A:4078:ALA:HA	1.98	0.45
1:A:1586:GLU:HG3	1:A:1765:ILE:H	1.81	0.45
1:A:3330:TYR:CE1	1:A:3334:PHE:CD2	3.05	0.45
1:A:3821:ASN:O	1:A:3825:ALA:HB2	2.17	0.45
1:A:3995:GLY:HA2	1:A:3998:ILE:CD1	2.46	0.45
1:A:1803:THR:HG21	1:A:1848:ASP:CG	2.37	0.45
1:A:2358:THR:CG2	1:A:2359:ILE:N	2.80	0.45
1:A:2458:LEU:HG	1:A:2484:LEU:HD21	1.99	0.45
1:A:2707:VAL:HG11	1:A:2712:LEU:CD1	2.45	0.45
1:A:2099:ASN:HA	1:A:2149:ARG:O	2.17	0.45
1:A:2494:LEU:HB2	1:A:2499:SER:N	2.32	0.45
1:A:3470:PHE:CE1	1:A:3488:VAL:HG21	2.52	0.45
1:A:1951:HIS:O	1:A:1955:LEU:HB2	2.17	0.45
1:A:2037:CYS:SG	1:A:2094:PHE:HB2	2.57	0.45
1:A:2417:CYS:O	1:A:2558:TYR:HA	2.17	0.45
1:A:2984:VAL:C	1:A:2986:PRO:HD3	2.37	0.45
1:A:1910:GLU:HB2	1:A:3846:MET:HA	1.98	0.45
1:A:2262:LEU:HA	1:A:2265:ILE:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3869:GLU:O	1:A:3870:LYS:C	2.56	0.45
1:A:1945:LEU:HD13	1:A:1994:VAL:HG21	1.98	0.44
1:A:2274:HIS:CE1	1:A:2326:LEU:O	2.54	0.44
1:A:2766:LYS:CE	1:A:2890:THR:HB	2.39	0.44
1:A:3308:ASN:O	1:A:3312:GLN:HB2	2.17	0.44
1:A:1611:LEU:O	1:A:1615:ILE:HG23	2.17	0.44
1:A:1759:LYS:HE3	1:A:1761:GLU:OE2	2.17	0.44
1:A:1822:CYS:HB2	1:A:1853:LEU:CD2	2.31	0.44
1:A:1973:LEU:O	1:A:1977:LEU:HG	2.18	0.44
1:A:2749:LEU:HD12	1:A:2773:VAL:HG12	1.99	0.44
1:A:3319:GLU:HA	1:A:3359:LYS:O	2.17	0.44
1:A:3330:TYR:CD1	1:A:3334:PHE:CD2	3.05	0.44
1:A:2354:SER:H	1:A:2357:SER:HB2	1.83	0.44
1:A:2411:LYS:HG2	1:A:2530:HIS:CE1	2.41	0.44
1:A:3702:MET:HB3	1:A:3767:PHE:HZ	1.83	0.44
1:A:1681:LYS:HE2	1:A:1939:PHE:CZ	2.53	0.44
1:A:3566:LEU:HD23	1:A:3587:LEU:HD11	1.99	0.44
1:A:2027:THR:HA	1:A:2028:PRO:HD3	1.48	0.44
1:A:1995:VAL:HG22	1:A:2022:PHE:HE2	1.80	0.44
1:A:2155:ASP:OD1	1:A:2195:GLU:HG3	2.17	0.44
1:A:2386:MET:HB3	1:A:2627:ARG:NE	2.32	0.44
1:A:2646:ARG:NH1	1:A:2687:GLY:H	2.15	0.44
1:A:3939:ILE:HG13	1:A:4010:LEU:HD23	1.98	0.44
1:A:1620:PHE:CA	1:A:1760:PHE:CE1	3.01	0.44
1:A:1793:CYS:SG	1:A:1918:GLU:HG2	2.57	0.44
1:A:1826:PHE:O	1:A:1826:PHE:CG	2.70	0.44
1:A:1968:PHE:N	1:A:1968:PHE:CD1	2.84	0.44
1:A:2385:VAL:HG23	1:A:2574:TYR:CD1	2.53	0.44
1:A:2783:GLN:HG2	1:A:2816:ILE:HB	1.99	0.44
1:A:3566:LEU:HD13	1:A:3570:LEU:HD11	1.86	0.44
1:A:2422:SER:H	1:A:2424:LYS:HZ1	1.65	0.44
1:A:2760:GLY:O	1:A:2761:ALA:HB3	2.18	0.44
1:A:2861:ARG:HD2	1:A:2866:LEU:HD13	2.00	0.44
1:A:1660:VAL:CG1	1:A:1728:TRP:CH2	3.01	0.44
