



## Full wwPDB EM Validation Report ⓘ

May 18, 2025 – 02:22 AM EDT

PDB ID : 9BMU / pdb\_00009bmu  
EMDB ID : EMD-44711  
Title : State-6 of motor domain from full-length human dynein-1 in 5 mM ADP  
Authors : Chai, P.; Zhang, K.  
Deposited on : 2024-05-02  
Resolution : 3.70 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev118  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

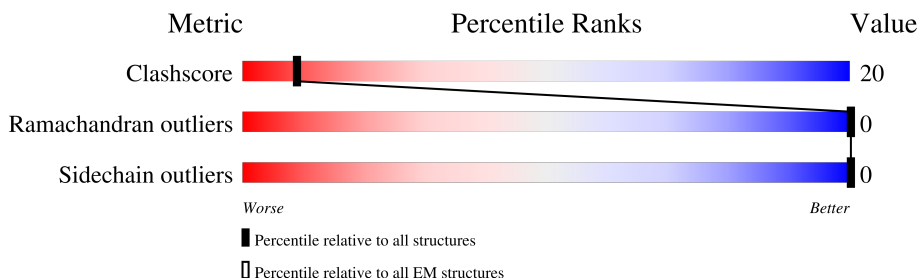
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	4646	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 21776 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 Cytoplasmic dynein 1 heavy chain 1.

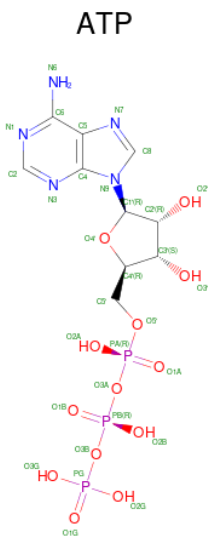
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2698	21664	13799	3740	4014	111	0	0

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	27	10	5	10	2	0
2	A	1	27	10	5	10	2	0
2	A	1	27	10	5	10	2	0

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



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











F4635	Y4636	E4637	R4638	V4642	T4645	GLU	E4414	P4324	A4241
S4595	S4596	S4597	S4598	S4599	S4600	S4601	K4418	N4326	A4242
S4602	S4603	S4604	S4605	S4606	S4607	S4608	L4423	A4327	L4243
S4609	S4610	S4611	S4612	S4613	S4614	S4615	R4428	E4328	K4244
S4616	S4617	S4618	S4619	S4620	S4621	S4622	Q4526	M4339	Q4249
S4623	S4624	S4625	S4626	S4627	S4628	S4629	M4532	M4343	S4250
S4630	S4631	S4632	S4633	S4634	S4635	S4636	S4533	L4344	I4251
S4637	S4638	S4639	S4640	S4641	S4642	S4643	W4534	K4345	Y4252
S4644	S4645	S4646	S4647	S4648	S4649	S4650	V4434	M4346	F4260
S4651	S4652	S4653	S4654	S4655	S4656	S4657	K4441	Q4347	D4261
S4658	S4659	S4660	S4661	S4662	S4663	S4664	K4442	MET	Q4262
S4665	S4666	S4667	S4668	S4669	S4670	S4671	K4443	LEU	R4263
S4672	S4673	S4674	S4675	S4676	S4677	S4678	Q4444	GLU	L4264
S4679	S4680	S4681	S4682	S4683	S4684	S4685	T4445	ASP	R4271
S4686	S4687	S4688	S4689	S4690	S4691	S4692	M4446	GLU	L4272
S4693	S4694	S4695	S4696	S4697	S4698	S4699	Y4447	ASP	T4275
S4700	S4701	S4702	S4703	S4704	S4705	S4706	L4448	ASP	R4276
S4707	S4708	S4709	S4710	S4711	S4712	S4713	R4449	ALA	T4277
S4714	S4715	S4716	S4717	S4718	S4719	S4720	I4452	TYR	F4278
S4721	S4722	S4723	S4724	S4725	S4726	S4727	M4453	ALA	F4282
S4728	S4729	S4730	S4731	S4732	S4733	S4734	E4454	GLU	K4287
S4735	S4736	S4737	S4738	S4739	S4740	S4741	L4455	THR	V4288
S4742	S4743	S4744	S4745	S4746	S4747	S4748	V4456	GLU	D4289
S4749	S4750	S4751	S4752	S4753	S4754	S4755	I4459	LYS	Q4290
S4756	S4757	S4758	S4759	S4760	S4761	S4762	L4460	THR	H4291
S4763	S4764	S4765	S4766	S4767	S4768	S4769	P4461	THR	K4292
S4770	S4771	S4772	S4773	S4774	S4775	S4776	W4464	ASP	D4293
S4777	S4778	S4779	S4780	S4781	S4782	S4783	S4465	SER	M4296
S4784	S4785	S4786	S4787	S4788	S4789	S4790	H4466	SER	P4297
S4791	S4792	S4793	S4794	S4795	S4796	S4797	G4472	GLY	I4300
S4798	S4799	S4800	S4801	S4802	S4803	S4804	M4473	ARG	R4301
S4805	S4806	S4807	S4808	S4809	S4810	S4811	T4474	P4374	R4302
S4812	S4813	S4814	S4815	S4816	S4817	S4818	V4475	A4375	E4303
S4819	S4820	S4821	S4822	S4823	S4824	S4825	I4476	W4376	E4304
S4826	S4827	S4828	S4829	S4830	S4831	S4832	Q4477	T4379	F4305
S4833	S4834	S4835	S4836	S4837	S4838	S4839	W4478	T4391	V4306
S4840	S4841	S4842	S4843	S4844	S4845	S4846	V4479	P4392	Q4307
S4847	S4848	S4849	S4850	S4851	S4852	S4853	F4482	Q4393	W4308
S4854	S4855	S4856	S4857	S4858	S4859	S4860	S4484	E4398	V4309
S4861	S4862	S4863	S4864	S4865	S4866	S4867	R4485	L4398	E4310
S4868	S4869	S4870	S4871	S4872	S4873	S4874	I4486	K4399	L4311
S4875	S4876	S4877	S4878	S4879	S4880	S4881	K4487	R4400	L4312
S4882	S4883	S4884	S4885	S4886	S4887	S4888	Q4488	T4401	P4313
S4889	S4890	S4891	S4892	S4893	S4894	S4895	L4489	V4402	D4314
S4896	S4897	S4898	S4899	S4900	S4901	S4902	I4492	I4405	T4315
S4903	S4904	S4905	S4906	S4907	S4908	S4909	L4504	S4319	P4318
S4910	S4911	S4912	S4913	S4914	S4915	S4916	K4505	W4320	S4319
S4917	S4918	S4919	S4920	S4921	S4922	S4923	R4633	L4321	W4320
S4924	S4925	S4926	S4927	S4928	S4929	S4930	S4634	F4413	L4321
S4931	S4932	S4933	S4934	S4935	S4936	S4937			

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	93339	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN 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	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.603	Depositor
Minimum map value	-0.336	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	329.984, 329.984, 329.984	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0312, 1.0312, 1.0312	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.20	0/22127	0.40	0/29993

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2229	GLY	Peptide

### 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	21664	0	21700	885	0
2	A	81	0	36	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	31	0	12	5	0
All	All	21776	0	21748	886	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 20.

