



Full wwPDB EM Validation Report ⓘ

Jun 12, 2025 – 10:18 AM EDT

PDB ID : 9NWE / pdb_00009nwe
EMDB ID : EMD-49876
Title : E3 ligase UBR4-KCMF1-calmodulin complex
Authors : Yang, Z.; Rape, M.P.
Deposited on : 2025-03-22
Resolution : 3.20 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev118
MolProbity : 4-5-2 with Phenix2.0rc1
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

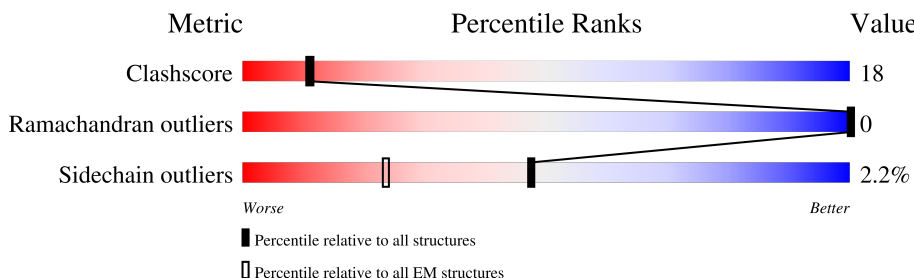
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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 ≥ 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	5205	
1	B	5205	
2	C	149	
2	D	149	
3	E	381	
3	F	381	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ZN	A	5203	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 29288 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 E3 ubiquitin-protein ligase UBR4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1660	Total	C	N	O	S	0	0
			13132	8325	2255	2465	87		
1	B	1660	Total	C	N	O	S	0	0
			13134	8325	2255	2467	87		

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP Q5T4S7
A	-20	ASP	-	expression tag	UNP Q5T4S7
A	-19	TYR	-	expression tag	UNP Q5T4S7
A	-18	LYS	-	expression tag	UNP Q5T4S7
A	-17	ASP	-	expression tag	UNP Q5T4S7
A	-16	HIS	-	expression tag	UNP Q5T4S7
A	-15	ASP	-	expression tag	UNP Q5T4S7
A	-14	GLY	-	expression tag	UNP Q5T4S7
A	-13	ASP	-	expression tag	UNP Q5T4S7
A	-12	TYR	-	expression tag	UNP Q5T4S7
A	-11	LYS	-	expression tag	UNP Q5T4S7
A	-10	ASP	-	expression tag	UNP Q5T4S7
A	-9	HIS	-	expression tag	UNP Q5T4S7
A	-8	ASP	-	expression tag	UNP Q5T4S7
A	-7	ILE	-	expression tag	UNP Q5T4S7
A	-6	ASP	-	expression tag	UNP Q5T4S7
A	-5	TYR	-	expression tag	UNP Q5T4S7
A	-4	LYS	-	expression tag	UNP Q5T4S7
A	-3	ASP	-	expression tag	UNP Q5T4S7
A	-2	ASP	-	expression tag	UNP Q5T4S7
A	-1	ASP	-	expression tag	UNP Q5T4S7
A	0	ASP	-	expression tag	UNP Q5T4S7
A	1	LYS	-	expression tag	UNP Q5T4S7
B	-21	MET	-	initiating methionine	UNP Q5T4S7
B	-20	ASP	-	expression tag	UNP Q5T4S7
B	-19	TYR	-	expression tag	UNP Q5T4S7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	LYS	-	expression tag	UNP Q5T4S7
B	-17	ASP	-	expression tag	UNP Q5T4S7
B	-16	HIS	-	expression tag	UNP Q5T4S7
B	-15	ASP	-	expression tag	UNP Q5T4S7
B	-14	GLY	-	expression tag	UNP Q5T4S7
B	-13	ASP	-	expression tag	UNP Q5T4S7
B	-12	TYR	-	expression tag	UNP Q5T4S7
B	-11	LYS	-	expression tag	UNP Q5T4S7
B	-10	ASP	-	expression tag	UNP Q5T4S7
B	-9	HIS	-	expression tag	UNP Q5T4S7
B	-8	ASP	-	expression tag	UNP Q5T4S7
B	-7	ILE	-	expression tag	UNP Q5T4S7
B	-6	ASP	-	expression tag	UNP Q5T4S7
B	-5	TYR	-	expression tag	UNP Q5T4S7
B	-4	LYS	-	expression tag	UNP Q5T4S7
B	-3	ASP	-	expression tag	UNP Q5T4S7
B	-2	ASP	-	expression tag	UNP Q5T4S7
B	-1	ASP	-	expression tag	UNP Q5T4S7
B	0	ASP	-	expression tag	UNP Q5T4S7
B	1	LYS	-	expression tag	UNP Q5T4S7

- Molecule 2 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	144	Total	C	N	O	S	0	0
			1134	696	182	247	9		
2	D	143	Total	C	N	O	S	0	0
			1127	692	181	245	9		

- Molecule 3 is a protein called E3 ubiquitin-protein ligase KCMF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	46	Total	C	N	O	S	0	0
			380	231	68	79	2		
3	F	45	Total	C	N	O	S	0	0
			371	226	67	76	2		

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

Mol	Chain	Residues	Atoms		AltConf
4	A	3	Total	Zn	0
			3	3	

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Mol	Chain	Residues	Atoms		AltConf
4	B	3	Total	Zn	0
			3	3	