1:A:2021:ILE:HG22	1:A:2022:PHE:HD1	1.82	0.44
1:A:2575:TYR:HD1	1:A:2578:ILE:HD11	1.83	0.44
1:A:3010:LEU:HD22	1:A:3320:LEU:HD12	1.99	0.44
1:A:3964:ALA:HB2	1:A:3993:VAL:HG11	1.99	0.44
1:A:1559:SER:CB	1:A:1572:ILE:HG22	2.47	0.43
1:A:2197:ASP:HB3	1:A:2549:ARG:HD2	1.99	0.43
1:A:3737:THR:HB	1:A:3740:THR:HG1	1.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1926:SER:HA	1:A:1929:ILE:CD1	2.48	0.43
1:A:2061:TYR:O	1:A:2064:GLN:HG2	2.17	0.43
1:A:2178:LEU:HB2	1:A:2182:GLU:H	1.83	0.43
1:A:3411:SER:O	1:A:3413:HIS:N	2.47	0.43
1:A:3461:ILE:C	1:A:3463:SER:N	2.70	0.43
1:A:3566:LEU:HA	1:A:3583:LEU:HD23	2.00	0.43
1:A:1953:LEU:HD11	1:A:1973:LEU:HB3	1.98	0.43
1:A:2404:PHE:CZ	1:A:2428:MET:HG2	2.53	0.43
1:A:3767:PHE:HB3	1:A:3769:VAL:HG23	2.00	0.43
1:A:4033:LEU:HD13	1:A:4035:GLN:CG	2.49	0.43
1:A:3509:LEU:CG	1:A:3513:VAL:HG21	2.45	0.43
1:A:1646:GLN:OE1	1:A:1763:ILE:HG12	2.18	0.43
1:A:2266:PHE:HD1	1:A:2326:LEU:HD21	1.83	0.43
1:A:2375:ILE:HG22	1:A:2376:PRO:O	2.18	0.43
1:A:3338:ASN:H	1:A:3341:GLU:HB2	1.82	0.43
1:A:4033:LEU:CD1	1:A:4035:GLN:N	2.82	0.43
1:A:4034:LEU:HD23	1:A:4034:LEU:C	2.38	0.43
1:A:1611:LEU:O	1:A:1615:ILE:HG12	2.19	0.43
1:A:3407:LEU:HD23	1:A:3518:PHE:CE2	2.53	0.43
1:A:2578:ILE:CG2	1:A:2630:TYR:HB2	2.49	0.43
1:A:4074:GLU:HA	1:A:4077:GLN:HE21	1.84	0.43
1:A:1741:LEU:O	1:A:1742:ASP:HB2	2.19	0.43
1:A:2738:MET:HG2	1:A:2769:LEU:HD21	2.00	0.43
1:A:2280:THR:HA	1:A:2283:LYS:HD2	1.99	0.43
1:A:2982:VAL:CG1	1:A:2983:GLY:N	2.82	0.43
1:A:3307:LEU:O	1:A:3311:LYS:N	2.27	0.43
1:A:3979:ASN:O	1:A:3981:PRO:CD	2.64	0.43
1:A:1998:LEU:CD1	1:A:2022:PHE:HZ	2.32	0.42
1:A:2072:LEU:HD11	1:A:2193:LEU:HD23	2.01	0.42
1:A:1830:VAL:O	1:A:1834:LEU:HG	2.19	0.42
1:A:2707:VAL:HG11	1:A:2712:LEU:HD12	2.00	0.42
1:A:1568:SER:HB2	1:A:1816:VAL:HG21	2.01	0.42
1:A:1991:GLU:O	1:A:1994:VAL:HB	2.19	0.42
1:A:2229:LEU:HD11	1:A:2285:GLU:HG3	2.02	0.42
1:A:2447:LYS:HE3	1:A:2493:LYS:HD3	2.00	0.42
1:A:2493:LYS:HG3	1:A:2494:LEU:N	2.33	0.42
1:A:2510:MET:O	1:A:2513:GLN:NE2	2.52	0.42
1:A:2512:LYS:O	1:A:2513:GLN:CB	2.66	0.42
1:A:3461:ILE:C	1:A:3463:SER:H	2.22	0.42
1:A:1650:LEU:O	1:A:1654:VAL:HG23	2.19	0.42
1:A:2141:ILE:CG2	1:A:2145:PHE:HB2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2503:VAL:HA	1:A:2506:LEU:HD12	2.01	0.42
1:A:2563:SER:C	1:A:2565:LYS:H	2.23	0.42
1:A:2609:THR:HA	1:A:2612:GLN:O	2.20	0.42