All (886) 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:3126:MET:HE3	1:A:3127:PRO:HD2	1.50	0.93
1:A:2603:MET:HE1	2:A:4703:ADP:C4	2.04	0.93
1:A:2688:GLU:HB2	1:A:2730:HIS:HE1	1.33	0.90
1:A:2619:GLY:HA2	1:A:2662:PHE:HB3	1.58	0.84
1:A:2473:ASN:HB2	1:A:2481:MET:HE1	1.60	0.83
1:A:2794:TYR:HE1	1:A:2836:ARG:HH21	1.30	0.80
1:A:2609:LEU:HD23	1:A:2660:VAL:HG21	1.65	0.78
1:A:4058:LEU:HA	1:A:4061:GLU:HG2	1.65	0.78
1:A:2995:ASP:OD1	1:A:3067:THR:OG1	2.02	0.78
1:A:2304:ASP:HA	1:A:2344:GLU:HB3	1.66	0.78
1:A:3154:LEU:HG	1:A:3516:TYR:HD2	1.49	0.78
1:A:3990:LEU:HD21	1:A:4008:PHE:HB2	1.65	0.77
1:A:1743:ASP:OD2	1:A:1804:ARG:NH2	2.17	0.77
1:A:2437:LEU:HD21	1:A:2451:ARG:HG3	1.67	0.77
1:A:2029:PRO:HG2	1:A:2032:LEU:HD12	1.66	0.76
1:A:3876:LEU:HD23	1:A:3878:GLN:H	1.51	0.75
1:A:2657:LYS:H	1:A:2705:ARG:HD2	1.51	0.75
1:A:2230:LYS:HE2	1:A:2344:GLU:HG3	1.68	0.75
1:A:2749:GLY:HA2	1:A:2770:THR:HG21	1.69	0.75
1:A:1888:CYS:HB2	1:A:2041:MET:HE1	1.69	0.74
1:A:2018:MET:HE2	1:A:2027:ASN:HA	1.70	0.74
1:A:3485:GLU:OE2	1:A:3489:TRP:NE1	2.16	0.74
1:A:2181:GLU:HG3	1:A:2244:LEU:HB2	1.68	0.74
1:A:4376:TRP:HA	1:A:4379:THR:HG22	1.69	0.74
1:A:3830:GLN:NE2	1:A:3834:ASP:OD2	2.21	0.74
1:A:2511:ARG:HH21	1:A:2735:TYR:HB3	1.53	0.73
1:A:1769:MET:HE3	1:A:1777:PRO:HD2	1.71	0.72
1:A:2584:TRP:CH2	1:A:2732:PRO:HB2	2.23	0.72
1:A:4106:LEU:HD23	1:A:4135:PRO:HD2	1.71	0.72
1:A:1816:VAL:HG13	1:A:1819:ARG:HH22	1.54	0.72
1:A:1631:PHE:HA	1:A:1944:ILE:HG22	1.70	0.72
1:A:2936:ILE:HG22	1:A:3068:MET:HB2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2895:ALA:HA	1:A:2898:LYS:HE2	1.72	0.72
1:A:4271:ARG:HD3	1:A:4633:ARG:HD2	1.70	0.72
1:A:3907:HIS:HD2	1:A:3991:LEU:HD11	1.54	0.72
1:A:4574:LYS:NZ	1:A:4625:GLU:OE2	2.22	0.72
1:A:1951:VAL:HG13	1:A:1953:ALA:H	1.54	0.71
1:A:2273:ARG:NH2	1:A:2329:ASN:O	2.24	0.71
1:A:3154:LEU:HG	1:A:3516:TYR:CD2	2.25	0.71
1:A:2221:MET:HG2	1:A:2343:PHE:HB2	1.72	0.71
1:A:2603:MET:HE1	2:A:4703:ADP:C5	2.25	0.70
1:A:3046:SER:OG	1:A:3049:GLU:OE1	2.09	0.70
1:A:2755:MET:HE1	1:A:2807:PHE:HA	1.72	0.70
1:A:3190:LYS:HB3	1:A:3503:ILE:HD11	1.72	0.70
1:A:3710:SER:O	1:A:3714:ASN:ND2	2.24	0.70
1:A:4400:ARG:HH21	1:A:4405:ILE:HG12	1.56	0.70
1:A:2680:ILE:HG12	1:A:2723:LEU:HD12	1.73	0.69
1:A:2831:ARG:HB3	1:A:2924:ARG:HH22	1.55	0.69
1:A:4154:LYS:HE3	1:A:4310:GLU:HA	1.73	0.69
1:A:3907:HIS:HE1	1:A:3937:ARG:HG3	1.57	0.69
1:A:1912:LYS:NZ	2:A:4701:ADP:O2B	2.26	0.69
1:A:2485:GLN:OE1	1:A:2488:ARG:NH1	2.26	0.69
1:A:2836:ARG:HG2	1:A:3091:LEU:HB3	1.73	0.69
1:A:4505:LYS:NZ	1:A:4554:ASP:O	2.25	0.68
1:A:3490:GLU:O	1:A:3493:SER:OG	2.09	0.68
1:A:1917:LYS:HG2	1:A:1927:VAL:HG21	1.74	0.68
1:A:3154:LEU:HB3	1:A:3171:ILE:HD13	1.75	0.68
1:A:2287:ILE:HA	1:A:2294:GLU:HG3	1.76	0.68
1:A:2220:LEU:HB2	1:A:2342:MET:HG3	1.76	0.68
1:A:3106:GLY:O	1:A:3110:THR:OG1	2.09	0.67
1:A:4393:GLN:OE1	1:A:4428:ARG:NH2	2.25	0.67
1:A:2213:ILE:HD11	1:A:2360:GLY:HA3	1.75	0.67
1:A:2054:LEU:HG	1:A:2097:LEU:HD22	1.76	0.67
1:A:2337:PRO:O	1:A:2340:ARG:NH1	2.27	0.67
1:A:4036:LYS:HG3	1:A:4038:ASN:H	1.60	0.67
1:A:2612:LEU:HB3	1:A:2615:MET:HE2	1.76	0.67
1:A:3971:PRO:HG2	1:A:3973:LEU:HD11	1.77	0.67
1:A:4301:ARG:NH1	1:A:4303:GLU:OE2	2.26	0.67
1:A:4525:ARG:HG2	1:A:4536:LEU:HD22	1.75	0.67
1:A:2457:SER:HB2	1:A:2732:PRO:HB3	1.77	0.67
1:A:1949:CYS:HA	1:A:2012:MET:HE3	1.74	0.67
1:A:2067:ASN:HB3	1:A:4537:GLU:HG2	1.77	0.67
1:A:4221:THR:HG23	1:A:4222:TRP:HD1	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2275:TRP:HE1	1:A:2285:ARG:NH2	1.93	0.67
1:A:3734:LEU:HD13	1:A:3783:LYS:HB3	1.77	0.67
1:A:1750:VAL:HG23	1:A:1811:LEU:HD21	1.76	0.66
1:A:2231:SER:OG	1:A:2344:GLU:OE2	2.12	0.66
1:A:3736:GLY:O	1:A:3740:LEU:N	2.27	0.66
1:A:2961:ILE:HD11	1:A:2998:ASN:HB3	1.76	0.66
1:A:2605:LEU:HD13	1:A:2662:PHE:HE2	1.60	0.66
1:A:2853:VAL:HA	1:A:2856:LYS:HG2	1.78	0.66
1:A:3727:LYS:O	1:A:3731:LEU:N	2.28	0.66
1:A:2245:GLU:OE1	1:A:2298:ARG:NH2	2.27	0.66
1:A:4248:ALA:O	1:A:4262:GLN:NE2	2.29	0.65
1:A:1961:ASN:ND2	1:A:2019:ASN:O	2.29	0.65
1:A:4194:LEU:HD21	1:A:4207:PHE:HD2	1.61	0.65
1:A:3950:LYS:NZ	1:A:3973:LEU:HG	2.12	0.65
1:A:2571:THR:H	1:A:2574:THR:HG22	1.61	0.65
1:A:2652:PRO:O	1:A:2705:ARG:NH2	2.29	0.65
1:A:4196:TYR:OH	1:A:4328:GLU:OE2	2.12	0.65
1:A:3892:LEU:HD12	1:A:3898:GLU:HG3	1.78	0.64
1:A:2747:ILE:HD11	2:A:4703:ADP:C6	2.33	0.64
1:A:4264:LEU:HD11	1:A:4637:GLU:HA	1.79	0.64
1:A:2536:ASP:OD1	1:A:2576:ARG:NH1	2.31	0.64
1:A:3057:GLN:HE22	1:A:3060:ARG:HH21	1.43	0.64
1:A:3567:LEU:HD12	1:A:3568:PRO:HD2	1.79	0.64
1:A:2660:VAL:HG12	1:A:2707:GLN:HG3	1.80	0.64
1:A:2269:ASP:HB2	1:A:2274:GLU:HG3	1.78	0.64
1:A:3553:LEU:O	1:A:3582:ARG:NH2	2.30	0.64
1:A:3989:ARG:HG3	1:A:4004:MET:HE2	1.81	0.63
1:A:1882:THR:HG23	1:A:2045:ASP:HB2	1.80	0.63
1:A:3885:MET:SD	1:A:4343:MET:HE1	2.39	0.63
1:A:3715:GLU:OE2	1:A:3718:LYS:NZ	2.31	0.63
1:A:4474:THR:H	1:A:4477:GLN:NE2	1.95	0.63
1:A:3981:THR:HG23	1:A:3984:GLY:H	1.64	0.63
1:A:2086:TYR:OH	1:A:2153:ASP:OD2	2.11	0.62
1:A:2527:PRO:HD2	1:A:2534:ILE:HD12	1.81	0.62
1:A:2831:ARG:HG3	1:A:2924:ARG:HH12	1.64	0.62
1:A:3654:ARG:HB2	1:A:3661:LEU:HB2	1.82	0.62
1:A:4043:MET:HE1	1:A:4125:PHE:HB3	1.81	0.62
1:A:1985:HIS:HA	1:A:1997:ILE:HG12	1.81	0.62
1:A:3974:TRP:HZ2	1:A:3985:GLN:HG2	1.64	0.62
1:A:4448:LEU:O	1:A:4452:ILE:HG12	1.99	0.62
1:A:1889:TYR:HD1	1:A:1919:LEU:HD13	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2073:PHE:HE2	1:A:2093:LEU:HA	1.65	0.62
1:A:3973:LEU:HB2	1:A:3992:LEU:HD11	1.80	0.62
1:A:4532:ASN:HB3	1:A:4534:TRP:CZ3	2.35	0.62
1:A:4034:GLU:O	1:A:4143:ARG:NH1	2.31	0.61
1:A:2284:LEU:HD22	1:A:2325:LEU:HD13	1.81	0.61
1:A:2605:LEU:HD11	1:A:2709:VAL:HG11	1.81	0.61
1:A:2934:LEU:HB3	1:A:3091:LEU:HA	1.80	0.61
1:A:3100:GLU:HA	1:A:3130:TYR:HE1	1.65	0.61
1:A:3194:LEU:HD11	1:A:3499:GLN:OE1	2.00	0.61
1:A:1908:ALA:HA	1:A:1912:LYS:HZ1	1.65	0.61
1:A:3588:LEU:HD11	1:A:3638:VAL:HG11	1.83	0.61
1:A:4312:LEU:HD12	1:A:4313:PRO:HD2	1.81	0.61
1:A:1708:GLU:O	1:A:1712:THR:HG23	2.00	0.61
1:A:1882:THR:HA	1:A:2048:LEU:HD23	1.83	0.61
1:A:2464:GLN:NE2	1:A:2468:ASN:OD1	2.34	0.61
1:A:2822:ILE:HD11	1:A:2858:PHE:CE2	2.36	0.61
1:A:3893:LYS:HZ3	1:A:3900:THR:HA	1.65	0.61
1:A:1836:PHE:HA	1:A:1839:LEU:HB2	1.83	0.61
1:A:2729:ARG:HG3	1:A:2730:HIS:HD2	1.66	0.61
1:A:1938:PHE:HB2	1:A:1967:MET:HE1	1.83	0.60
1:A:4176:ARG:NH1	1:A:4220:ASP:OD1	2.33	0.60
1:A:2134:GLN:HG2	1:A:2168:VAL:HG21	1.83	0.60
1:A:4190:ILE:HG23	1:A:4201:TRP:HZ2	1.66	0.60
1:A:1654:PHE:HE1	1:A:1702:LEU:HD11	1.66	0.60
1:A:1882:THR:HG22	1:A:1884:LEU:H	1.66	0.60
1:A:2223:VAL:HG21	1:A:2348:LEU:HD11	1.84	0.60
1:A:4192:GLU:OE1	1:A:4195:ARG:NH1	2.35	0.60
1:A:3044:LEU:HD22	1:A:3049:GLU:HG3	1.84	0.60
1:A:3067:THR:O	1:A:3068:MET:HE2	2.02	0.60
1:A:1796:VAL:HG22	1:A:1808:LEU:HB3	1.84	0.60
1:A:2037:ARG:HH22	1:A:4250:SER:HG	1.48	0.60
1:A:2461:MET:HG2	1:A:2583:THR:HG21	1.84	0.60
1:A:3500:MET:O	1:A:3503:ILE:HG22	2.01	0.60
1:A:1626:PHE:HE1	1:A:1706:GLU:HG3	1.67	0.60
1:A:1891:THR:HG21	1:A:2039:LEU:HD21	1.84	0.60
1:A:3646:ASN:OD1	1:A:3650:ASN:ND2	2.35	0.59
1:A:3909:LEU:HB3	1:A:4344:LEU:HD13	1.83	0.59
1:A:3993:ILE:HD11	1:A:4000:ARG:HB2	1.83	0.59
1:A:2588:HIS:HA	1:A:2707:GLN:OE1	2.02	0.59
1:A:2901:TYR:OH	1:A:2909:LEU:N	2.34	0.59
1:A:3558:GLU:OE2	1:A:3562:TRP:NE1	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3849:VAL:O	1:A:3855:ARG:NH1	2.36	0.59
1:A:1721:VAL:HA	1:A:1724:VAL:HG12	1.84	0.59
1:A:3010:THR:HG23	1:A:3017:VAL:HG22	1.84	0.59
1:A:1755:GLN:NE2	1:A:1814:GLU:OE2	2.34	0.59
1:A:2037:ARG:NH2	1:A:4250:SER:OG	2.30	0.58
1:A:2327:LEU:HD12	1:A:2331:GLU:HB3	1.85	0.58
1:A:2484:GLU:OE2	1:A:2488:ARG:NH2	2.36	0.58
1:A:2112:LYS:HD2	1:A:2113:ARG:HH12	1.69	0.58
1:A:2863:ARG:O	1:A:2863:ARG:NH1	2.29	0.58
1:A:3877:HIS:HA	1:A:3880:HIS:CE1	2.38	0.58
1:A:2592:VAL:HG13	1:A:2733:VAL:HG23	1.85	0.58
1:A:3872:ALA:HB1	1:A:3880:HIS:CD2	2.38	0.58
1:A:4629:LYS:HD2	1:A:4629:LYS:O	2.03	0.58
1:A:2275:TRP:HZ2	1:A:2281:THR:HG21	1.68	0.58
1:A:4443:LYS:HD3	1:A:4444:GLN:H	1.67	0.58
1:A:2203:TRP:CH2	1:A:2236:VAL:HG11	2.39	0.58
1:A:3046:SER:HG	1:A:3049:GLU:CD	2.11	0.58
1:A:3826:GLN:HB3	1:A:4140:ARG:HD3	1.84	0.58
1:A:3993:ILE:HD13	1:A:4004:MET:HB2	1.84	0.58
1:A:1880:VAL:HG21	1:A:2049:ILE:HA	1.86	0.58
1:A:2205:GLU:O	1:A:2209:GLN:HG3	2.03	0.58
1:A:3172:THR:HG21	1:A:3694:SER:HB3	1.84	0.58
1:A:1930:PHE:CD2	1:A:1941:MET:HE1	2.39	0.58
1:A:2452:LEU:HD22	1:A:2729:ARG:HD2	1.84	0.58
1:A:3985:GLN:O	1:A:3989:ARG:HG2	2.04	0.57
1:A:2840:ASP:O	1:A:2843:ARG:HG2	2.03	0.57
1:A:3132:LYS:HE3	1:A:3132:LYS:HA	1.86	0.57
1:A:3785:GLU:O	1:A:3789:ILE:HG13	2.04	0.57
1:A:3884:ALA:HB1	1:A:4009:VAL:HG21	1.85	0.57
1:A:3909:LEU:HD11	1:A:4343:MET:HG2	1.86	0.57
1:A:2813:LEU:HD21	1:A:2816:LEU:HG	1.87	0.57
1:A:2934:LEU:HD23	1:A:3091:LEU:HD12	1.86	0.57
1:A:4171:LYS:HG3	1:A:4172:SER:H	1.69	0.57
1:A:2179:ARG:HD3	1:A:2208:LEU:HD11	1.87	0.57
1:A:2469:VAL:HG13	1:A:2481:MET:HE2	1.86	0.57
1:A:3691:ASP:OD1	1:A:3692:LEU:N	2.38	0.57
1:A:2635:PHE:HE2	1:A:2706:ILE:HD13	1.70	0.57
1:A:2944:THR:OG1	1:A:2948:ARG:NH2	2.38	0.57
1:A:4423:LEU:HD13	1:A:4466:HIS:HD2	1.69	0.57
1:A:1748:GLN:HG3	1:A:1749:LEU:HD22	1.86	0.57
1:A:2275:TRP:HB2	1:A:2329:ASN:HD22	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3950:LYS:O	1:A:3954:ASP:N	2.31	0.57
1:A:1884:LEU:HD13	1:A:2044:PRO:HA	1.86	0.56
1:A:1840:SER:OG	1:A:1841:GLN:OE1	2.20	0.56
1:A:2814:GLU:OE1	1:A:2814:GLU:N	2.38	0.56
1:A:1889:TYR:CD1	1:A:1919:LEU:HD13	2.40	0.56
1:A:2480:PRO:O	1:A:2482:GLN:NE2	2.37	0.56
1:A:2943:LYS:HG2	1:A:3094:PHE:CD2	2.40	0.56
1:A:3204:GLY:HA2	1:A:3207:LYS:HE2	1.88	0.56
1:A:3066:PHE:CE1	1:A:3068:MET:HE3	2.41	0.56
1:A:2639:CYS:HA	1:A:2652:PRO:HA	1.87	0.56
1:A:3948:ILE:HA	1:A:3951:VAL:HG12	1.87	0.56
1:A:4538:GLU:OE1	1:A:4594:LYS:NZ	2.29	0.56
1:A:3654:ARG:N	1:A:3661:LEU:O	2.39	0.56
1:A:2211:TYR:O	1:A:2214:THR:OG1	2.20	0.56
1:A:2369:LEU:HD11	1:A:2374:ILE:HD11	1.87	0.56
1:A:2623:SER:N	1:A:2626:THR:OG1	2.39	0.56
1:A:3628:ARG:HH21	1:A:3670:ASP:HB2	1.71	0.56
1:A:1985:HIS:HB2	1:A:1997:ILE:HG21	1.87	0.56
1:A:2195:ASP:N	1:A:2198:GLU:OE1	2.38	0.56
1:A:2266:GLY:HA3	1:A:2275:TRP:CH2	2.41	0.56
1:A:3520:PHE:HB3	1:A:3524:MET:HB2	1.88	0.56
1:A:2091:ARG:HB2	2:A:4701:ADP:O3'	2.06	0.56
1:A:2388:ASP:OD1	1:A:2389:GLU:N	2.39	0.56
1:A:2744:LEU:HA	1:A:2747:ILE:HG22	1.88	0.56
1:A:2826:ALA:HA	1:A:2850:ILE:HD11	1.88	0.56
1:A:3133:LEU:HD11	1:A:3141:GLU:HB3	1.86	0.56
1:A:4534:TRP:CG	1:A:4594:LYS:HZ3	2.24	0.56
1:A:1839:LEU:O	1:A:1843:ARG:NH1	2.38	0.55
1:A:2620:LEU:N	1:A:2662:PHE:O	2.40	0.55
1:A:2864:GLU:OE2	1:A:2864:GLU:N	2.38	0.55
1:A:4010:SER:HB2	1:A:4015:GLU:HA	1.88	0.55
1:A:3088:ARG:NH2	2:A:4703:ADP:O3B	2.38	0.55
1:A:2688:GLU:HB2	1:A:2730:HIS:CE1	2.26	0.55
1:A:3570:ASP:OD1	1:A:3571:ASP:N	2.39	0.55
1:A:3874:GLY:HA3	1:A:4144:ILE:HG13	1.89	0.55
1:A:3907:HIS:CD2	1:A:3991:LEU:HD11	2.40	0.55
1:A:4227:ALA:HB2	1:A:4233:ILE:HD12	1.88	0.55
1:A:4577:LEU:HG	1:A:4635:PHE:CE2	2.41	0.55
1:A:2536:ASP:HA	1:A:2576:ARG:HH11	1.72	0.55
1:A:2464:GLN:HG2	1:A:2583:THR:HA	1.89	0.55
1:A:4485:ARG:O	1:A:4488:GLN:HG2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2452:LEU:HD22	1:A:2729:ARG:HB2	1.88	0.55
1:A:4205:TYR:OH	1:A:4261:ASP:OD2	2.17	0.55
1:A:4483:SER:C	1:A:4487:LYS:HZ3	2.15	0.55
1:A:1628:ARG:HG3	1:A:1657:MET:HE3	1.89	0.55
1:A:2811:ARG:HB3	1:A:2812:PRO:HD3	1.88	0.55
1:A:4129:GLU:OE2	1:A:4131:ASN:ND2	2.40	0.55
1:A:1706:GLU:O	1:A:1710:ARG:HG3	2.07	0.54
1:A:2755:MET:CE	1:A:2807:PHE:HA	2.36	0.54
1:A:2964:HIS:NE2	1:A:2966:LYS:HB3	2.22	0.54
1:A:3161:LEU:HB3	1:A:3168:THR:HG22	1.89	0.54
1:A:3790:VAL:HG13	1:A:3794:VAL:HB	1.88	0.54
1:A:2288:ILE:HD12	1:A:2333:LEU:HD23	1.89	0.54
1:A:2992:PHE:HD2	1:A:3064:VAL:HG23	1.72	0.54
1:A:4318:PRO:HB2	1:A:4325:ASN:HA	1.89	0.54
1:A:4301:ARG:O	1:A:4304:GLU:HG2	2.07	0.54
1:A:2581:LEU:HD13	1:A:2591:LEU:HD21	1.90	0.54
1:A:2615:MET:HG3	1:A:2658:TRP:HB2	1.89	0.54
1:A:2797:ARG:HH21	1:A:3087:ASN:ND2	2.06	0.54
1:A:2876:TRP:CH2	1:A:2953:MET:HG2	2.43	0.54
1:A:2943:LYS:HA	1:A:3094:PHE:HE2	1.73	0.54
1:A:3639:GLU:HG2	1:A:3686:VAL:HG21	1.90	0.54
1:A:2202:MET:SD	1:A:2202:MET:N	2.80	0.54
1:A:2507:ARG:HG2	1:A:2510:MET:HE1	1.89	0.54
1:A:2038:SER:C	1:A:2039:LEU:HD22	2.33	0.54
1:A:2148:LYS:HE2	1:A:2361:MET:HB3	1.90	0.54
1:A:3723:ASP:OD1	1:A:3724:VAL:N	2.40	0.54
1:A:4107:MET:O	1:A:4111:LYS:HG2	2.07	0.54
1:A:2609:LEU:HG	1:A:2612:LEU:HD12	1.90	0.54
1:A:3872:ALA:HB1	1:A:3880:HIS:HD2	1.72	0.54
1:A:2509:LYS:O	1:A:2513:GLU:HG3	2.08	0.54
1:A:3606:ASP:OD1	1:A:3607:ARG:N	2.41	0.54
1:A:4036:LYS:HZ1	1:A:4038:ASN:HB2	1.73	0.54
1:A:4609:VAL:HG22	1:A:4642:VAL:HB	1.89	0.53
1:A:1748:GLN:HE22	1:A:1872:TYR:HA	1.73	0.53
1:A:2628:PRO:HB3	1:A:2682:PHE:CD2	2.43	0.53
1:A:2726:ARG:NH2	3:A:4702:ATP:O3G	2.38	0.53
1:A:1879:LEU:HD22	2:A:4701:ADP:C6	2.43	0.53
1:A:1892:MET:N	1:A:1892:MET:HE2	2.22	0.53
1:A:3030:MET:HE1	1:A:3051:TYR:HD1	1.73	0.53
1:A:3974:TRP:NE1	1:A:3976:GLU:OE2	2.40	0.53
1:A:4095:MET:HG3	1:A:4097:LYS:NZ	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4605:VAL:N	1:A:4624:PHE:O	2.25	0.53
1:A:2594:CYS:HA	1:A:2712:CYS:O	2.09	0.53
1:A:2882:ILE:HD12	1:A:2883:PRO:HD2	1.90	0.53
1:A:3129:VAL:HG21	1:A:3149:PHE:HB2	1.90	0.53
1:A:4160:THR:HG23	1:A:4212:LEU:HD21	1.91	0.53
1:A:1677:SER:OG	1:A:1678:SER:N	2.42	0.53
1:A:2948:ARG:HG3	1:A:2958:VAL:HG21	1.91	0.53
1:A:2347:ASP:OD1	1:A:2348:LEU:N	2.40	0.53
1:A:2568:VAL:HG21	1:A:2607:SER:HB2	1.91	0.53
1:A:4190:ILE:HG23	1:A:4201:TRP:CZ2	2.43	0.53
1:A:4446:ASN:OD1	1:A:4447:TYR:N	2.41	0.53
1:A:2275:TRP:HE1	1:A:2285:ARG:HH21	1.55	0.53
1:A:3193:GLU:O	1:A:3196:GLU:HG3	2.09	0.53
1:A:2453:ARG:HB2	1:A:2729:ARG:HA	1.90	0.53
1:A:2615:MET:HG3	1:A:2658:TRP:O	2.08	0.53
1:A:2640:GLU:HG2	1:A:2653:VAL:HG22	1.91	0.53
1:A:3950:LYS:HZ2	1:A:3973:LEU:HG	1.74	0.53
1:A:4405:ILE:O	1:A:4411:ARG:NH1	2.39	0.53
1:A:4461:PRO:HG2	1:A:4464:TRP:CE3	2.44	0.53
1:A:4489:LEU:HA	1:A:4492:ILE:HG12	1.91	0.53
1:A:1905:PHE:HE1	1:A:2038:SER:HB3	1.74	0.52
1:A:2234:TRP:CE2	1:A:2302:VAL:HG21	2.44	0.52
1:A:3949:ALA:O	1:A:3952:GLN:NE2	2.42	0.52
1:A:4071:ILE:HG21	1:A:4099:VAL:HA	1.91	0.52
1:A:2300:TRP:CG	1:A:2342:MET:HE1	2.44	0.52
1:A:3986:ALA:O	1:A:3990:LEU:HD23	2.09	0.52
1:A:1961:ASN:HD21	1:A:2019:ASN:HB3	1.75	0.52
1:A:2584:TRP:HE3	1:A:2591:LEU:HD22	1.73	0.52
1:A:3147:CYS:O	1:A:3150:VAL:HG12	2.09	0.52
1:A:4475:VAL:O	1:A:4479:VAL:HG23	2.09	0.52
1:A:2768:PRO:HB2	1:A:2858:PHE:HE1	1.74	0.52
1:A:2819:GLU:HA	1:A:2861:ILE:HD11	1.90	0.52
1:A:3751:GLN:O	1:A:3755:GLU:HG2	2.09	0.52
1:A:4098:ASN:HB2	1:A:4100:HIS:CE1	2.44	0.52
1:A:1766:LEU:HD22	1:A:1778:LEU:HD11	1.90	0.52
1:A:2969:GLY:HA2	1:A:3004:PHE:HE2	1.75	0.52
1:A:1816:VAL:HA	1:A:1819:ARG:NH1	2.25	0.52
1:A:2747:ILE:HG23	1:A:2748:TYR:CD2	2.45	0.52
1:A:2422:ILE:HG23	1:A:2487:GLU:HG2	1.92	0.52
1:A:1884:LEU:HD21	1:A:2041:MET:SD	2.50	0.52
1:A:2511:ARG:HD3	1:A:2535:ILE:HD13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3585:ARG:NH1	1:A:3694:SER:O	2.42	0.52
1:A:4156:ASN:ND2	1:A:4188:ALA:HA	2.25	0.52
1:A:4402:VAL:HA	1:A:4405:ILE:HD12	1.91	0.52
1:A:2837:LEU:O	1:A:2843:ARG:NH2	2.43	0.52
1:A:2486:LEU:O	1:A:2490:ILE:HG12	2.10	0.52
1:A:1672:VAL:HA	1:A:1691:SER:HA	1.91	0.51
1:A:1698:ILE:HD12	1:A:1701:TRP:NE1	2.24	0.51
1:A:1713:LEU:HD22	1:A:1749:LEU:HD21	1.92	0.51
1:A:2437:LEU:HD22	1:A:2455:LEU:HD21	1.90	0.51
1:A:2492:ARG:HH22	1:A:2525:PRO:HB2	1.75	0.51
1:A:2684:ARG:HD2	1:A:2726:ARG:HB3	1.92	0.51
1:A:3544:ARG:NH1	1:A:3546:ASP:OD1	2.43	0.51
1:A:2835:ASP:OD1	1:A:2921:ARG:NH1	2.44	0.51
1:A:2874:SER:HB3	1:A:2884:VAL:HG21	1.92	0.51
1:A:2900:PHE:O	1:A:2904:GLU:N	2.43	0.51
1:A:3990:LEU:HD22	1:A:4004:MET:HG3	1.92	0.51
1:A:4452:ILE:O	1:A:4456:VAL:HG23	2.10	0.51
1:A:3649:LEU:HD12	1:A:3695:ARG:HH21	1.75	0.51
1:A:4251:ILE:HG22	1:A:4252:TYR:CD2	2.45	0.51
1:A:4489:LEU:HD11	1:A:4515:PHE:HE1	1.75	0.51
1:A:1666:LEU:HG	1:A:1673:VAL:HA	1.92	0.51
1:A:2472:TYR:HD2	1:A:2481:MET:HE3	1.75	0.51
1:A:2481:MET:SD	1:A:2481:MET:N	2.83	0.51
1:A:3115:LEU:HD13	1:A:3143:ILE:HD13	1.92	0.51
1:A:4088:VAL:HG23	1:A:4118:PRO:HA	1.93	0.51
1:A:4098:ASN:HB2	1:A:4100:HIS:HE1	1.75	0.51
1:A:1905:PHE:CE1	1:A:2038:SER:HB3	2.46	0.51
1:A:2222:MET:HE1	1:A:2342:MET:HB3	1.92	0.51
1:A:2311:TRP:H	1:A:2311:TRP:CD1	2.28	0.51
1:A:4002:LEU:O	1:A:4006:HIS:ND1	2.43	0.51
1:A:4066:ILE:HD11	1:A:4095:MET:HB2	1.93	0.51
1:A:4240:TRP:CD1	1:A:4275:THR:HG1	2.29	0.51
1:A:1736:ASN:O	1:A:1740:THR:HG23	2.11	0.51
1:A:2595:GLY:HA2	1:A:2735:TYR:CE1	2.46	0.51
1:A:2614:ASP:C	1:A:2657:LYS:HD2	2.36	0.51
1:A:3888:ALA:HA	1:A:4013:LEU:HD21	1.93	0.51
1:A:4186:PHE:O	1:A:4189:ILE:HG22	2.10	0.51
1:A:1633:GLY:O	1:A:1637:LEU:N	2.41	0.51
1:A:3700:ASN:HD22	1:A:3702:THR:HG22	1.75	0.51
1:A:3716:VAL:HB	1:A:3836:TYR:OH	2.10	0.51
1:A:2423:MET:HG3	1:A:2427:PHE:HE2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2093:LEU:O	1:A:2097:LEU:HG	2.10	0.51
1:A:1662:SER:HB2	1:A:1679:ARG:HD3	1.92	0.51
1:A:1632:VAL:O	1:A:1943:ARG:NH1	2.44	0.50
1:A:2787:ASP:OD1	1:A:2788:THR:N	2.44	0.50
1:A:2935:LEU:HD13	1:A:2943:LYS:HB3	1.93	0.50
1:A:3603:GLU:HG2	1:A:3604:TYR:CD1	2.46	0.50
1:A:2785:THR:OG1	1:A:2787:ASP:OD1	2.24	0.50
1:A:2935:LEU:HB2	1:A:3067:THR:HG22	1.92	0.50
1:A:3607:ARG:HG3	1:A:3632:PRO:HG3	1.93	0.50
1:A:4154:LYS:HB2	1:A:4312:LEU:HD23	1.92	0.50
1:A:2277:ASP:HB3	1:A:2285:ARG:HH22	1.76	0.50
1:A:2231:SER:HA	1:A:2234:TRP:CD1	2.47	0.50
1:A:2670:ASP:HA	1:A:2721:LYS:HE3	1.92	0.50
1:A:3045:ASP:OD1	1:A:3046:SER:N	2.42	0.50
1:A:3495:THR:HG23	1:A:3496:PHE:HD1	1.76	0.50
1:A:3576:ASN:ND2	1:A:3700:ASN:O	2.45	0.50
1:A:3017:VAL:HB	1:A:3020:LEU:HG	1.93	0.50
1:A:3544:ARG:NH2	1:A:3546:ASP:OD2	2.44	0.50
1:A:3818:LEU:HD22	1:A:4346:MET:SD	2.51	0.50
1:A:4075:GLU:O	1:A:4079:GLN:HG2	2.12	0.50
1:A:1778:LEU:HB3	1:A:1826:ILE:HD11	1.94	0.50
1:A:3810:SER:HB3	1:A:3890:ILE:HD12	1.94	0.50
1:A:4109:LEU:HD12	1:A:4112:LYS:HD3	1.93	0.50
1:A:4321:LEU:HD23	1:A:4321:LEU:H	1.77	0.50
1:A:2600:GLY:O	1:A:2604:THR:OG1	2.21	0.50
1:A:3742:LEU:HD12	1:A:3776:GLU:HB3	1.94	0.50
1:A:3950:LYS:HE3	1:A:3973:LEU:HA	1.94	0.50
1:A:4095:MET:HG3	1:A:4097:LYS:HZ1	1.77	0.50
1:A:3207:LYS:HZ3	1:A:3754:ASN:HB3	1.77	0.49
1:A:3586:TYR:O	1:A:3696:VAL:HG13	2.11	0.49
1:A:2210:LEU:O	1:A:2214:THR:HG23	2.11	0.49
1:A:2461:MET:HG3	1:A:2584:TRP:HE1	1.77	0.49
1:A:2909:LEU:HA	2:A:4704:ADP:C2	2.47	0.49
1:A:3021:PHE:CE2	1:A:3029:LEU:HB2	2.48	0.49
1:A:3213:ASP:O	1:A:3216:GLU:HG2	2.12	0.49
1:A:3839:VAL:HG21	1:A:3863:LEU:HA	1.94	0.49
1:A:1880:VAL:HG21	1:A:2049:ILE:HG12	1.95	0.49
1:A:2964:HIS:HA	1:A:3643:PRO:HB2	1.94	0.49
1:A:3733:LYS:C	1:A:3736:GLY:H	2.21	0.49
1:A:4042:LEU:HD23	1:A:4126:LEU:HB2	1.94	0.49
1:A:4277:SER:HA	1:A:4282:PHE:CD1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4423:LEU:HD13	1:A:4466:HIS:CD2	2.45	0.49
1:A:2609:LEU:HB3	1:A:2617:VAL:HG22	1.95	0.49
1:A:2912:PHE:CZ	1:A:2915:VAL:HG23	2.48	0.49
1:A:2757:ARG:HA	1:A:2763:ARG:HH11	1.76	0.49
1:A:4306:VAL:O	1:A:4309:VAL:HG12	2.12	0.49
1:A:4430:ASP:O	1:A:4434:VAL:HG23	2.12	0.49
1:A:2075:LEU:HD22	1:A:4526:GLN:OE1	2.13	0.49
1:A:2667:ASN:HB3	1:A:2723:LEU:HD21	1.95	0.49
1:A:2890:ARG:NH1	1:A:2911:LEU:O	2.43	0.49
1:A:2946:LEU:O	1:A:2950:VAL:HG23	2.12	0.49
1:A:4110:GLU:HG3	1:A:4137:ASN:OD1	2.12	0.49
1:A:1886:ASP:OD1	1:A:1886:ASP:N	2.44	0.49
1:A:1896:LEU:HD21	1:A:2013:ALA:HB2	1.94	0.49
1:A:2280:PHE:CE1	1:A:2301:ILE:HG21	2.48	0.49
1:A:2897:LEU:CD1	1:A:2911:LEU:HD21	2.42	0.49
1:A:4398:LEU:HD12	1:A:4414:GLU:HA	1.94	0.49
1:A:1665:ILE:O	1:A:1674:LEU:N	2.39	0.49
1:A:2935:LEU:HD23	1:A:3092:ASN:OD1	2.13	0.49
1:A:2912:PHE:CE2	1:A:2914:GLU:HB2	2.48	0.49
1:A:3893:LYS:NZ	1:A:3900:THR:HA	2.27	0.49
1:A:4052:SER:O	1:A:4055:VAL:HG12	2.13	0.49
1:A:4300:ILE:N	1:A:4304:GLU:OE2	2.33	0.49
1:A:2813:LEU:CD2	1:A:2816:LEU:HG	2.41	0.49
1:A:3660:VAL:HG13	1:A:3671:LEU:HB3	1.94	0.48
1:A:3870:ARG:NH2	1:A:4034:GLU:HB2	2.27	0.48
1:A:1644:SER:OG	1:A:1645:LYS:NZ	2.41	0.48
1:A:2685:GLN:HE21	1:A:2692:PHE:HA	1.78	0.48
1:A:2773:MET:HG3	1:A:2802:TRP:CZ3	2.48	0.48
1:A:2886:GLN:OE1	1:A:2886:GLN:N	2.36	0.48
1:A:1900:LEU:HB2	1:A:2035:LEU:O	2.13	0.48
1:A:2228:SER:O	1:A:2369:LEU:HB2	2.14	0.48
1:A:2571:THR:H	1:A:2574:THR:CG2	2.25	0.48
1:A:3149:PHE:O	1:A:3153:THR:HG23	2.14	0.48
1:A:3187:PHE:CE1	1:A:3191:ARG:HG3	2.49	0.48
1:A:3598:GLU:OE2	1:A:3598:GLU:N	2.28	0.48
1:A:3784:VAL:O	1:A:3787:THR:OG1	2.26	0.48
1:A:4099:VAL:HG22	1:A:4128:MET:HB3	1.96	0.48
1:A:2723:LEU:HB2	1:A:2728:LEU:HD11	1.95	0.48
1:A:3744:GLN:O	1:A:3747:LYS:HG3	2.12	0.48
1:A:3817:SER:O	1:A:3820:GLN:HG2	2.12	0.48
1:A:3839:VAL:HG12	1:A:3840:LEU:HD23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1766:LEU:HD21	1:A:1778:LEU:HD21	1.95	0.48
1:A:1825:LEU:HD11	1:A:1838:TRP:CE3	2.49	0.48
1:A:1979:GLN:HB3	1:A:2035:LEU:HD13	1.96	0.48