1:A:3024:LEU:HD13	1:A:3303:LYS:HG3	1.92	0.42
1:A:3544:LYS:O	1:A:3548:LEU:HB2	2.19	0.42
1:A:3728:GLU:CG	1:A:4079:LYS:HE2	2.49	0.42
1:A:1992:LYS:HG2	1:A:2024:SER:HB2	1.92	0.42
1:A:2109:LEU:CD1	1:A:2129:LEU:HD23	2.49	0.42
1:A:2225:LYS:HD2	1:A:2281:PHE:CZ	2.55	0.42
1:A:2640:THR:O	1:A:2643:SER:HB3	2.20	0.42
1:A:3414:MET:O	1:A:3418:ILE:HG12	2.19	0.42
1:A:3785:TYR:CE2	1:A:3859:VAL:HG13	2.54	0.42
1:A:2786:ILE:HD12	1:A:3460:PRO:CG	2.50	0.42
1:A:3628:ILE:HG13	1:A:3705:LEU:HD23	2.00	0.42
1:A:3696:MET:SD	1:A:3760:LEU:HD23	2.59	0.42
1:A:4033:LEU:HD12	1:A:4033:LEU:C	2.39	0.42
1:A:1727:LEU:O	1:A:1731:VAL:HG23	2.20	0.42
1:A:1898:LEU:HD11	1:A:1908:LEU:CD2	2.50	0.42
1:A:3784:ASN:ND2	1:A:3865:ALA:O	2.52	0.42
1:A:3810:SER:HB3	1:A:3837:GLY:HA2	2.01	0.42
1:A:1702:LEU:HA	1:A:1702:LEU:HD23	1.86	0.42
1:A:1939:PHE:CD1	1:A:1939:PHE:N	2.87	0.42
1:A:2012:LEU:HD12	1:A:2013:VAL:N	2.35	0.42
1:A:4045:LEU:O	1:A:4048:ILE:HG22	2.19	0.42
1:A:1672:TYR:O	1:A:1676:VAL:HG23	2.19	0.42
1:A:1781:THR:HG21	1:A:1919:PHE:CE1	2.55	0.42
1:A:2568:SER:HA	1:A:2597:VAL:HG21	2.02	0.42
1:A:3505:ILE:O	1:A:3510:ARG:NH1	2.53	0.42
1:A:2492:PRO:CB	1:A:2502:VAL:HG11	2.49	0.41
1:A:2829:GLU:HA	1:A:2832:ASN:HD22	1.84	0.41
1:A:3464:ARG:O	1:A:3467:SER:O	2.38	0.41
1:A:3579:GLU:O	1:A:3582:GLU:N	2.43	0.41
1:A:1706:LEU:HD21	1:A:1935:GLN:CG	2.48	0.41
1:A:1992:LYS:CG	1:A:2024:SER:CB	2.78	0.41
1:A:2095:ASP:OD1	1:A:2149:ARG:NH2	2.53	0.41
1:A:2178:LEU:HB3	1:A:2179:PRO:HD2	2.01	0.41
1:A:2758:LEU:HD22	1:A:2917:MET:SD	2.60	0.41
1:A:3785:TYR:CD1	1:A:3785:TYR:N	2.87	0.41
1:A:1742:ASP:HB3	1:A:1745:ASN:HD22	1.86	0.41
1:A:1929:ILE:H	1:A:1929:ILE:HD12	1.86	0.41
1:A:1965:HIS:HD2	1:A:2212:LEU:HD23	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2111:LYS:CD	1:A:2161:GLU:CG	2.84	0.41
1:A:1575:LEU:O	1:A:1576:GLU:HB3	2.20	0.41
1:A:1966:TYR:CZ	1:A:2006:LEU:HD23	2.55	0.41
1:A:2001:VAL:O	1:A:2004:PRO:HD2	2.20	0.41
1:A:2053:PHE:HB2	1:A:2219:VAL:HB	2.02	0.41
1:A:2708:ASN:O	1:A:2712:LEU:HD13	2.20	0.41
1:A:2755:HIS:HB3	1:A:2912:CYS:SG	2.60	0.41
1:A:3365:ARG:HD2	1:A:3368:ASP:OD2	2.19	0.41
1:A:4033:LEU:HD12	1:A:4035:GLN:H	1.84	0.41
1:A:2420:PRO:HD3	1:A:2536:ASN:HD21	1.85	0.41
1:A:2760:GLY:HA3	1:A:2766:LYS:HD3	2.01	0.41
1:A:2819:GLU:HB3	1:A:2891:ILE:HG22	2.03	0.41
1:A:2860:THR:HG21	1:A:2867:LEU:HD12	2.02	0.41
1:A:3671:VAL:HA	1:A:3674:ILE:HG22	2.03	0.41
1:A:3848:LEU:O	1:A:3849:SER:C	2.59	0.41
1:A:2306:ASP:HB2	1:A:2309:SER:HB3	2.02	0.41
1:A:2762:SER:O	1:A:2763:ARG:CB	2.68	0.41
1:A:3832:SER:O	1:A:3836:GLY:N	2.45	0.41
1:A:3846:MET:HG3	1:A:3847:SER:N	2.35	0.41
1:A:4033:LEU:CD1	1:A:4035:GLN:H	2.34	0.41
1:A:2225:LYS:HG2	1:A:2229:LEU:HD12	2.02	0.41
1:A:2786:ILE:HD12	1:A:3460:PRO:HG2	2.03	0.41
1:A:2891:ILE:HD11	1:A:2903:ILE:HD11	2.03	0.41
1:A:2044:ARG:HH21	1:A:2093:ILE:HD11	1.85	0.41
1:A:2099:ASN:HD22	1:A:2151:TRP:HE1	1.68	0.41
1:A:2852:LEU:HG	1:A:2856:LEU:HD13	2.03	0.41
1:A:3544:LYS:HE3	1:A:3607:PHE:CD1	2.55	0.41
1:A:3570:LEU:HD23	1:A:3580:ASN:CG	2.41	0.41
1:A:3590:LEU:HD12	1:A:3593:GLU:HB2	2.02	0.41
1:A:1823:ASP:HB3	1:A:1852:ARG:O	2.16	0.41
1:A:2034:ILE:HD12	1:A:2061:TYR:CE2	2.55	0.41
1:A:2039:LYS:HG2	1:A:2049:MET:HG3	2.03	0.41
1:A:2138:ASN:ND2	1:A:2185:PRO:O	2.52	0.41
1:A:2141:ILE:HG22	1:A:2145:PHE:CB	2.51	0.41
1:A:3534:LEU:HD12	1:A:3618:TYR:CZ	2.52	0.41
1:A:4020:ASN:ND2	1:A:4028:ARG:HD3	2.35	0.41
1:A:2905:SER:HA	1:A:2906:PRO:HD2	1.85	0.41
1:A:3772:TRP:HZ3	1:A:3780:ASN:HD22	1.68	0.41
1:A:3809:GLU:HB3	1:A:3810:SER:H	1.54	0.41
1:A:2517:LYS:NZ	1:A:2520:GLU:OE1	2.48	0.40
1:A:2985:ASN:N	1:A:2986:PRO:CD	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3330:TYR:CZ	1:A:3346:LEU:HD13	2.55	0.40
1:A:3612:ASP:C	1:A:3615:VAL:HG22	2.41	0.40
1:A:1822:CYS:SG	1:A:1850:PHE:CA	3.04	0.40
1:A:2489:ILE:HD11	1:A:2506:LEU:HD13	2.02	0.40
1:A:2661:VAL:HG12	1:A:2916:TRP:CE2	2.57	0.40
1:A:2977:TYR:HD1	1:A:2981:LYS:HG3	1.86	0.40
1:A:3708:PHE:CZ	1:A:3720:LEU:HD21	2.57	0.40
1:A:1715:LEU:HG	1:A:1727:LEU:HD22	2.02	0.40
1:A:2034:ILE:HG13	1:A:2061:TYR:CE2	2.57	0.40
1:A:2088:ILE:HG12	1:A:2151:TRP:CZ2	2.55	0.40
1:A:2488:GLU:CG	1:A:2491:LEU:HD12	2.51	0.40
1:A:1965:HIS:HD2	1:A:2212:LEU:HD21	1.85	0.40
1:A:2109:LEU:HB3	1:A:2113:SER:HB2	2.03	0.40
1:A:2332:GLY:HA2	1:A:2335:GLN:CG	2.51	0.40
1:A:2336:ARG:HG2	1:A:2355:ASP:CG	2.41	0.40
1:A:3682:VAL:HG13	1:A:3686:PHE:HD2	1.87	0.40
1:A:3737:THR:CB	1:A:3740:THR:OG1	2.56	0.40
1:A:3886:ALA:N	1:A:3887:PRO:CD	2.84	0.40
1:A:3978:ASN:O	1:A:3981:PRO:HD3	2.20	0.40
1:A:1744:LEU:HD22	1:A:1760:PHE:CD2	2.56	0.40
1:A:1968:PHE:HD1	1:A:1968:PHE:N	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	2237/2286 (98%)	2137 (96%)	93 (4%)	7 (0%)	41 77