1:A:3730:ASP:O	1:A:3734:LEU:N	2.43	0.48
1:A:3730:ASP:O	1:A:3734:LEU:HG	2.14	0.48
1:A:4260:PHE:HE2	1:A:4618:LEU:HD11	1.79	0.48
1:A:4482:PHE:O	1:A:4486:ILE:HG12	2.14	0.48
1:A:2548:TRP:CE2	1:A:2576:ARG:HG2	2.49	0.48
1:A:2558:GLU:CD	1:A:2560:HIS:H	2.22	0.48
1:A:2622:PHE:HD2	1:A:2666:ILE:HA	1.79	0.48
1:A:3596:ALA:HB2	1:A:3701:PHE:CD1	2.49	0.48
1:A:1633:GLY:HA2	1:A:1943:ARG:NH2	2.28	0.48
1:A:2912:PHE:HE2	1:A:2914:GLU:HB2	1.78	0.48
1:A:2934:LEU:HD12	1:A:3066:PHE:O	2.13	0.48
1:A:3544:ARG:HH11	1:A:3547:ILE:HB	1.77	0.48
1:A:4318:PRO:HB3	1:A:4327:ALA:HB3	1.96	0.48
1:A:3046:SER:N	1:A:3049:GLU:OE2	2.47	0.48
1:A:3133:LEU:HD12	1:A:3134:PRO:HD2	1.96	0.48
1:A:3909:LEU:HD21	1:A:4343:MET:HB3	1.94	0.48
1:A:4097:LYS:HA	1:A:4127:THR:CG2	2.44	0.48
1:A:1914:GLU:OE2	2:A:4701:ADP:H3'	2.14	0.47
1:A:2352:THR:O	1:A:2356:VAL:HG23	2.13	0.47
1:A:2373:MET:HE1	3:A:4702:ATP:C4	2.50	0.47
1:A:2936:ILE:HD11	1:A:3091:LEU:HD21	1.95	0.47
1:A:2726:ARG:HH21	3:A:4702:ATP:PG	2.37	0.47
1:A:3635:VAL:HB	1:A:3679:LEU:HD23	1.97	0.47
1:A:2461:MET:CG	1:A:2584:TRP:HE1	2.28	0.47
1:A:1937:ASP:OD2	1:A:1940:ALA:HB3	2.14	0.47
1:A:2050:ALA:O	1:A:2054:LEU:HB2	2.15	0.47
1:A:3021:PHE:CD2	1:A:3025:GLU:HG3	2.50	0.47
1:A:4232:ASN:OD1	1:A:4233:ILE:N	2.47	0.47
1:A:1698:ILE:HD12	1:A:1701:TRP:HE1	1.79	0.47
1:A:1975:VAL:HA	1:A:1978:ILE:HG22	1.96	0.47
1:A:3012:LEU:HD11	1:A:3064:VAL:HG11	1.96	0.47
1:A:3214:GLN:O	1:A:3218:LEU:HG	2.14	0.47
1:A:3624:GLU:O	1:A:3628:ARG:HG2	2.15	0.47
1:A:3819:LYS:HE3	1:A:3826:GLN:OE1	2.15	0.47
1:A:1850:GLN:HE21	1:A:1855:GLN:HE21	1.62	0.47
1:A:2412:MET:O	1:A:2415:ILE:HG22	2.15	0.47
1:A:3491:LYS:HA	1:A:3494:GLU:OE1	2.15	0.47
1:A:4181:PHE:HE2	1:A:4296:MET:HE1	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2038:SER:O	1:A:2039:LEU:HD22	2.15	0.47
1:A:2511:ARG:NH2	1:A:2735:TYR:HB3	2.26	0.47
1:A:2910:VAL:HG22	2:A:4704:ADP:N1	2.29	0.47
1:A:3833:LEU:O	1:A:3837:HIS:ND1	2.38	0.47
1:A:4179:LEU:HD23	1:A:4179:LEU:HA	1.76	0.47
1:A:4556:CYS:O	1:A:4591:ARG:HA	2.13	0.47
1:A:1665:ILE:N	1:A:1675:GLY:O	2.34	0.47
1:A:1809:GLU:OE2	1:A:2057:GLN:NE2	2.46	0.47
1:A:2369:LEU:HD21	1:A:2374:ILE:CG1	2.44	0.47
1:A:2968:THR:HG23	1:A:2970:GLU:HG3	1.96	0.47
1:A:3517:ALA:HA	1:A:3520:PHE:HD2	1.80	0.47
1:A:3544:ARG:O	1:A:3547:ILE:HG22	2.15	0.47
1:A:3950:LYS:HA	1:A:3953:ALA:HB3	1.96	0.47
1:A:4303:GLU:O	1:A:4306:VAL:HB	2.15	0.47
1:A:1940:ALA:O	1:A:1944:ILE:HG12	2.15	0.47
1:A:2185:VAL:HG13	1:A:2239:LYS:HD2	1.96	0.47
1:A:3576:ASN:HB3	1:A:3701:PHE:CE2	2.49	0.47
1:A:3796:THR:O	1:A:3799:GLN:HG3	2.15	0.47
1:A:3907:HIS:CE1	1:A:3937:ARG:HG3	2.46	0.47
1:A:1683:GLU:HG3	1:A:1685:MET:HE3	1.96	0.47
1:A:2230:LYS:HZ2	1:A:2345:VAL:C	2.23	0.47
1:A:2412:MET:HA	1:A:2415:ILE:HG22	1.97	0.47
1:A:2781:GLN:OE1	1:A:2794:TYR:HB2	2.14	0.47
1:A:2138:ILE:HD12	1:A:2168:VAL:HG22	1.96	0.46
1:A:3886:LEU:HD22	1:A:4343:MET:HE2	1.97	0.46
1:A:4525:ARG:HD3	1:A:4592:TRP:CH2	2.49	0.46
1:A:1949:CYS:HA	1:A:2012:MET:CE	2.42	0.46
1:A:1964:GLU:OE2	1:A:1964:GLU:N	2.33	0.46
1:A:2934:LEU:N	1:A:3090:VAL:O	2.41	0.46
1:A:3591:ASP:OD1	1:A:3591:ASP:N	2.48	0.46
1:A:3733:LYS:HA	1:A:3736:GLY:HA3	1.98	0.46
1:A:4318:PRO:HG3	1:A:4328:GLU:HG2	1.97	0.46
1:A:4485:ARG:O	1:A:4489:LEU:HG	2.16	0.46
1:A:1626:PHE:CZ	1:A:1628:ARG:HB3	2.51	0.46
1:A:1891:THR:CG2	1:A:2039:LEU:HD21	2.45	0.46
1:A:3935:VAL:HG22	1:A:3996:PHE:HE1	1.80	0.46
1:A:3945:LYS:HE3	1:A:3945:LYS:HB3	1.82	0.46
1:A:3993:ILE:HG21	1:A:4004:MET:HG2	1.98	0.46
1:A:2981:ARG:NH2	1:A:3025:GLU:OE2	2.48	0.46
1:A:3620:ARG:NH1	1:A:3644:VAL:HG11	2.30	0.46
1:A:4086:THR:O	1:A:4090:SER:OG	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4554:ASP:N	1:A:4557:SER:OG	2.48	0.46
1:A:3121:ILE:O	1:A:3540:ASN:ND2	2.46	0.46
1:A:3653:VAL:HG12	1:A:3662:ILE:HD11	1.98	0.46
1:A:2223:VAL:O	1:A:2363:TRP:HA	2.15	0.46
1:A:2573:ASP:OD1	1:A:2576:ARG:NH2	2.49	0.46
1:A:2869:ARG:O	1:A:2871:ILE:HD12	2.15	0.46
1:A:4411:ARG:O	1:A:4414:GLU:HG3	2.16	0.46
1:A:3034:LYS:HE3	1:A:3038:GLN:NE2	2.31	0.46
1:A:3167:ARG:CZ	1:A:3685:THR:HA	2.46	0.46
1:A:4260:PHE:CE2	1:A:4608:PRO:HB3	2.51	0.46
1:A:2943:LYS:HG2	1:A:3094:PHE:HD2	1.78	0.46
1:A:3204:GLY:O	1:A:3207:LYS:HG2	2.15	0.46
1:A:3653:VAL:HA	1:A:3662:ILE:HG12	1.98	0.46
1:A:2085:HIS:HB3	1:A:2348:LEU:HD12	1.98	0.46
1:A:2142:CYS:O	1:A:2146:VAL:HB	2.15	0.46
1:A:2596:PRO:HB2	1:A:2738:TYR:CZ	2.50	0.46
1:A:2747:ILE:HD11	2:A:4703:ADP:C5	2.51	0.46
1:A:2827:HIS:NE2	1:A:2881:TYR:OH	2.46	0.46
1:A:2873:TYR:CE2	1:A:2883:PRO:HD3	2.51	0.46
1:A:3017:VAL:HG12	1:A:3019:GLY:H	1.80	0.46
1:A:3113:MET:HG2	1:A:3115:LEU:HG	1.98	0.46
1:A:3807:ALA:O	1:A:3811:ILE:HD12	2.16	0.46
1:A:4190:ILE:HD12	1:A:4201:TRP:CZ2	2.51	0.46
1:A:2075:LEU:HD11	1:A:4536:LEU:HD12	1.98	0.46
1:A:2623:SER:HA	1:A:2668:LEU:HD23	1.97	0.46
1:A:3790:VAL:HG22	1:A:3794:VAL:HG21	1.97	0.46
1:A:4260:PHE:CD2	1:A:4608:PRO:HB3	2.50	0.46
1:A:4606:THR:OG1	1:A:4623:ASP:OD2	2.27	0.46
1:A:1912:LYS:HG2	1:A:2041:MET:HG3	1.98	0.45
1:A:2873:TYR:HB3	1:A:2881:TYR:CZ	2.51	0.45
1:A:3797:VAL:O	1:A:3800:GLN:HG2	2.16	0.45
1:A:1816:VAL:HG22	1:A:1819:ARG:HH12	1.82	0.45
1:A:2577:HIS:CE1	1:A:2736:VAL:HG22	2.51	0.45
1:A:2680:ILE:HD12	1:A:2680:ILE:HA	1.80	0.45
1:A:3175:HIS:CE1	1:A:3585:ARG:HH12	2.33	0.45
1:A:2382:LEU:HD12	1:A:2463:HIS:CE1	2.51	0.45
1:A:2969:GLY:HA2	1:A:3004:PHE:CE2	2.51	0.45
1:A:3627:LEU:HD13	1:A:3669:ILE:HG21	1.99	0.45
1:A:4543:VAL:HG21	1:A:4622:VAL:HB	1.97	0.45
1:A:1838:TRP:CZ2	1:A:1843:ARG:HG2	2.51	0.45
1:A:2230:LYS:HE2	1:A:2344:GLU:CG	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2446:ILE:N	1:A:2505:ASP:OD2	2.50	0.45
1:A:2449:LEU:HD12	1:A:2453:ARG:NH2	2.32	0.45
1:A:2654:GLN:N	1:A:2654:GLN:OE1	2.50	0.45
1:A:4036:LYS:HD2	1:A:4037:PRO:HD2	1.98	0.45
1:A:4050:ASP:N	1:A:4050:ASP:OD1	2.49	0.45
1:A:4196:TYR:O	1:A:4200:GLY:N	2.36	0.45
1:A:3168:THR:O	1:A:3169:MET:HE2	2.16	0.45
1:A:4221:THR:HG23	1:A:4222:TRP:CD1	2.46	0.45
1:A:2960:GLN:HB3	1:A:2993:ILE:HG13	1.98	0.45
1:A:3586:TYR:HA	1:A:3587:PRO:HD3	1.82	0.45
1:A:4009:VAL:HG13	1:A:4018:MET:HE1	1.97	0.45
1:A:4454:GLU:HG3	1:A:4459:ILE:HG23	1.99	0.45
1:A:1738:TYR:HE1	1:A:1741:TRP:HZ3	1.64	0.45
1:A:2370:SER:HB3	1:A:2373:MET:HB2	1.99	0.45
1:A:2496:TYR:CE1	1:A:2500:TRP:HD1	2.34	0.45
1:A:3191:ARG:CZ	1:A:3500:MET:HE1	2.47	0.45
1:A:4532:ASN:HB3	1:A:4534:TRP:HZ3	1.79	0.45
1:A:1877:ASP:OD2	1:A:1878:LYS:N	2.50	0.45
1:A:2149:LEU:HD11	1:A:2157:LEU:HD22	1.99	0.45
1:A:2255:ASP:HA	1:A:2304:ASP:O	2.16	0.45
1:A:2275:TRP:CZ2	1:A:2277:ASP:HA	2.52	0.45
1:A:4303:GLU:O	1:A:4307:GLN:OE1	2.34	0.45
1:A:4312:LEU:HD12	1:A:4313:PRO:CD	2.46	0.45
1:A:2152:GLU:O	1:A:2155:PRO:HD2	2.16	0.45
1:A:2219:GLY:HA2	1:A:2341:ILE:O	2.17	0.45
1:A:2219:GLY:HA3	1:A:2319:LEU:HD22	1.99	0.45
1:A:3021:PHE:CE2	1:A:3025:GLU:HG3	2.52	0.45
1:A:3951:VAL:HG23	1:A:3957:PHE:CD2	2.52	0.45
1:A:4182:LEU:HD11	1:A:4272:LEU:HB3	1.99	0.45
1:A:4414:GLU:O	1:A:4418:LYS:HG2	2.17	0.45
1:A:4578:SER:O	1:A:4638:ARG:NH2	2.50	0.45
1:A:1821:VAL:HG21	1:A:1841:GLN:HG3	1.99	0.45
1:A:1886:ASP:HA	1:A:1889:TYR:HB2	1.98	0.45
1:A:2138:ILE:HD11	1:A:2168:VAL:HG13	1.99	0.45
1:A:2538:GLU:HB3	1:A:2548:TRP:NE1	2.32	0.45
1:A:3819:LYS:HA	1:A:3825:TYR:O	2.16	0.45
1:A:4110:GLU:HA	1:A:4113:LEU:HG	1.99	0.45
1:A:1659:ALA:HB1	1:A:1873:LEU:HD13	1.99	0.44
1:A:2105:ARG:HA	1:A:2108:ILE:HG12	1.98	0.44
1:A:2237:LEU:HG	1:A:2300:TRP:HH2	1.82	0.44
1:A:2609:LEU:HA	1:A:2612:LEU:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2691:GLY:HA2	1:A:2703:LEU:HD23	1.98	0.44
1:A:2777:TYR:HB2	1:A:2799:MET:HE1	1.99	0.44
1:A:3950:LYS:HZ1	1:A:3973:LEU:HG	1.82	0.44
1:A:2223:VAL:HG22	1:A:2348:LEU:HD21	1.99	0.44
1:A:2435:LYS:O	1:A:2438:GLU:HG3	2.16	0.44
1:A:2608:ALA:O	1:A:2612:LEU:HG	2.17	0.44
1:A:3006:GLU:OE1	1:A:3009:ASN:ND2	2.49	0.44
1:A:3789:ILE:O	1:A:3793:GLU:HG3	2.17	0.44
1:A:3825:TYR:CE1	1:A:3875:MET:HA	2.52	0.44
1:A:3870:ARG:HH22	1:A:4034:GLU:HB2	1.82	0.44
1:A:1852:ASP:HB3	1:A:1855:GLN:NE2	2.32	0.44
1:A:2553:PRO:HD2	1:A:2570:PRO:HB2	1.99	0.44
1:A:3882:THR:HG22	1:A:4339:MET:SD	2.57	0.44
1:A:2238:LEU:HB2	1:A:2300:TRP:CZ3	2.52	0.44
1:A:2427:PHE:CE1	1:A:2433:VAL:HG21	2.53	0.44
1:A:2464:GLN:CB	1:A:2583:THR:HG23	2.48	0.44
1:A:2677:GLN:HB2	1:A:2680:ILE:HG22	1.99	0.44
1:A:3999:ASP:OD1	1:A:4000:ARG:N	2.50	0.44
1:A:4030:ILE:HG21	1:A:4145:PHE:HZ	1.81	0.44
1:A:4604:VAL:HA	1:A:4625:GLU:HA	1.98	0.44
1:A:1938:PHE:CB	1:A:1967:MET:HE1	2.48	0.44
1:A:2427:PHE:CD1	1:A:2433:VAL:HG21	2.52	0.44
1:A:2666:ILE:O	1:A:2669:PRO:HD2	2.17	0.44
1:A:2729:ARG:HG3	1:A:2730:HIS:CD2	2.48	0.44
1:A:2755:MET:SD	1:A:2807:PHE:HD1	2.40	0.44
1:A:2852:THR:C	1:A:2856:LYS:HZ2	2.25	0.44
1:A:3783:LYS:HA	1:A:3783:LYS:HD3	1.66	0.44
1:A:4293:ASP:OD1	1:A:4293:ASP:N	2.50	0.44
1:A:4565:LEU:HD13	1:A:4585:LEU:HD21	1.98	0.44
1:A:2563:ALA:HA	1:A:2751:PHE:CE2	2.53	0.44
1:A:2688:GLU:HG3	1:A:2689:HIS:ND1	2.32	0.44
1:A:3154:LEU:HB3	1:A:3171:ILE:CD1	2.46	0.44
1:A:3214:GLN:O	1:A:3217:GLU:HG3	2.17	0.44
1:A:3544:ARG:NH1	1:A:3547:ILE:HB	2.33	0.44
1:A:1928:LEU:HD23	1:A:1948:LEU:HD21	2.00	0.44
1:A:2103:VAL:O	1:A:2106:GLU:HG3	2.17	0.44
1:A:2460:SER:HB2	1:A:2589:LYS:NZ	2.33	0.44
1:A:2857:HIS:C	1:A:2858:PHE:HD1	2.25	0.44
1:A:3512:ALA:O	1:A:3516:TYR:HB2	2.17	0.44
1:A:3846:LEU:HD22	1:A:3855:ARG:NH1	2.32	0.44
1:A:1713:LEU:CD2	1:A:1749:LEU:HD21	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2624:SER:HB2	1:A:2670:ASP:OD2	2.18	0.44
1:A:3653:VAL:O	1:A:3654:ARG:NE	2.49	0.44
1:A:3704:THR:HG23	1:A:3707:SER:H	1.82	0.44
1:A:4577:LEU:HD22	1:A:4638:ARG:NE	2.33	0.44
1:A:2304:ASP:OD1	1:A:2726:ARG:NH2	2.50	0.44
1:A:2316:ASN:O	1:A:2358:ARG:NH1	2.50	0.44
1:A:2980:LEU:HD21	1:A:3011:LEU:HD11	1.99	0.44
1:A:3628:ARG:HH12	1:A:3669:ILE:HG23	1.83	0.44
1:A:4173:PRO:HG2	1:A:4176:ARG:HE	1.83	0.44
1:A:4297:PRO:HG3	1:A:4308:TRP:CG	2.53	0.44
1:A:2231:SER:HB2	3:A:4702:ATP:O2A	2.18	0.43
1:A:2296:GLN:OE1	1:A:2296:GLN:N	2.47	0.43
1:A:2726:ARG:O	1:A:2729:ARG:HG2	2.16	0.43
1:A:2838:VAL:HA	1:A:3093:TRP:CD2	2.53	0.43
1:A:4346:MET:HA	1:A:4346:MET:HE2	2.00	0.43
1:A:1633:GLY:HA2	1:A:1943:ARG:CZ	2.48	0.43
1:A:1872:TYR:CZ	1:A:1874:GLY:HA2	2.53	0.43
1:A:1888:CYS:O	1:A:1892:MET:HG2	2.17	0.43
1:A:2203:TRP:HH2	1:A:2236:VAL:HG11	1.79	0.43
1:A:2309:PRO:HD3	1:A:2350:TYR:O	2.18	0.43
1:A:2453:ARG:NH1	1:A:2733:VAL:HG12	2.33	0.43
1:A:4541:LEU:HB3	1:A:4592:TRP:CZ3	2.52	0.43
1:A:2104:LYS:HB2	1:A:2136:ILE:HD13	1.99	0.43
1:A:2494:LEU:O	1:A:2498:ILE:HG13	2.18	0.43
1:A:4507:ILE:HG23	1:A:4509:VAL:HG13	2.00	0.43
1:A:2831:ARG:HH21	1:A:2921:ARG:HH21	1.65	0.43
1:A:3098:SER:OG	1:A:3099:THR:N	2.52	0.43
1:A:4324:PRO:HD3	1:A:4638:ARG:HG2	2.01	0.43
1:A:1667:ASN:OD1	1:A:1667:ASN:N	2.50	0.43
1:A:1716:LEU:HG	1:A:1745:TYR:HD1	1.82	0.43
1:A:1745:TYR:O	1:A:1807:LYS:HE2	2.18	0.43
1:A:1945:PHE:HZ	1:A:1978:ILE:HG21	1.83	0.43
1:A:2377:ASN:C	1:A:2377:ASN:HD22	2.26	0.43
1:A:3851:ASP:O	1:A:3855:ARG:HG3	2.19	0.43
1:A:3914:ILE:HB	1:A:3937:ARG:HD2	2.00	0.43
1:A:3947:LEU:HD11	1:A:3973:LEU:HD23	2.00	0.43
1:A:3960:TRP:HZ3	1:A:3996:PHE:HD2	1.66	0.43
1:A:4036:LYS:HZ2	1:A:4038:ASN:H	1.65	0.43
1:A:4055:VAL:HG11	1:A:4095:MET:HE2	2.00	0.43
1:A:4110:GLU:HB3	1:A:4111:LYS:NZ	2.34	0.43
1:A:3057:GLN:NE2	1:A:3060:ARG:HH21	2.11	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3638:VAL:HG12	1:A:3681:THR:HB	2.00	0.43
1:A:1701:TRP:O	1:A:1705:VAL:HG23	2.18	0.43
1:A:1850:GLN:HE21	1:A:1855:GLN:NE2	2.17	0.43
1:A:2135:GLU:HG2	1:A:2168:VAL:HG23	2.00	0.43
1:A:2603:MET:HA	1:A:2606:PHE:HB2	2.01	0.43
1:A:2957:SER:O	1:A:2991:ALA:N	2.48	0.43
1:A:3614:PHE:CE2	1:A:3641:TYR:HA	2.54	0.43
1:A:4097:LYS:HA	1:A:4127:THR:HG22	2.01	0.43
1:A:4194:LEU:HD22	1:A:4201:TRP:NE1	2.33	0.43
1:A:4287:LYS:HE3	1:A:4287:LYS:HB2	1.66	0.43
1:A:4577:LEU:HD23	1:A:4577:LEU:HA	1.87	0.43
1:A:1826:ILE:O	1:A:1829:LYS:HD2	2.19	0.43
1:A:2135:GLU:HG2	1:A:2168:VAL:CG2	2.49	0.43
1:A:4413:PHE:HD2	1:A:4504:LEU:HD21	1.83	0.43
1:A:2071:PRO:O	1:A:2075:LEU:HG	2.18	0.43
1:A:2460:SER:HB2	1:A:2589:LYS:HZ2	1.84	0.43
1:A:2512:ALA:O	1:A:2516:GLU:HG3	2.18	0.43
1:A:3730:ASP:C	1:A:3733:LYS:H	2.27	0.43
1:A:3756:VAL:O	1:A:3759:ARG:HG2	2.18	0.43
1:A:1816:VAL:HA	1:A:1819:ARG:HH12	1.84	0.43
1:A:2650:LEU:HD22	1:A:2692:PHE:HE2	1.84	0.43
1:A:2685:GLN:NE2	1:A:2692:PHE:HA	2.34	0.43
1:A:4485:ARG:HA	1:A:4488:GLN:OE1	2.18	0.43
1:A:2373:MET:SD	3:A:4702:ATP:C2	3.11	0.42
1:A:2778:THR:O	1:A:2782:GLU:OE1	2.36	0.42
1:A:3100:GLU:HA	1:A:3130:TYR:CE1	2.51	0.42
1:A:2679:VAL:O	1:A:2683:ILE:HD12	2.18	0.42
1:A:3973:LEU:HD13	1:A:3992:LEU:HD13	2.01	0.42
1:A:4189:ILE:HG13	1:A:4321:LEU:HB2	2.00	0.42
1:A:2823:ARG:HG3	1:A:2873:TYR:HE1	1.84	0.42
1:A:2856:LYS:HG3	1:A:2857:HIS:ND1	2.34	0.42
1:A:3506:ASP:OD1	1:A:3543:PHE:HB2	2.19	0.42
1:A:3554:SER:OG	1:A:3559:ARG:NH1	2.48	0.42
1:A:3636:GLN:HA	1:A:3680:SER:OG	2.19	0.42
1:A:3957:PHE:CZ	1:A:3961:LEU:HD13	2.54	0.42
1:A:3966:PRO:HG3	1:A:3997:ARG:NH1	2.34	0.42
1:A:1861:MET:HE2	1:A:1890:LEU:HB2	2.01	0.42
1:A:2768:PRO:HB2	1:A:2858:PHE:CE1	2.54	0.42
1:A:3487:GLU:O	1:A:3491:LYS:HG2	2.18	0.42
1:A:3544:ARG:NH1	1:A:3544:ARG:HB3	2.33	0.42
1:A:2375:PHE:CD2	1:A:2427:PHE:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2386:PRO:HG3	1:A:2413:LEU:HD13	2.02	0.42
1:A:1880:VAL:CG2	1:A:2049:ILE:HG12	2.50	0.42
1:A:2074:LYS:HA	1:A:2074:LYS:HD2	1.81	0.42
1:A:2154:ILE:HB	1:A:2155:PRO:HD3	2.01	0.42
1:A:2614:ASP:HA	1:A:2657:LYS:NZ	2.33	0.42
1:A:2735:TYR:CE2	1:A:2737:ASP:HB3	2.55	0.42
1:A:2837:LEU:HD13	1:A:2842:GLU:HB3	2.02	0.42
1:A:3612:THR:O	1:A:3635:VAL:HA	2.19	0.42
1:A:3641:TYR:CD2	1:A:3692:LEU:HD21	2.55	0.42
1:A:4107:MET:HE3	1:A:4107:MET:HB3	1.95	0.42
1:A:1910:THR:N	2:A:4701:ADP:O2B	2.51	0.42
1:A:2420:ALA:HA	1:A:2423:MET:HG2	2.02	0.42
1:A:2507:ARG:O	1:A:2511:ARG:HG3	2.19	0.42
1:A:3191:ARG:NH1	1:A:3500:MET:HE1	2.35	0.42
1:A:4241:SER:HA	1:A:4244:LYS:HE3	2.00	0.42
1:A:1802:PRO:O	1:A:1805:ARG:HB3	2.19	0.42
1:A:2220:LEU:HD12	1:A:2342:MET:HG3	2.00	0.42
1:A:2595:GLY:HA3	1:A:2736:VAL:O	2.20	0.42
1:A:2748:TYR:CZ	1:A:2799:MET:HB3	2.55	0.42
1:A:4017:PHE:HB3	1:A:4018:MET:HE2	2.02	0.42
1:A:1923:LEU:HD12	1:A:1954:TRP:CH2	2.55	0.42
1:A:1965:GLU:OE1	1:A:1965:GLU:N	2.52	0.42
1:A:2242:GLU:HG3	1:A:2248:GLU:HA	2.01	0.42
1:A:2831:ARG:HD3	1:A:2921:ARG:HG2	2.02	0.42
1:A:2960:GLN:HA	1:A:2993:ILE:O	2.19	0.42
1:A:3895:THR:HB	1:A:3898:GLU:OE2	2.19	0.42
1:A:4296:MET:HE2	1:A:4296:MET:HA	2.01	0.42
1:A:1818:GLN:HA	1:A:1821:VAL:HG12	2.01	0.42
1:A:1946:VAL:HG22	1:A:1950:GLN:HE22	1.85	0.42
1:A:2157:LEU:HD12	1:A:2157:LEU:HA	1.83	0.42
1:A:2254:ILE:HG23	1:A:2279:LEU:HD23	2.01	0.42
1:A:2789:GLN:OE1	1:A:2790:PRO:HD2	2.20	0.42
1:A:2910:VAL:HG21	1:A:3105:VAL:HG22	2.02	0.42
1:A:2929:PRO:O	1:A:2930:GLN:HG3	2.20	0.42
1:A:3563:GLN:OE1	1:A:3567:LEU:HD23	2.19	0.42
1:A:3781:THR:O	1:A:3785:GLU:HG2	2.19	0.42
1:A:3907:HIS:CG	1:A:3941:LEU:HD11	2.55	0.42
1:A:4313:PRO:HB2	1:A:4315:THR:HG22	2.01	0.42
1:A:1628:ARG:O	1:A:1631:PHE:HD2	2.03	0.41
1:A:1843:ARG:NH2	1:A:1860:GLN:HG2	2.35	0.41
1:A:2387:LEU:HD22	1:A:2467:ARG:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2465:ALA:HB2	1:A:2493:TYR:CE1	2.55	0.41
1:A:2739:PRO:HD2	1:A:2796:PRO:HG3	2.02	0.41
1:A:2964:HIS:CD2	1:A:2966:LYS:HB3	2.55	0.41
1:A:3731:LEU:HD12	1:A:3790:VAL:HG21	2.02	0.41
1:A:4178:ARG:NH1	1:A:4278:PHE:HA	2.34	0.41
1:A:2932:HIS:ND1	1:A:3064:VAL:HG12	2.35	0.41
1:A:3109:PHE:HB3	1:A:3180:ILE:HG21	2.02	0.41
1:A:3495:THR:HG23	1:A:3496:PHE:CD1	2.55	0.41
1:A:3888:ALA:O	1:A:4012:ASN:ND2	2.52	0.41
1:A:4507:ILE:HD12	1:A:4507:ILE:HA	1.92	0.41
2:A:4703:ADP:N3	2:A:4703:ADP:H2'	2.35	0.41
1:A:2518:ILE:HA	1:A:2521:ILE:HG12	2.01	0.41
1:A:3005:LEU:HD23	1:A:3009:ASN:HD21	1.86	0.41
1:A:3814:THR:O	1:A:3818:LEU:HD23	2.20	0.41
1:A:4069:ILE:O	1:A:4096:LEU:HA	2.21	0.41
1:A:1632:VAL:HG12	1:A:1656:LYS:HD2	2.01	0.41
1:A:2671:MET:SD	1:A:2677:GLN:HG3	2.61	0.41
1:A:2959:TYR:N	1:A:2991:ALA:O	2.53	0.41
1:A:3101:ALA:O	1:A:3105:VAL:HG23	2.19	0.41
1:A:3649:LEU:HB2	1:A:3695:ARG:HE	1.86	0.41
1:A:3824:LEU:HA	1:A:4139:LEU:HD13	2.03	0.41
1:A:3931:GLN:O	1:A:3935:VAL:HG23	2.20	0.41
1:A:4027:LEU:HD22	1:A:4058:LEU:HD22	2.02	0.41
1:A:4288:VAL:HB	1:A:4320:TRP:CD1	2.54	0.41
1:A:4391:ILE:HD11	1:A:4479:VAL:HG13	2.01	0.41
1:A:2316:ASN:HB2	1:A:2358:ARG:CZ	2.51	0.41
1:A:2584:TRP:HB3	1:A:2591:LEU:HD23	2.02	0.41
1:A:3096:ASP:OD1	1:A:3097:TRP:N	2.54	0.41
1:A:3164:ARG:HH21	1:A:4374:PRO:N	2.18	0.41
1:A:3208:ILE:O	1:A:3212:VAL:HG23	2.20	0.41
1:A:4222:TRP:CZ3	1:A:4242:ALA:HB1	2.56	0.41
1:A:4264:LEU:HD12	1:A:4264:LEU:HA	1.82	0.41
1:A:1801:PRO:HA	1:A:1802:PRO:HD3	1.96	0.41
1:A:2431:GLY:O	1:A:2435:LYS:HE2	2.21	0.41
1:A:2538:GLU:HB3	1:A:2548:TRP:CE2	2.55	0.41
1:A:3014:ASN:ND2	1:A:3016:GLU:OE2	2.54	0.41
1:A:3683:ASP:HB3	1:A:3686:VAL:HB	2.01	0.41
1:A:3893:LYS:HD2	1:A:3893:LYS:HA	1.79	0.41
1:A:4038:ASN:HA	1:A:4118:PRO:HG3	2.02	0.41
1:A:4131:ASN:OD1	1:A:4134:VAL:HG23	2.21	0.41
1:A:2677:GLN:O	1:A:2680:ILE:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3518:GLY:HA3	1:A:3579:MET:HE1	2.03	0.41
1:A:3865:GLN:HE22	1:A:4017:PHE:HA	1.85	0.41
1:A:3881:ILE:HD13	1:A:4006:HIS:CD2	2.55	0.41
1:A:3966:PRO:HD2	1:A:4000:ARG:HG3	2.02	0.41
1:A:1637:LEU:O	1:A:1641:ILE:HG12	2.21	0.41
1:A:1691:SER:OG	1:A:1694:GLU:OE1	2.36	0.41
1:A:1755:GLN:HG2	1:A:1814:GLU:OE2	2.21	0.41
1:A:1792:LEU:HD22	1:A:1808:LEU:HD22	2.03	0.41
1:A:1914:GLU:CD	2:A:4701:ADP:H3'	2.45	0.41
1:A:1975:VAL:O	1:A:1978:ILE:HG22	2.21	0.41
1:A:2211:TYR:O	1:A:2215:GLN:HG2	2.20	0.41
1:A:2578:GLU:OE2	1:A:2608:ALA:HA	2.21	0.41
1:A:4187:HIS:ND1	1:A:4212:LEU:HD13	2.35	0.41
1:A:4455:LEU:HD21	1:A:4464:TRP:CH2	2.56	0.41
1:A:4607:LEU:HB2	1:A:4622:VAL:HG23	2.02	0.41
1:A:1682:GLU:HB2	1:A:1803:LEU:HD21	2.03	0.41
1:A:1782:LEU:O	1:A:1786:GLU:HG2	2.21	0.41
1:A:1797:LEU:HD21	1:A:2128:ALA:HB2	2.03	0.41
1:A:2383:ARG:NH2	1:A:2424:GLN:OE1	2.48	0.41
1:A:2605:LEU:HD11	1:A:2709:VAL:CG1	2.50	0.41
1:A:2703:LEU:HD12	1:A:2706:ILE:HD12	2.03	0.41
1:A:2827:HIS:O	1:A:2831:ARG:HG2	2.20	0.41
1:A:2838:VAL:HG12	1:A:3093:TRP:CD1	2.55	0.41
1:A:3503:ILE:HG13	1:A:3552:TYR:OH	2.20	0.41
1:A:3733:LYS:HA	1:A:3733:LYS:HD3	1.87	0.41
1:A:3786:GLU:O	1:A:3790:VAL:HG23	2.21	0.41
1:A:3824:LEU:HD11	1:A:4044:CYS:SG	2.60	0.41
1:A:3898:GLU:OE1	1:A:3898:GLU:N	2.41	0.41
1:A:4543:VAL:HG11	1:A:4624:PHE:CZ	2.56	0.41
1:A:4607:LEU:HD23	1:A:4607:LEU:HA	1.87	0.41
1:A:1904:PRO:HA	1:A:2039:LEU:HB2	2.03	0.41
1:A:2259:ILE:HG12	1:A:2263:HIS:HB2	2.03	0.41
1:A:2628:PRO:HG3	1:A:2679:VAL:HA	2.02	0.41
1:A:2956:LEU:CD2	1:A:2989:LYS:HB3	2.51	0.41
1:A:4194:LEU:HD21	1:A:4207:PHE:CD2	2.48	0.41
1:A:1746:GLN:O	1:A:1750:VAL:HG22	2.20	0.40
1:A:1916:VAL:HG11	1:A:1956:CYS:HB2	2.03	0.40
1:A:2492:ARG:NH2	1:A:2525:PRO:HB2	2.35	0.40
1:A:2504:GLY:O	1:A:2735:TYR:N	2.54	0.40
1:A:2616:GLU:O	1:A:2660:VAL:HG22	2.20	0.40
1:A:3913:GLU:OE1	1:A:3913:GLU:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4194:LEU:HD22	1:A:4201:TRP:HE1	1.86	0.40
1:A:1735:PRO:O	1:A:1739:ILE:HD12	2.21	0.40
1:A:2114:GLU:O	1:A:2118:ARG:HG2	2.21	0.40
1:A:2687:VAL:HG13	1:A:2730:HIS:ND1	2.36	0.40
1:A:2847:ASP:HA	1:A:2850:ILE:HG22	2.02	0.40
1:A:3044:LEU:HB3	1:A:3049:GLU:CG	2.51	0.40
1:A:4109:LEU:O	1:A:4112:LYS:HG2	2.21	0.40
1:A:4318:PRO:HA	1:A:4321:LEU:CD2	2.51	0.40
1:A:2114:GLU:OE2	1:A:2118:ARG:NH2	2.46	0.40
1:A:2238:LEU:HD11	1:A:2249:GLY:HA3	2.03	0.40
1:A:2269:ASP:CB	1:A:2274:GLU:HG3	2.47	0.40
1:A:2282:HIS:O	1:A:2286:LYS:HG2	2.21	0.40
1:A:2778:THR:O	1:A:2781:GLN:HB2	2.20	0.40
1:A:2976:LEU:HD23	1:A:2976:LEU:HA	1.89	0.40
1:A:3207:LYS:O	1:A:3211:THR:HG23	2.21	0.40
1:A:3690:PRO:HA	1:A:3693:CYS:SG	2.61	0.40
1:A:4553:LEU:HD23	1:A:4553:LEU:H	1.86	0.40
1:A:1904:PRO:O	1:A:1912:LYS:HD2	2.21	0.40
1:A:1940:ALA:HA	1:A:1943:ARG:HG2	2.03	0.40
1:A:2113:ARG:HA	1:A:2113:ARG:NE	2.37	0.40
1:A:2184:LYS:HE3	1:A:2243:ARG:HH12	1.85	0.40
1:A:2511:ARG:HD3	1:A:2535:ILE:CD1	2.51	0.40
1:A:2793:ILE:O	1:A:2793:ILE:HG13	2.21	0.40
1:A:3821:ILE:HG22	1:A:4345:LYS:HD2	2.03	0.40
1:A:3916:LEU:HD11	1:A:3937:ARG:HE	1.87	0.40
1:A:3973:LEU:HD22	1:A:3992:LEU:HD22	2.03	0.40
1:A:4180:TYR:O	1:A:4183:LEU:HG	2.20	0.40
1:A:4239:PRO:HB2	1:A:4242:ALA:HB3	2.04	0.40
1:A:1882:THR:HG22	1:A:1884:LEU:N	2.33	0.40
1:A:1886:ASP:HA	1:A:1889:TYR:HD2	1.87	0.40
1:A:2241:LEU:HB3	1:A:2298:ARG:NH2	2.36	0.40
1:A:2603:MET:HG3	1:A:2604:THR:N	2.37	0.40
1:A:2680:ILE:HD11	1:A:2727:PHE:CZ	2.57	0.40
1:A:3734:LEU:HB3	1:A:3783:LYS:HB3	2.04	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	2684/4646 (58%)	2592 (97%)	92 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	2397/4125 (58%)	2397 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1651	GLN
1	A	1790	ASN
1	A	1817	HIS
1	A	1850	GLN
1	A	1863	ASN
1	A	2003	ASN
1	A	2212	GLN
1	A	2215	GLN
1	A	2491	GLN
1	A	2730	HIS
1	A	2791	HIS