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2990	GLY
1	A	3306	TRP
1	A	3482	GLY
1	A	2519	PRO
1	A	3980	ILE
1	A	2562	PRO
1	A	2028	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	2039/2078 (98%)	1968 (96%)	71 (4%)	36 59

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1794	PHE
1	A	1826	PHE
1	A	1852	ARG
1	A	1923	SER
1	A	1944	SER
1	A	1971	ARG
1	A	1992	LYS
1	A	1999	LYS
1	A	2012	LEU
1	A	2057	CYS
1	A	2078	CYS
1	A	2109	LEU
1	A	2202	THR
1	A	2218	ASP
1	A	2295	ILE
1	A	2346	PHE
1	A	2357	SER
1	A	2386	MET
1	A	2424	LYS
1	A	2428	MET

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Mol	Chain	Res	Type
1	A	2461	HIS
1	A	2472	THR
1	A	2476	LYS
1	A	2526	ILE
1	A	2544	ILE
1	A	2563	SER
1	A	2566	SER
1	A	2611	LEU
1	A	2638	ARG
1	A	2694	LEU
1	A	2822	ILE
1	A	2833	THR
1	A	2843	LEU
1	A	2853	LEU
1	A	2856	LEU
1	A	2865	LEU
1	A	2873	LEU
1	A	2875	ASP
1	A	2911	ARG
1	A	2920	TRP
1	A	3301	PHE
1	A	3329	ILE
1	A	3332	THR
1	A	3355	LYS
1	A	3372	THR
1	A	3400	SER
1	A	3418	ILE
1	A	3531	ASP
1	A	3538	ASN
1	A	3548	LEU
1	A	3565	ARG
1	A	3601	LEU
1	A	3618	TYR
1	A	3677	LEU
1	A	3717	GLU
1	A	3729	SER
1	A	3735	LYS
1	A	3737	THR
1	A	3744	LEU
1	A	3811	LEU
1	A	3871	PHE
1	A	3884	LEU

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Mol	Chain	Res	Type
1	A	3906	THR
1	A	3917	THR
1	A	3943	THR
1	A	3950	PHE
1	A	3960	ASP
1	A	3982	TRP
1	A	4004	LEU
1	A	4016	CYS
1	A	4040	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1622	GLN
1	A	1646	GLN
1	A	1736	GLN
1	A	1745	ASN
1	A	1851	ASN
1	A	1873	GLN
1	A	1899	ASN
1	A	1951	HIS
1	A	1965	HIS
1	A	1979	ASN
1	A	2068	GLN
1	A	2099	ASN
1	A	2274	HIS
1	A	2282	ASN
1	A	2293	HIS
1	A	2383	HIS
1	A	2409	ASN
1	A	2459	HIS
1	A	2530	HIS
1	A	2536	ASN
1	A	2634	ASN
1	A	2683	ASN
1	A	2688	ASN
1	A	3323	ASN
1	A	3338	ASN
1	A	3420	ASN
1	A	3497	HIS
1	A	3521	ASN
1	A	3542	GLN

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Mol	Chain	Res	Type
1	A	3588	ASN
1	A	3624	HIS
1	A	3780	ASN
1	A	3890	GLN
1	A	4020	ASN
1	A	4077	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 Tomogram visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5758. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

6.1 Orthogonal projections [i](#)



X



Y



Z

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

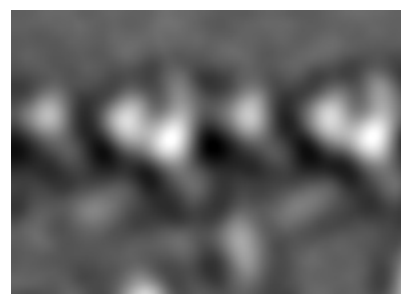
6.2 Central slices [i](#)