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Mol	Chain	Res	Type
1	A	3057	GLN
1	A	3158	ASN
1	A	3650	ASN
1	A	3667	GLN
1	A	3700	ASN
1	A	3714	ASN
1	A	3772	ASN
1	A	3792	GLN
1	A	3820	GLN
1	A	3852	HIS
1	A	3907	HIS
1	A	4191	GLN
1	A	4291	HIS
1	A	4466	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ATP	A	4702	-	28,33,33	0.99	2 (7%)	34,52,52	0.65	1 (2%)
2	ADP	A	4701	-	24,29,29	0.86	0	29,45,45	1.32	5 (17%)
2	ADP	A	4704	-	24,29,29	0.81	0	29,45,45	1.28	2 (6%)
2	ADP	A	4703	-	24,29,29	0.83	0	29,45,45	1.33	4 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	A	4702	-	-	5/18/38/38	0/3/3/3
2	ADP	A	4701	-	-	5/12/32/32	0/3/3/3
2	ADP	A	4704	-	-	5/12/32/32	0/3/3/3
2	ADP	A	4703	-	-	5/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	4702	ATP	PA-O3A	-2.72	1.56	1.59
3	A	4702	ATP	PB-O3B	-2.64	1.56	1.59

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4704	ADP	N3-C2-N1	-3.69	123.66	128.67
2	A	4701	ADP	N3-C2-N1	-3.35	124.12	128.67
2	A	4703	ADP	N3-C2-N1	-3.21	124.32	128.67
2	A	4703	ADP	C4'-O4'-C1'	2.90	112.58	109.92
2	A	4704	ADP	C4-C5-N7	-2.67	106.52	109.34
2	A	4703	ADP	C4-C5-N7	-2.53	106.66	109.34
2	A	4701	ADP	C4-C5-N7	-2.43	106.77	109.34
3	A	4702	ATP	C5-C6-N6	2.36	123.90	120.31
2	A	4701	ADP	C2'-C3'-C4'	2.31	107.07	102.61
2	A	4703	ADP	O4'-C1'-N9	-2.15	105.89	108.75
2	A	4701	ADP	C4'-O4'-C1'	2.12	111.87	109.92
2	A	4701	ADP	O3B-PB-O2B	2.06	115.55	107.80