X Index: 25



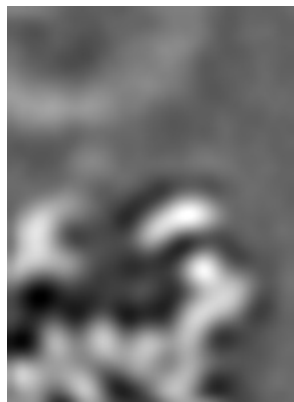
Y Index: 18



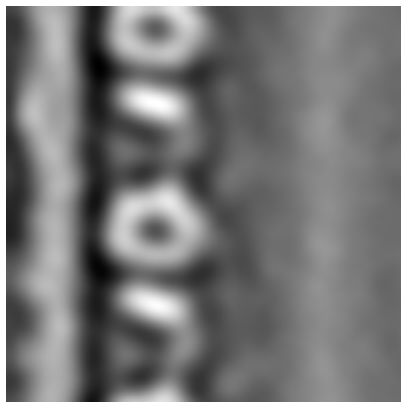
Z Index: 25

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

6.3 Largest variance slices [i](#)



X Index: 29



Y Index: 15



Z Index: 11

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

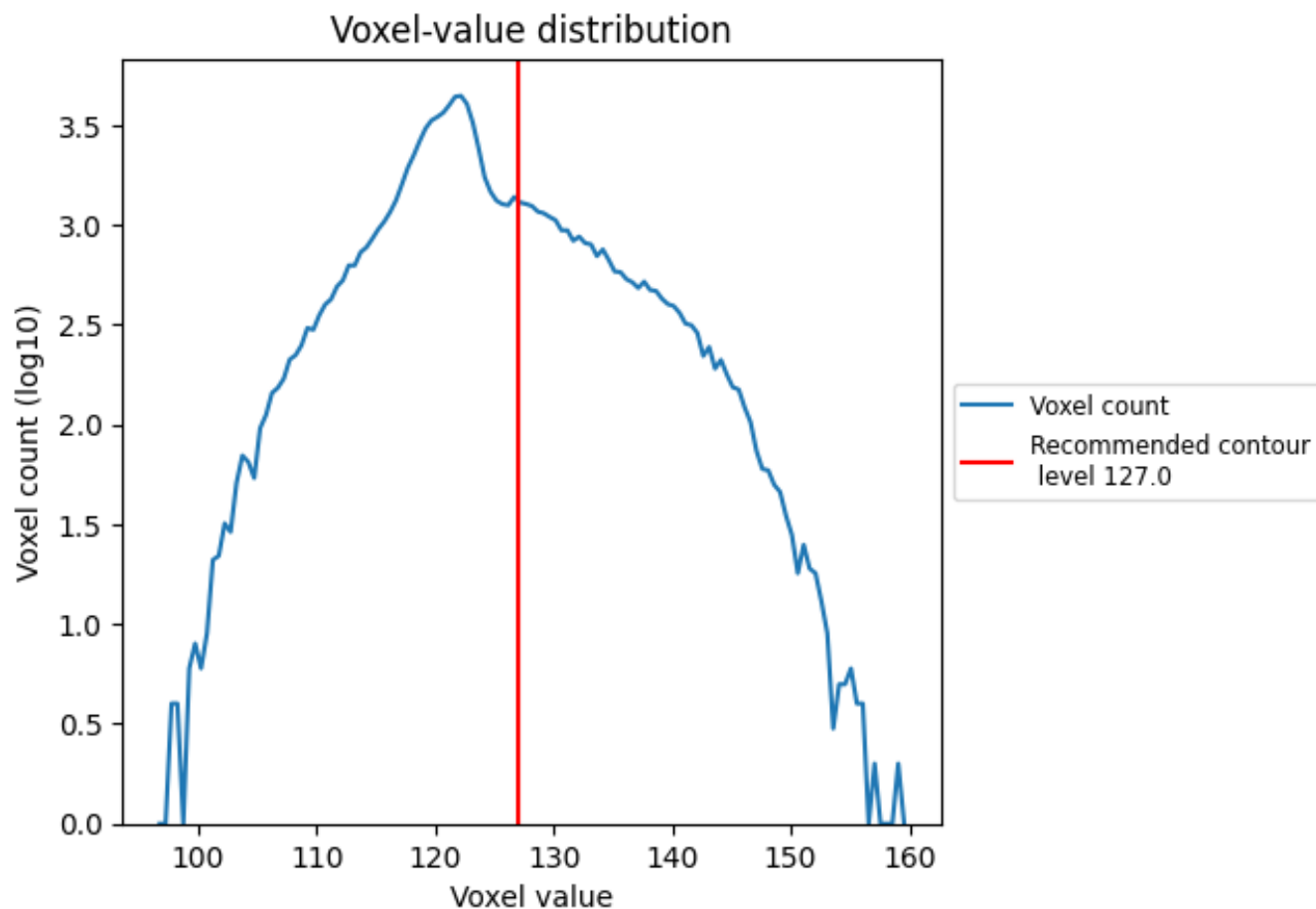
6.4 Mask visualisation [i](#)

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

7 Tomogram analysis [i](#)

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

7.1 Voxel-value distribution [i](#)



The voxel-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic.

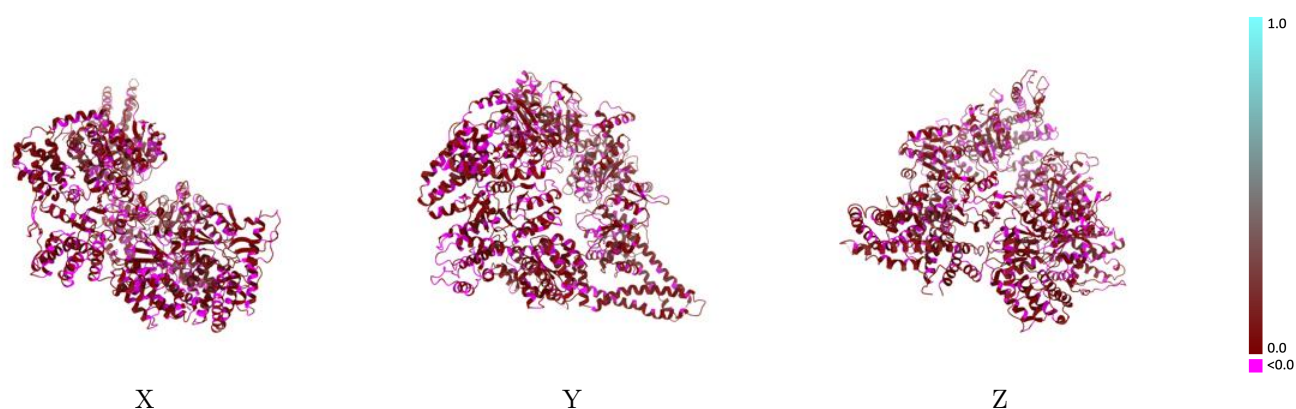
8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-5758 and PDB model 3J68. Per-residue inclusion information can be found in section 3 on page 4.

8.1 Map-model overlay [i](#)

This section was not generated.

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

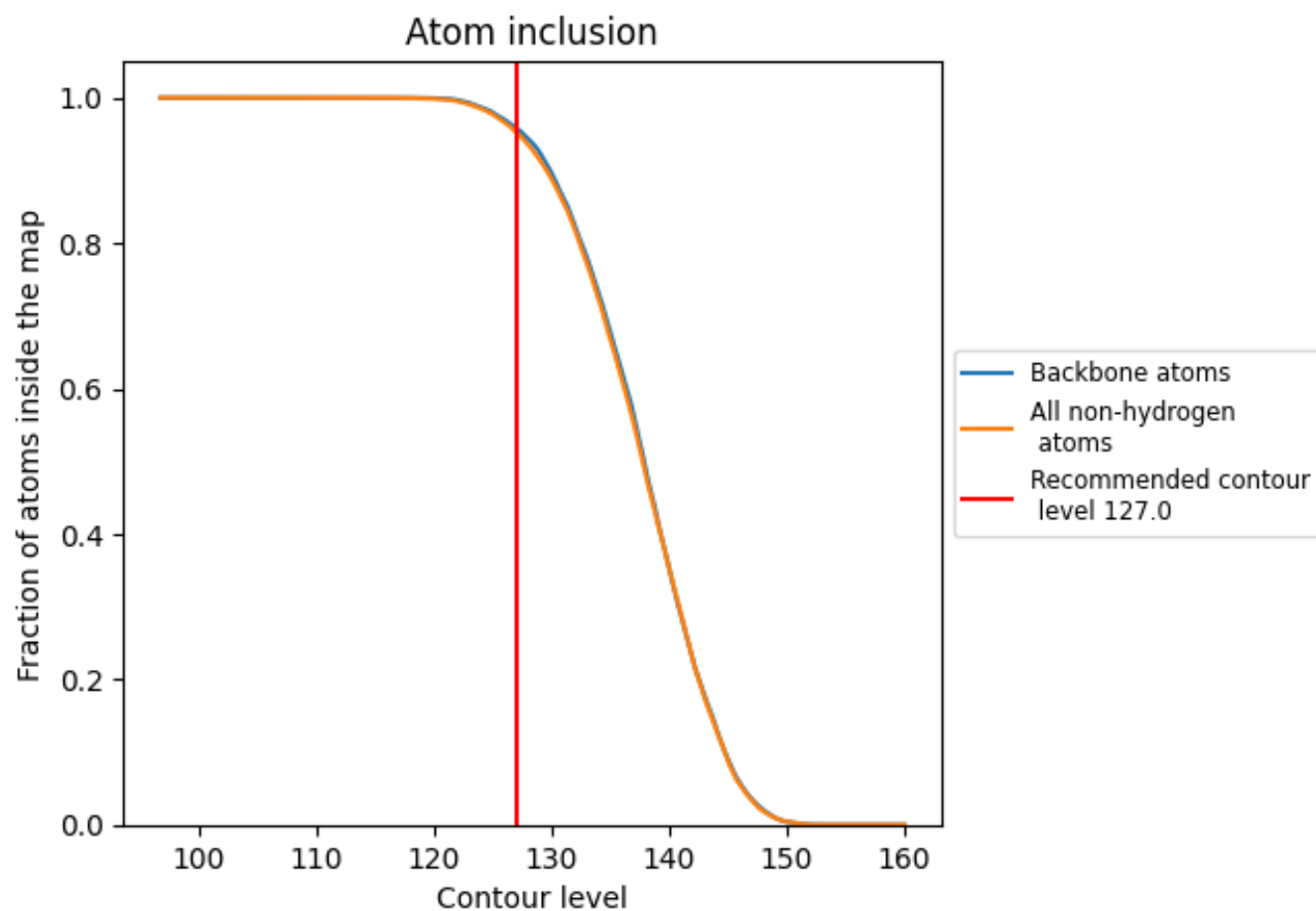


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

8.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (127.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9533	<div></div> 0.0400
A	<div></div> 0.9533	<div></div> 0.0400