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	4703	ADP	C5'-O5'-PA-O2A
2	A	4703	ADP	C5'-O5'-PA-O3A
2	A	4704	ADP	C5'-O5'-PA-O1A
2	A	4704	ADP	C5'-O5'-PA-O2A
2	A	4704	ADP	C5'-O5'-PA-O3A
2	A	4704	ADP	O4'-C4'-C5'-O5'
3	A	4702	ATP	C5'-O5'-PA-O1A
3	A	4702	ATP	C5'-O5'-PA-O2A
3	A	4702	ATP	C5'-O5'-PA-O3A
3	A	4702	ATP	O4'-C4'-C5'-O5'
2	A	4703	ADP	O4'-C4'-C5'-O5'
3	A	4702	ATP	C3'-C4'-C5'-O5'
2	A	4701	ADP	O4'-C4'-C5'-O5'
2	A	4704	ADP	C3'-C4'-C5'-O5'
2	A	4703	ADP	C3'-C4'-C5'-O5'
2	A	4701	ADP	C3'-C4'-C5'-O5'
2	A	4701	ADP	C5'-O5'-PA-O1A
2	A	4701	ADP	C5'-O5'-PA-O2A
2	A	4701	ADP	C5'-O5'-PA-O3A
2	A	4703	ADP	C4'-C5'-O5'-PA

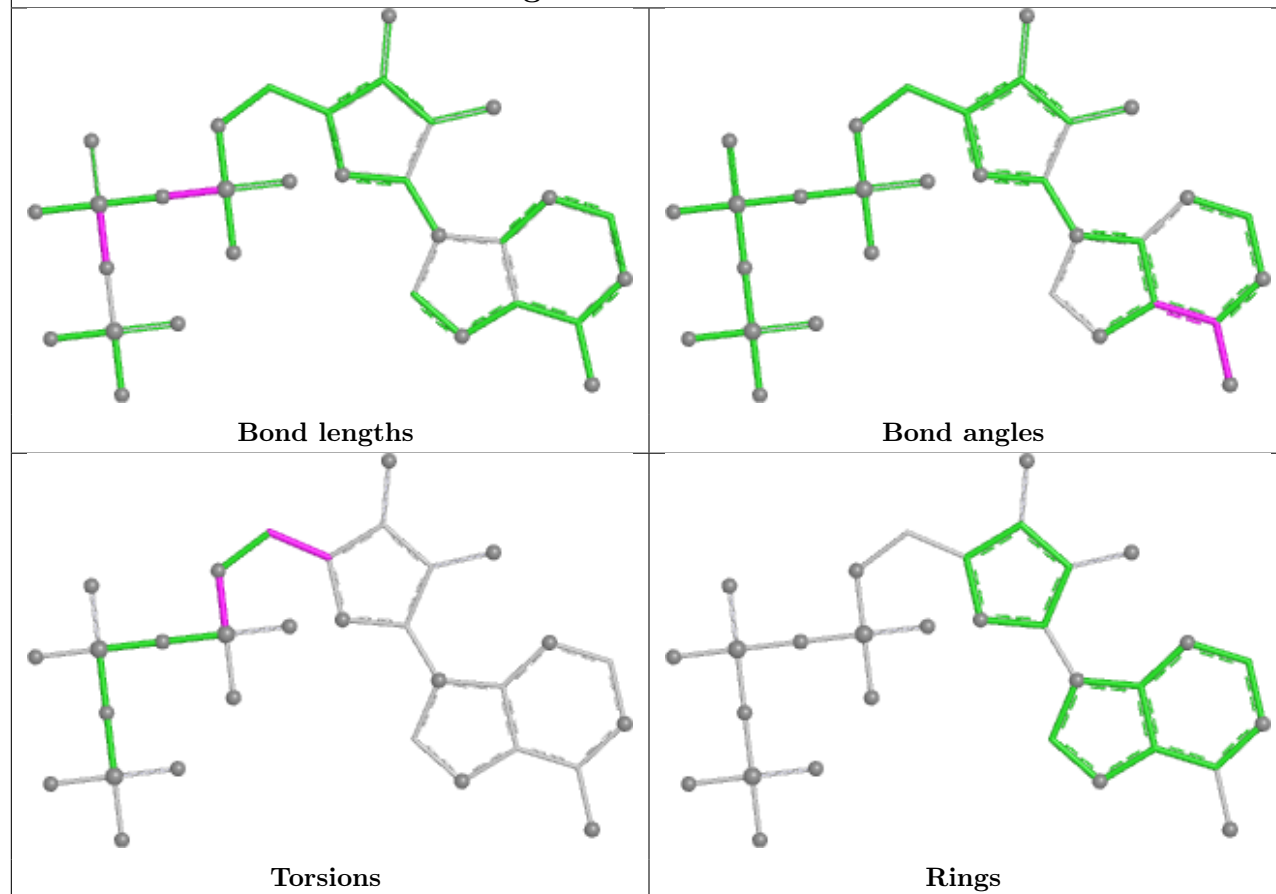
There are no ring outliers.

4 monomers are involved in 19 short contacts:

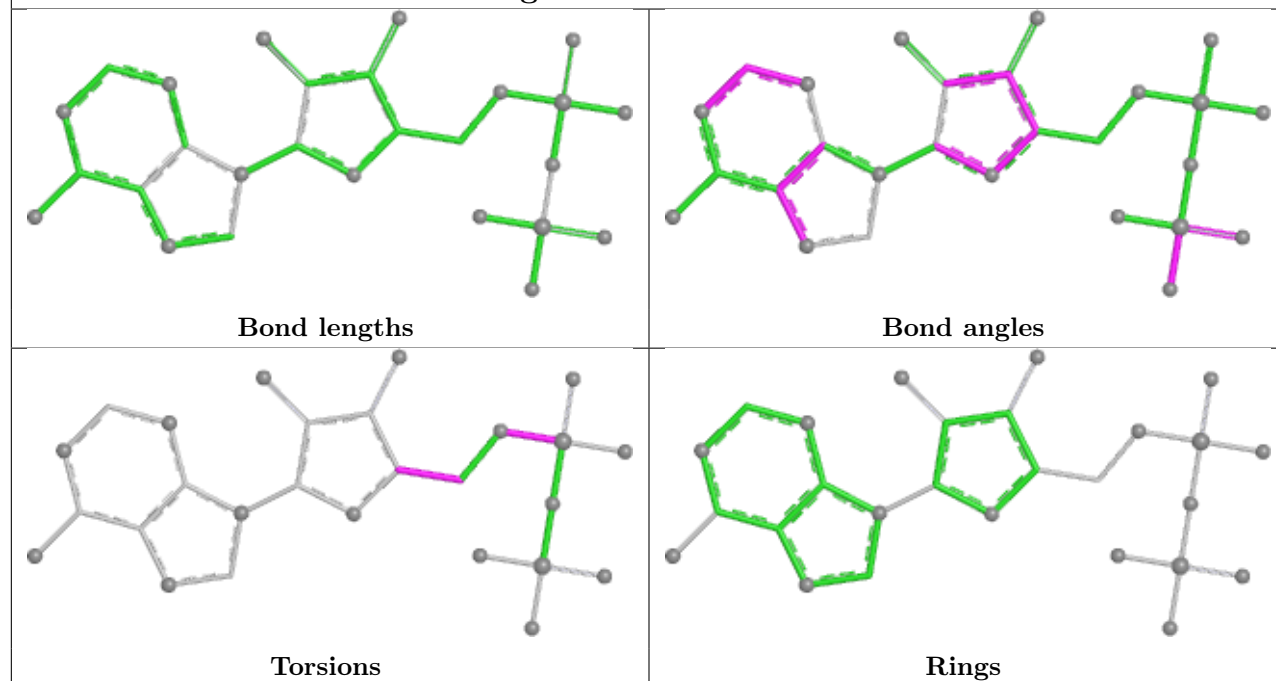
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4702	ATP	5	0
2	A	4701	ADP	6	0
2	A	4704	ADP	2	0
2	A	4703	ADP	6	0

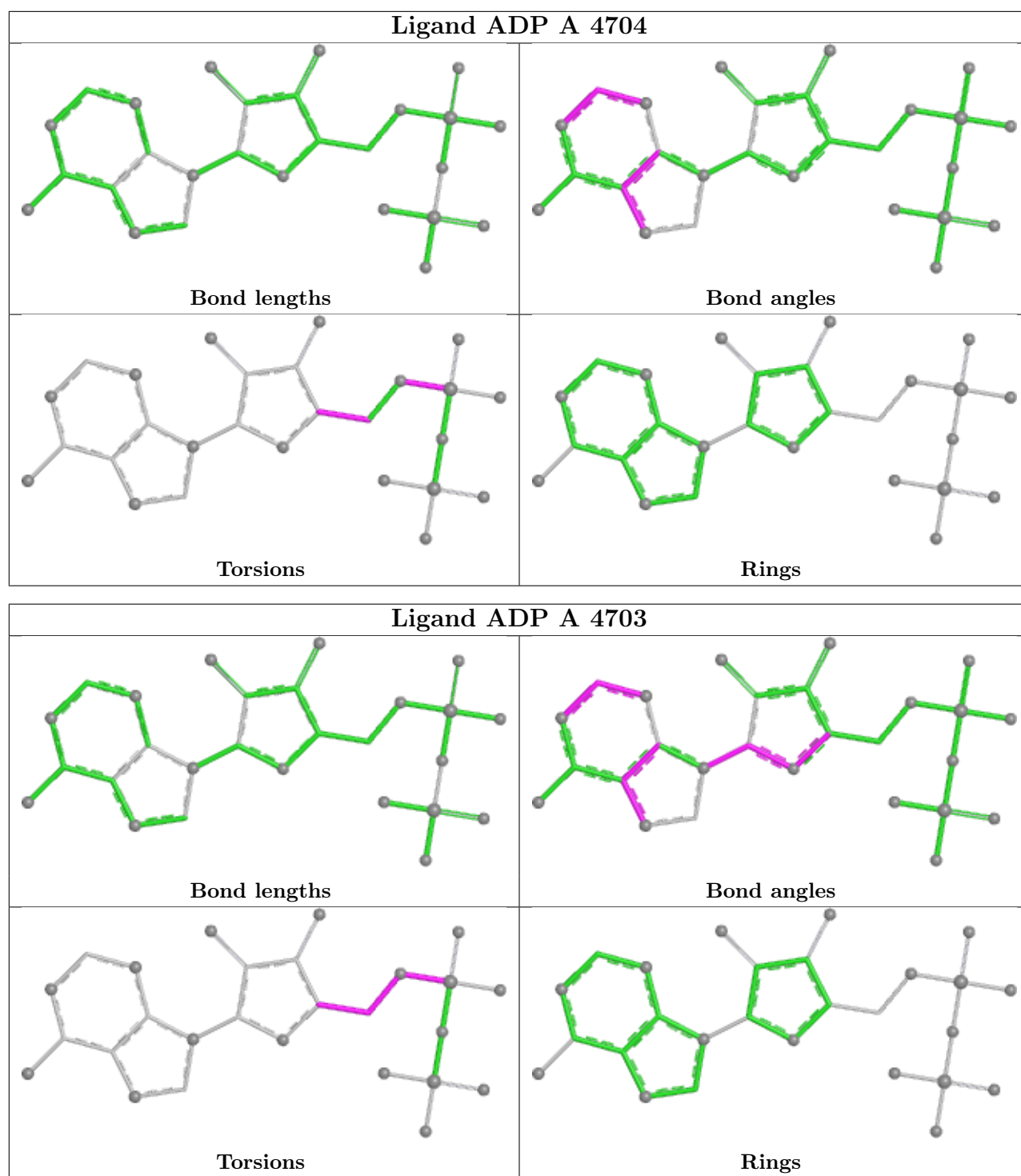
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

## Ligand ATP A 4702



## Ligand ADP A 4701





## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.



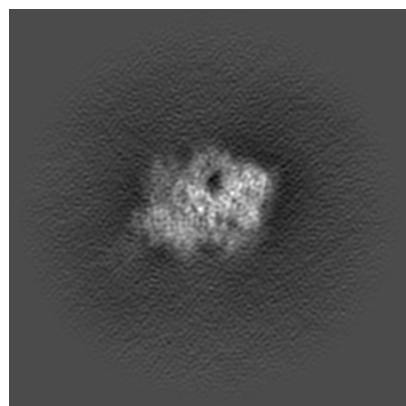
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44711. These allow visual inspection of the internal detail of the map and identification of artifacts.

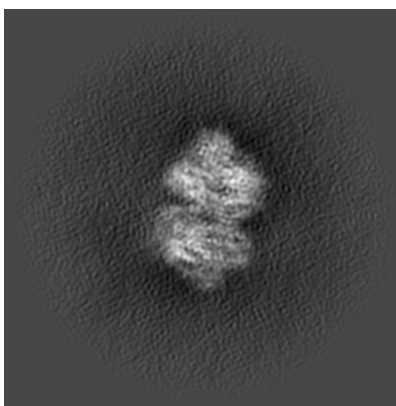
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

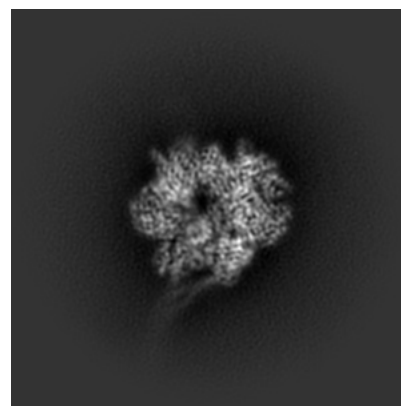
#### 6.1.1 Primary map



X

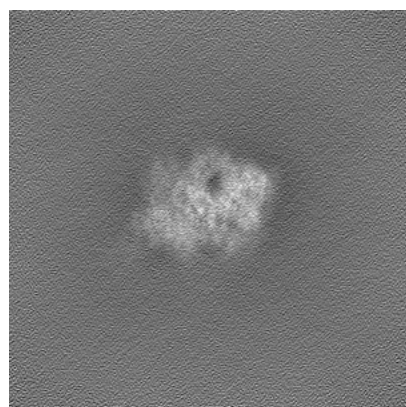


Y

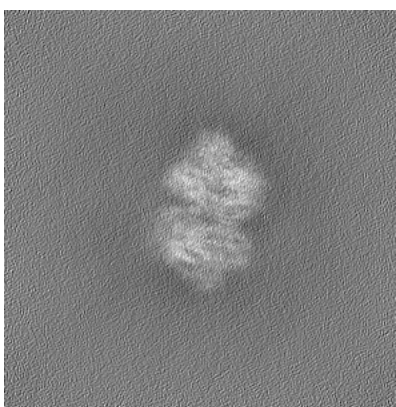


Z

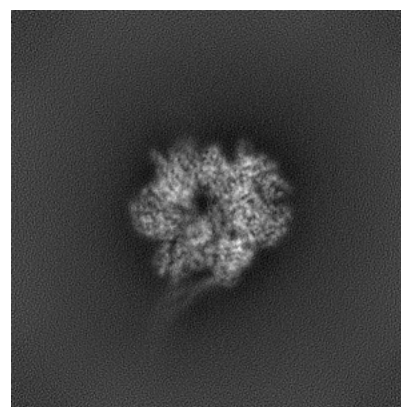
#### 6.1.2 Raw map



X



Y

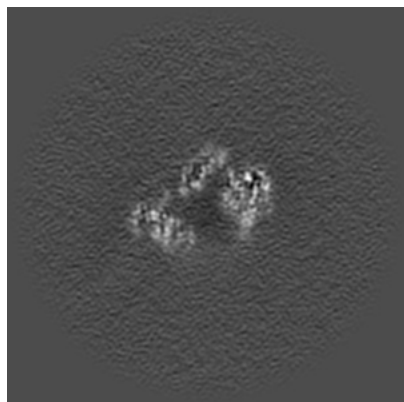


Z

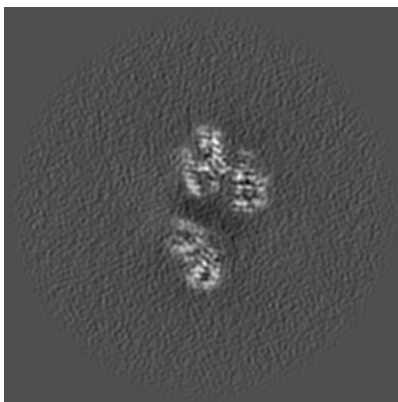
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

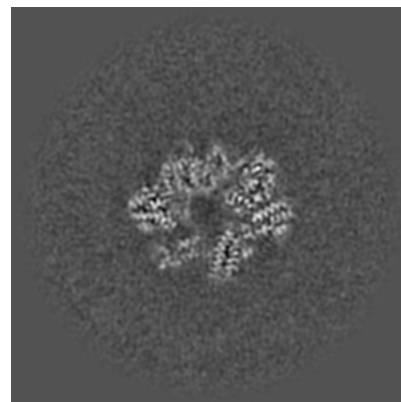
### 6.2.1 Primary map



X Index: 160

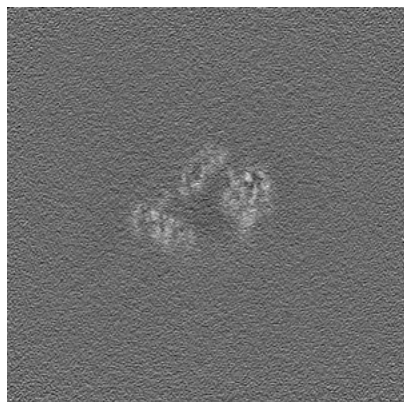


Y Index: 160

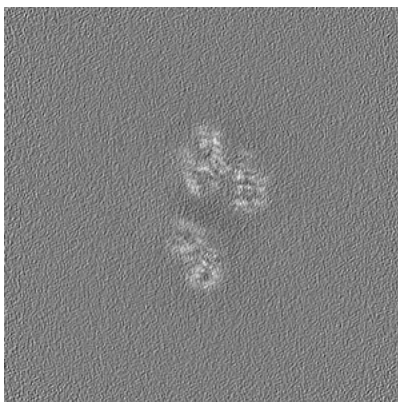


Z Index: 160

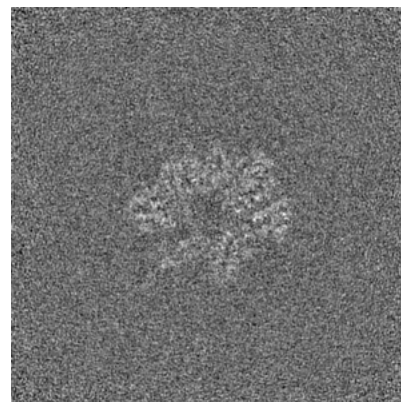
### 6.2.2 Raw map



X Index: 160



Y Index: 160

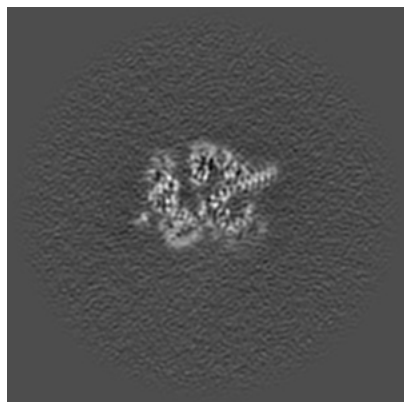


Z Index: 160

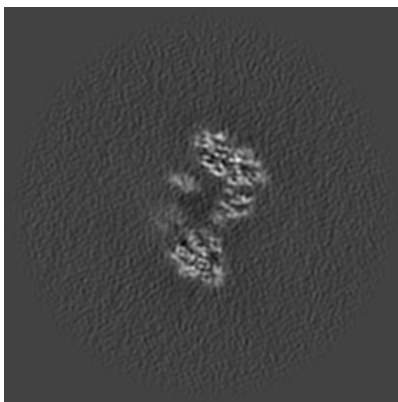
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

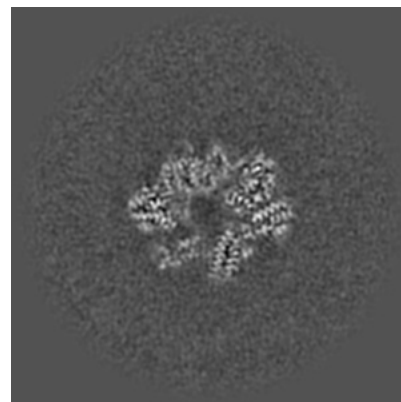
### 6.3.1 Primary map



X Index: 182

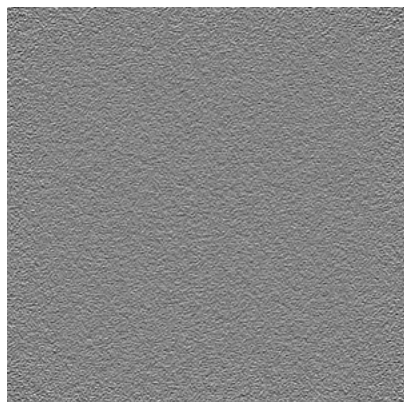


Y Index: 150

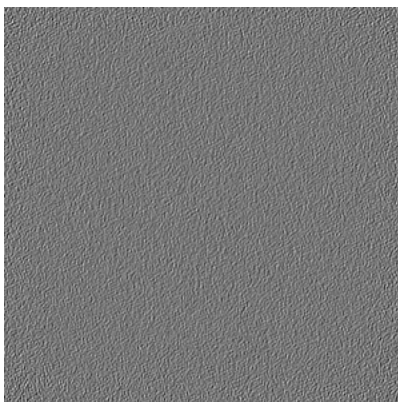


Z Index: 160

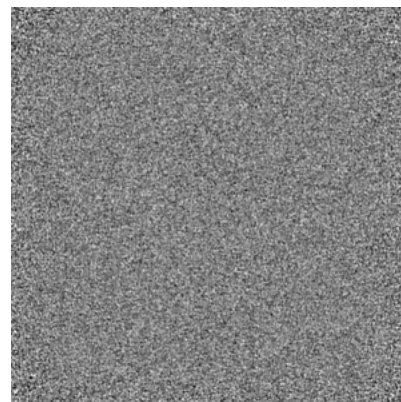
### 6.3.2 Raw map



X Index: 0



Y Index: 0



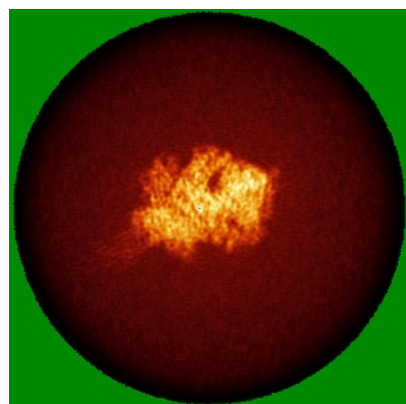
Z Index: 0

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

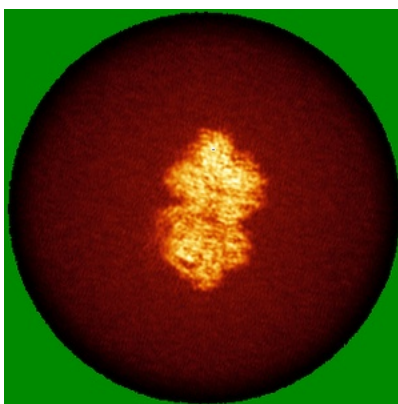


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

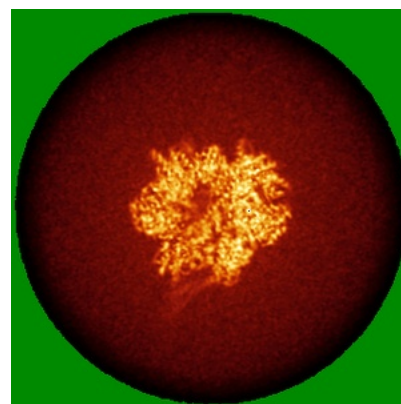
### 6.4.1 Primary map



X

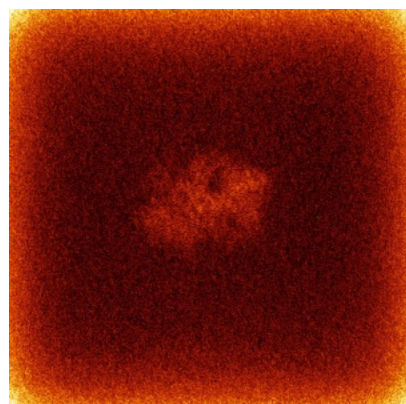


Y

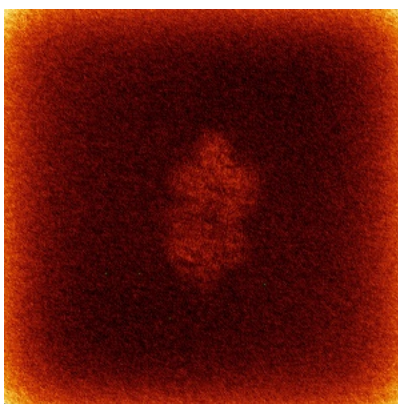


Z

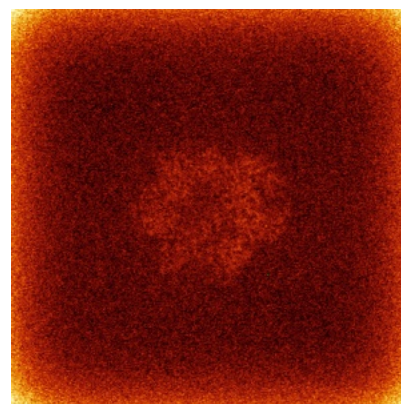
### 6.4.2 Raw map



X



Y

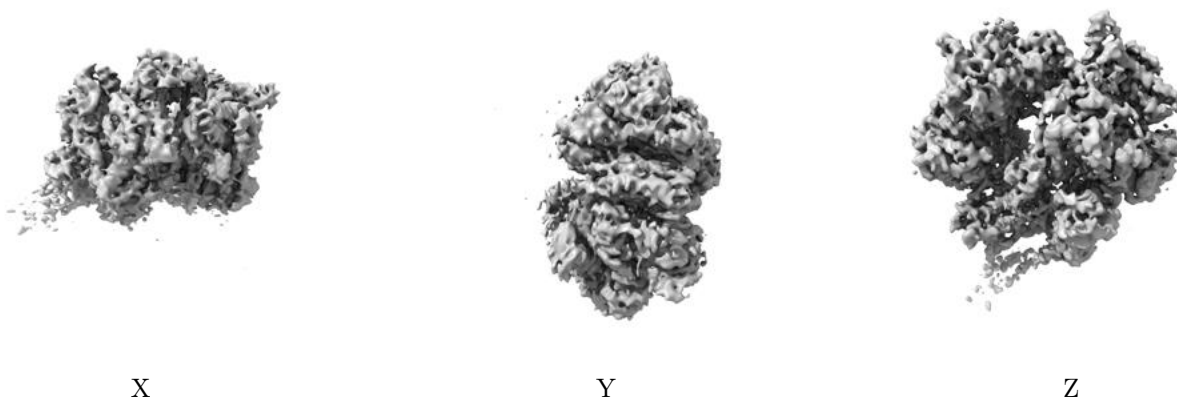


Z

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

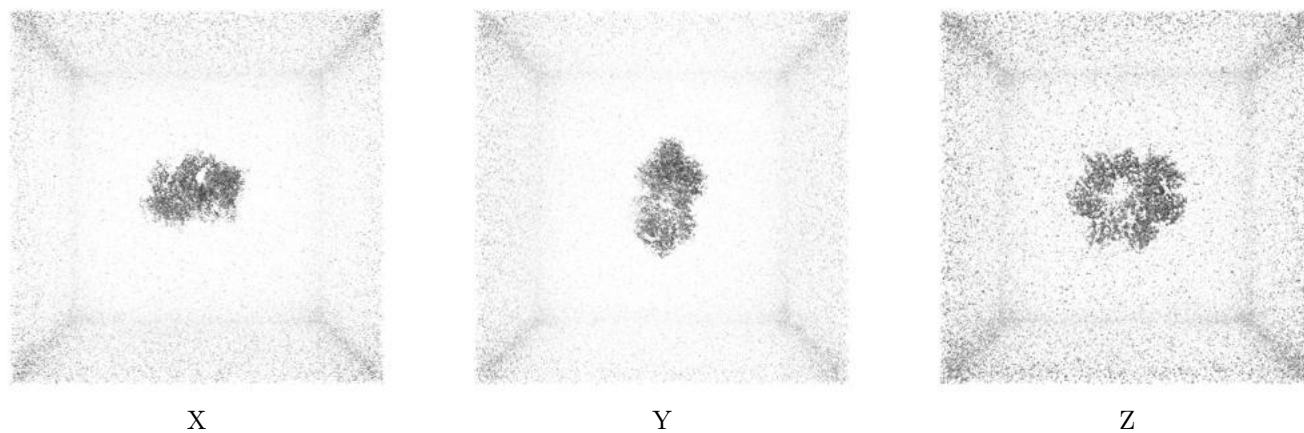
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

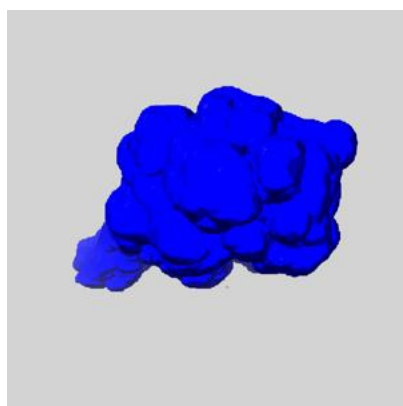
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

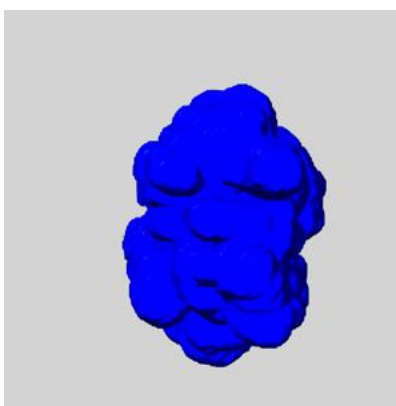
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

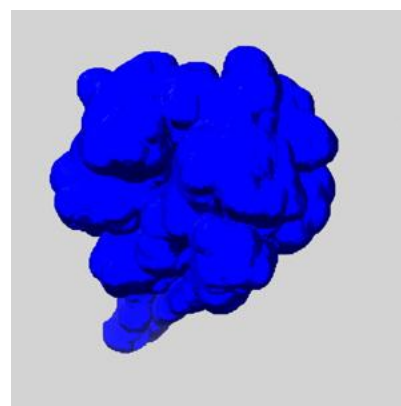
### 6.6.1 emd\_44711\_msk\_1.map [i](#)



X



Y

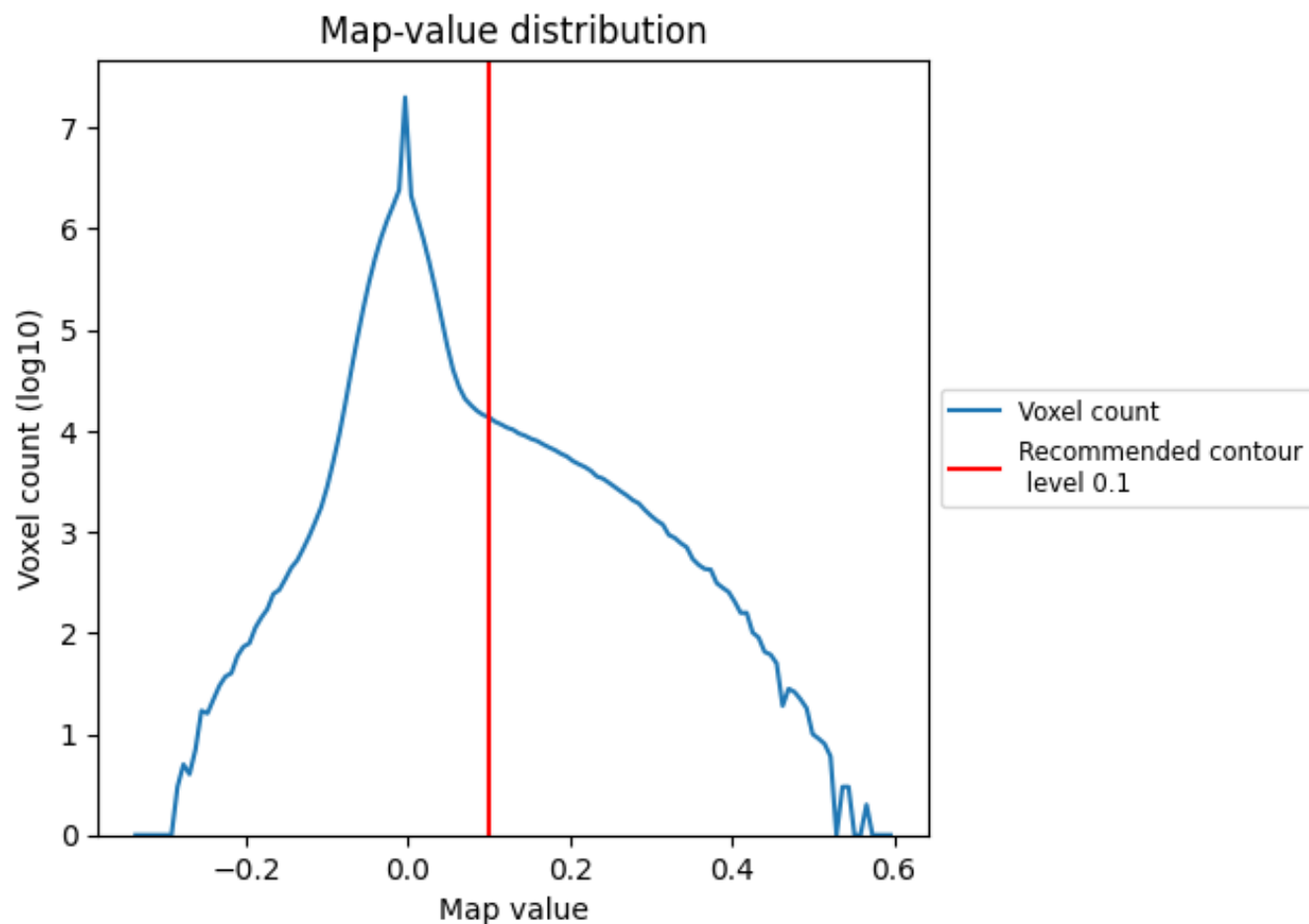


Z

## 7 Map analysis [i](#)

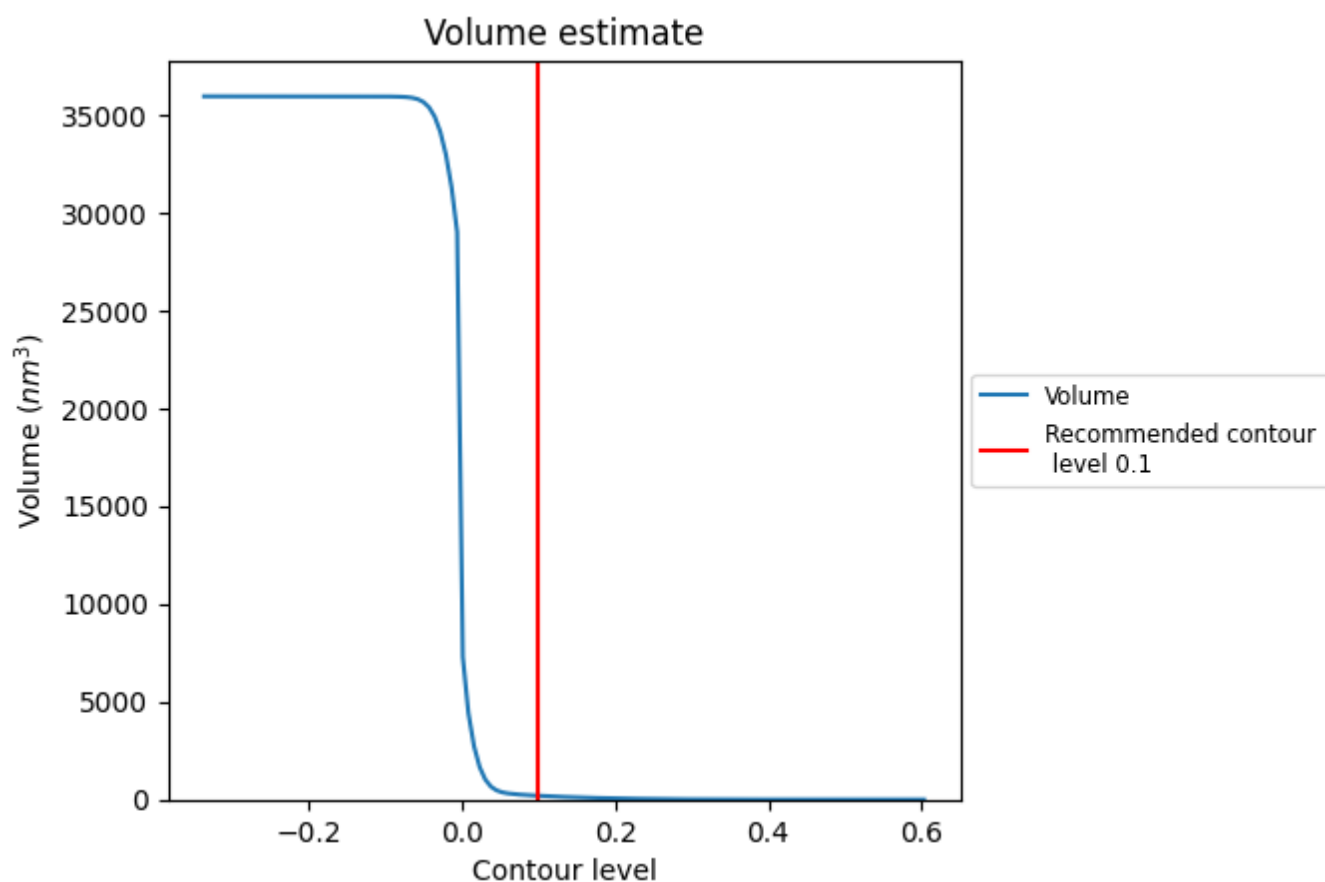
This section contains the results of statistical analysis of the map.

### 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](#)

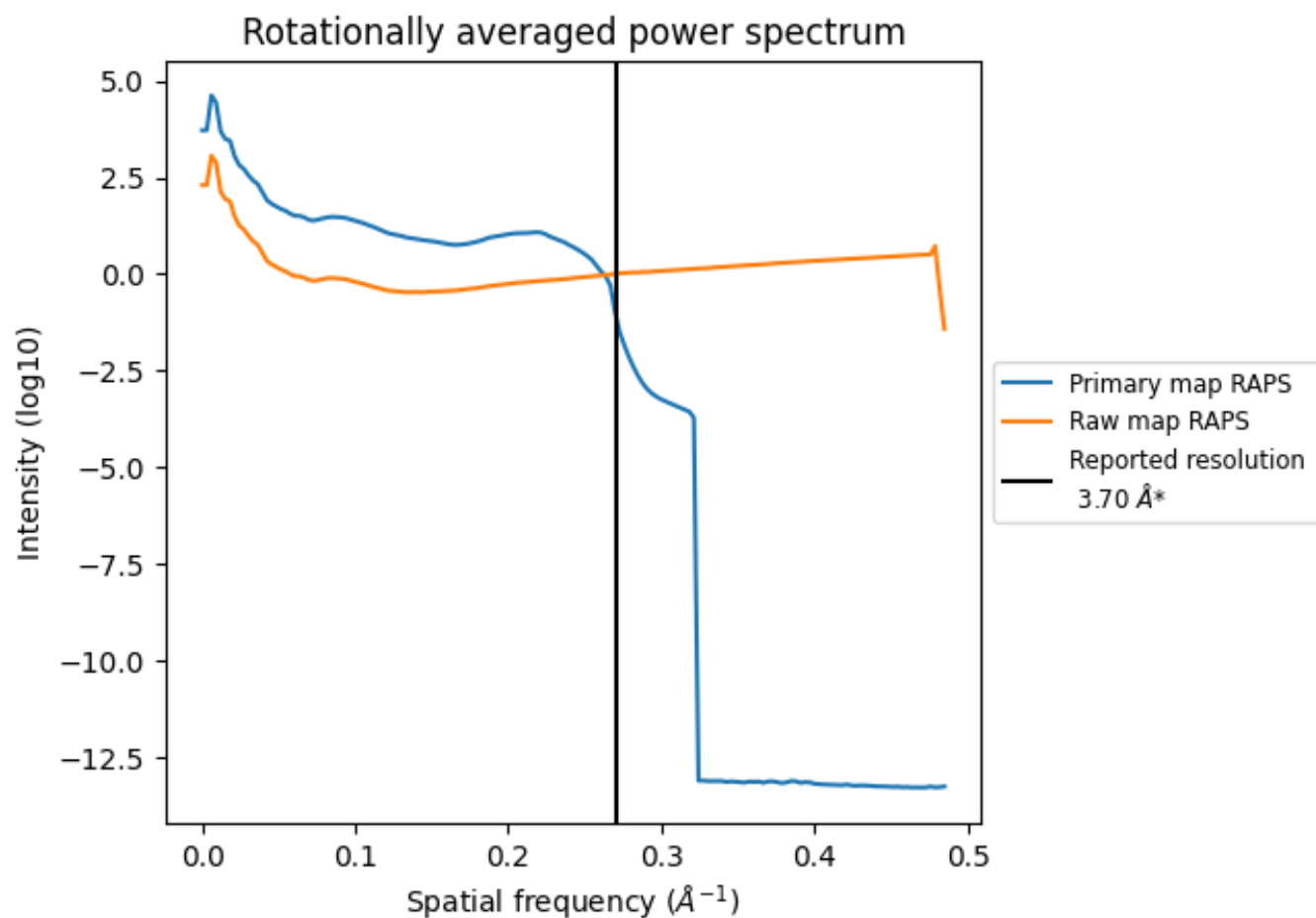


The volume at the recommended contour level is 195 nm<sup>3</sup>; this corresponds to an approximate mass of 176 kDa.

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 ⓘ

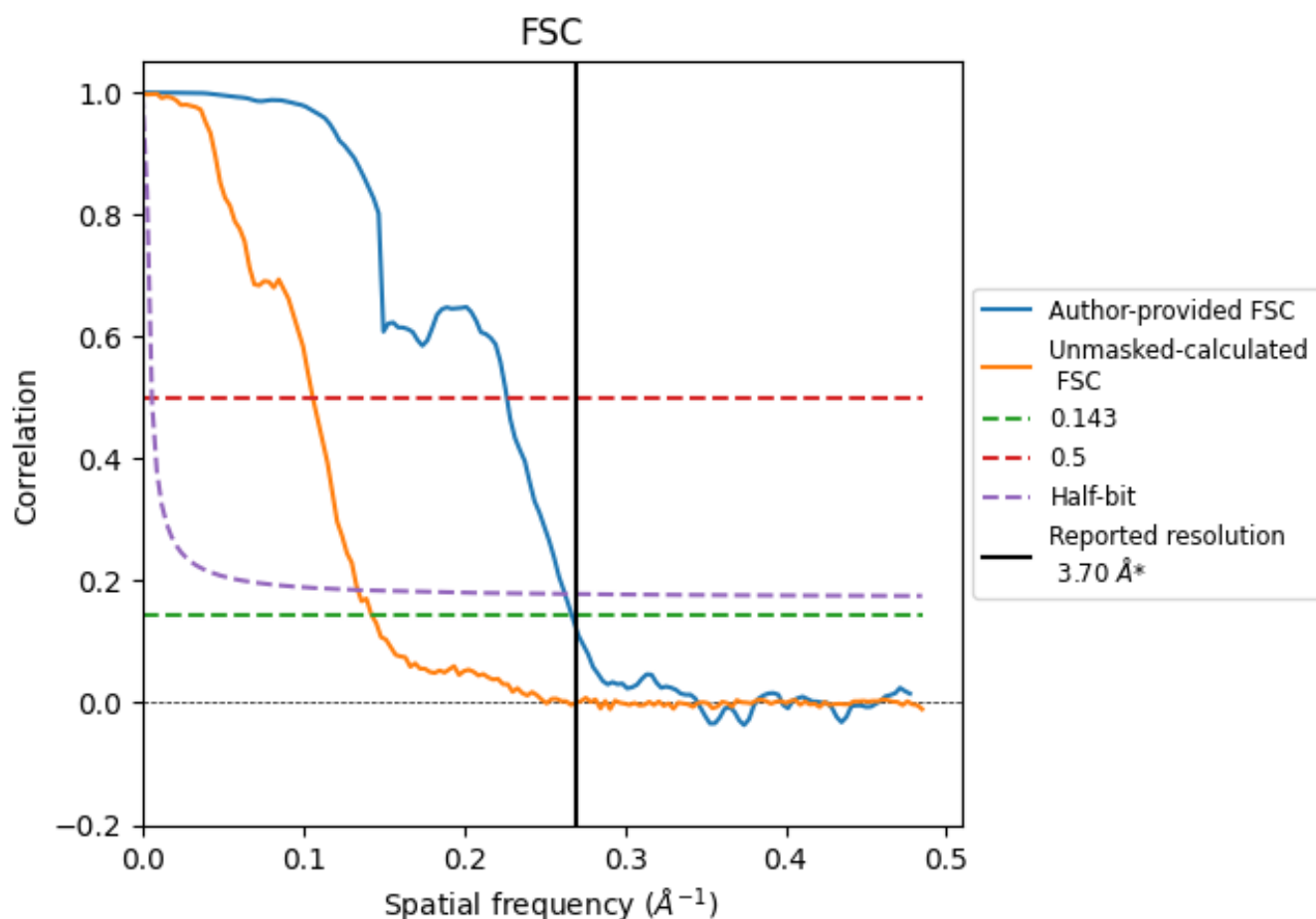


\*Reported resolution corresponds to spatial frequency of 0.270 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.270  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

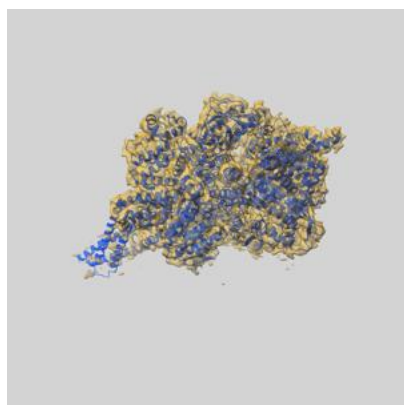
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.74	4.41	3.81
Unmasked-calculated*	7.00	9.43	7.46

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.00 differs from the reported value 3.7 by more than 10 %

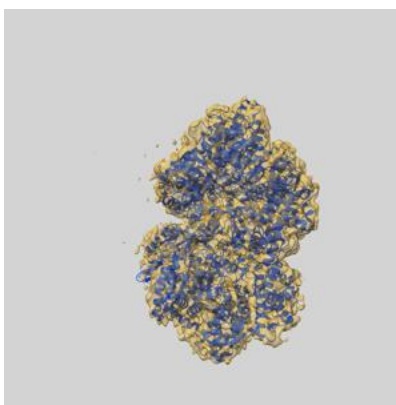
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44711 and PDB model 9BMU. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

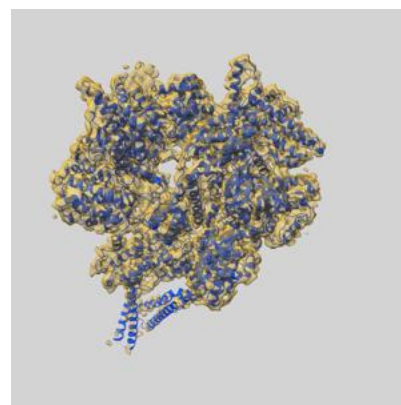
### 9.1 Map-model overlay [i](#)



X



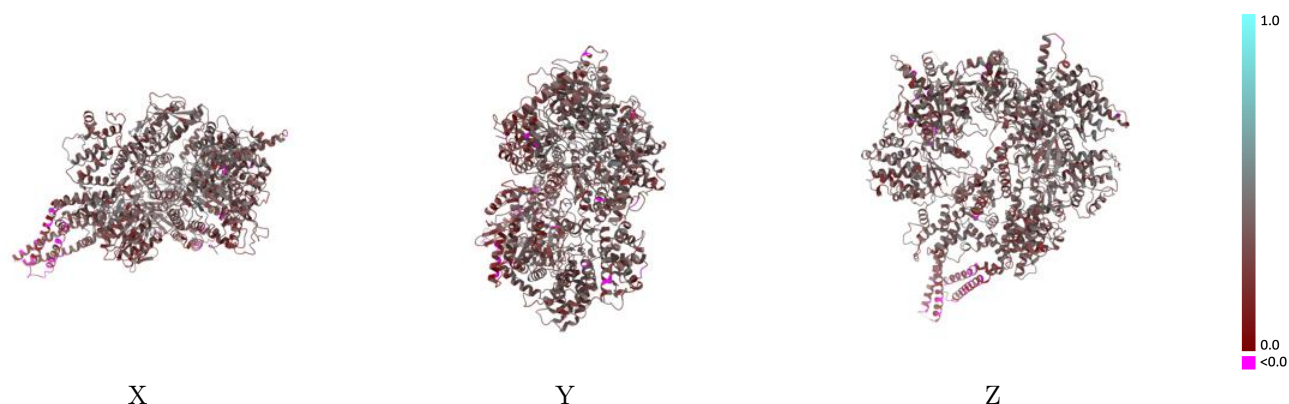
Y



Z

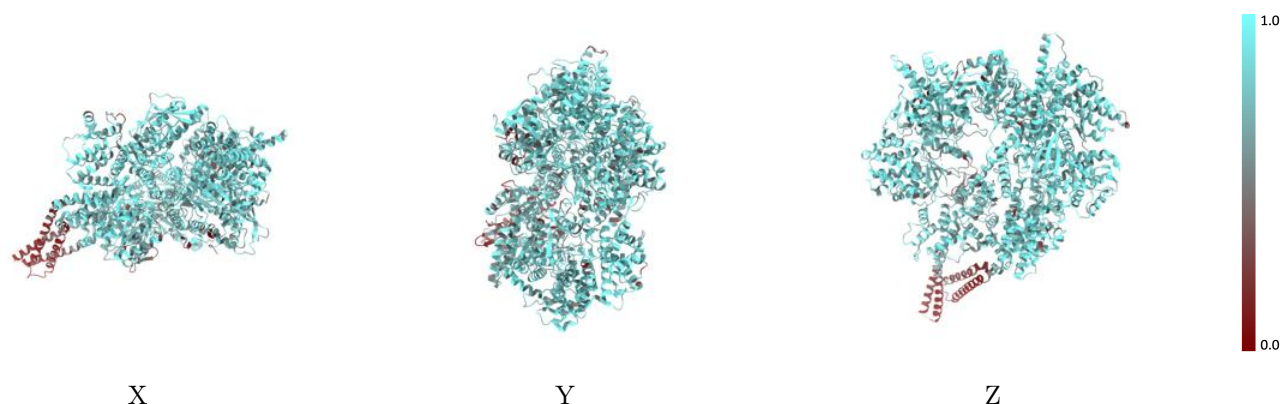
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



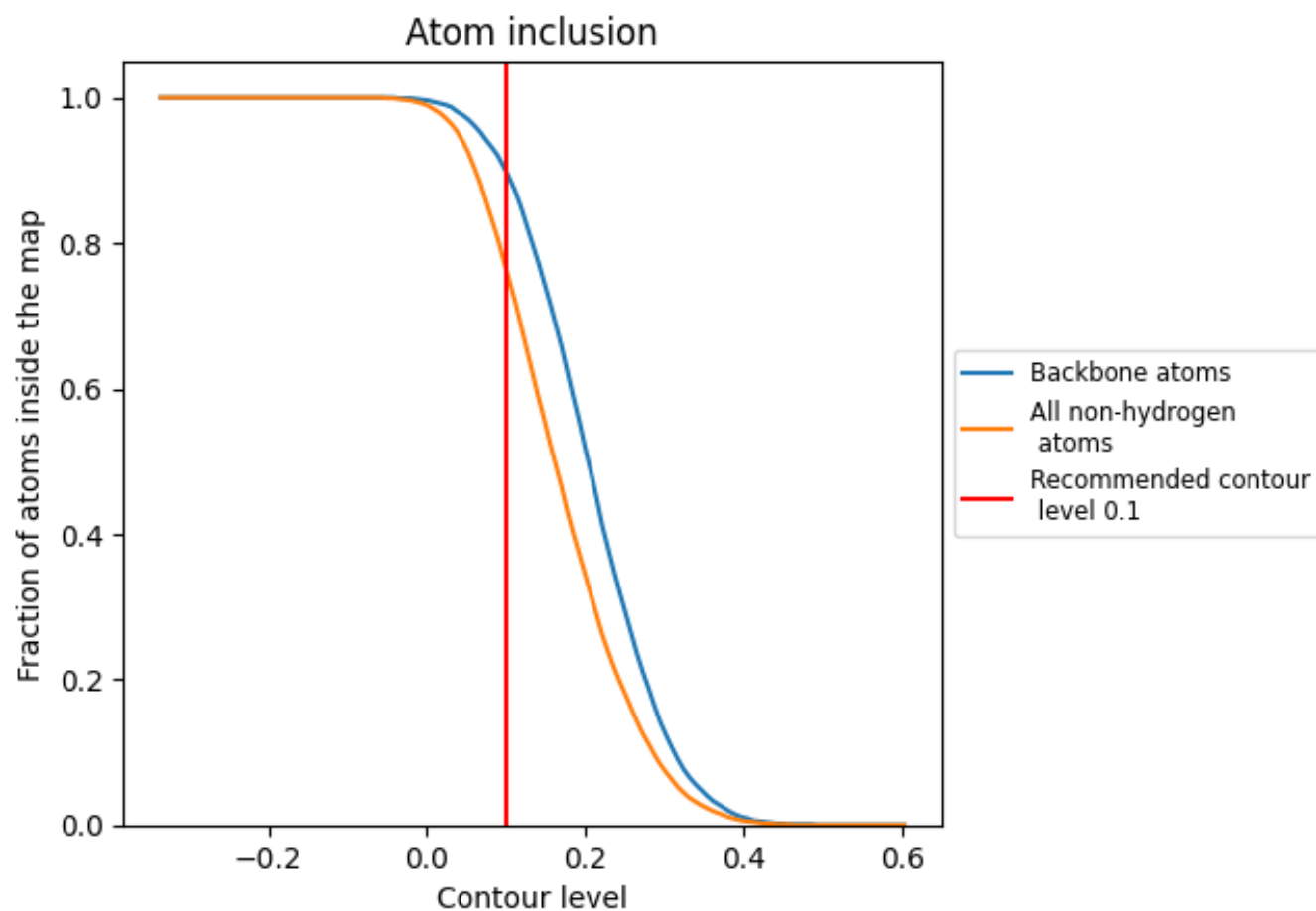
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 76% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7650	<div></div> 0.3330
A	<div></div> 0.7650	<div></div> 0.3330