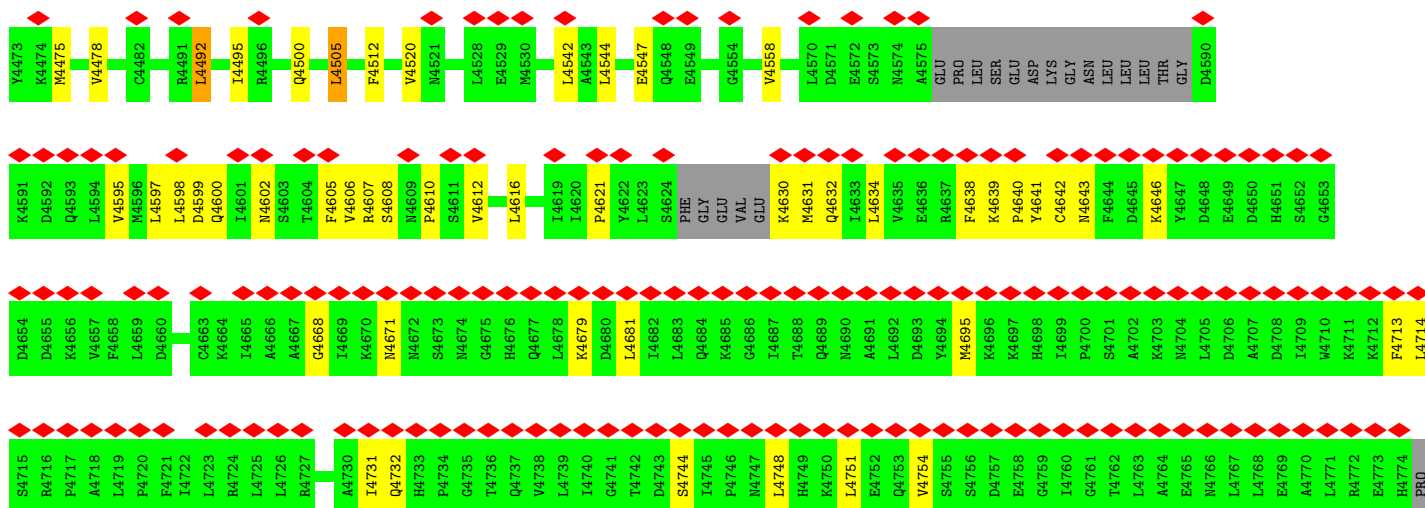
- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
5	C	2	Total	Ca	0
			2	2	
5	D	2	Total	Ca	0
			2	2	



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N4412	T4352	L4273	R4134	VAL	S3966	V3879	S3791	C3677	Q3443	SER	D3298	K3199
K4413	L4353	R4274	T4135	GLU	S3967	V3880	V3792	G3678	L3447	LYS	S3299	I3200
L4414	E4354	L4276	C4146	ALA	L3968	N3793	R3793	E3679	SER	SER	V3300	Q3201
T4415	K4355	V4277	V4149	LEU	Q3969	E3881	R3794	N3680	THR	THR	F3302	Q3202
S4416	D4356	V4278	V4155	THR	Y3970	H3882	L3799	V3681	LYS	LYS	F3303	R3207
L4417	P4357	Q4279	I4155	T4044	K3972	L3884	A3800	Y3682	S3453	SER	L3304	R3211
D4418	Q4358	R4280	T4281	P4047	L3973	L3887	Q3801	D3580	I3454	LYS	Q3305	K3212
L4419	Q4359	L4282	R4158	W4059	L3974	R3888	E3802	K3582	W3455	LYS	Q3307	L3213
P4420	E4360	L4283	K4159	W4059	L3975	R3888	Y3803	R3583	P3456	GLU	S3308	L3214
D4421	D4361	L4284	L4165	W4071	L3979	A3889	C3807	R3588	L3458	GLU	F3309	L3215
A4422	E4362	E4286	L4170	L4075	S3980	N3893	I3818	Y3692	A3459	GLU	V3311	F3216
E4423	L4363	T4287	K3981	L4076	K3981	P3894	Q3819	R3595	A3460	LYS	D3312	Q3226
V4424	Q4364	P4076	C3985	P4076	C3985	A3895	Q3819	K3605	Y3461	GLU	V3315	L3227
V4425	G4365	L4077	C3986	L4077	L3986	R3897	K3820	L3605	K3464	LYS	V3318	R3228
K4426	E4366	R4078	E3987	G4079	E3987	R3898	V3821	K3606	A3465	GLY	L3319	H3231
L4427	R4367	G4079	L3988	L4080	L3988	L3899	F3822	E3826	K3466	GLU	L3320	L3233
V4428	M4367	I4080	R3989	I4080	L3989	L3900	R3825	Y3827	V3469	THR	L3323	H3232
V4429	Q4368	D4081	R3991	G4082	L3990	V3901	K3826	K3628	D3470	SER	L3324	L3234
C4430	G4369	N4083	R3991	N4083	L3991	Q3903	E3827	L3631	K3478	GLY	C3325	L3235
T4431	M4370	G4084	L3994	G4084	L3994	G3904	L3828	L3632	L3497	GLU	C3326	L3236
T4432	P4371	K4085	F3997	K4085	F3997	L3905	L3833	L3633	S3490	THR	C3327	H3237
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E4435	S4374	T4307	M3999	A4086	L3999	I3906	R3836	L3642	V3494	GLY	C3330	K3241
E4436	S4375	A4308	V4001	A4086	L3999	I3906	R3836	L3642	V3494	GLY	C3331	L3242
E4437	M4376	L4200	V4001	A4086	L3999	I3906	R3836	L3642	V3494	GLY	C3332	E3245
P4437	P4377	A4311	V4001	A4086	L3999	I3906	R3836	L3642	V3494	GLY	C3333	L3249
M4438	G4378	C4313	V4001	A4086	L3999	I3906	R3836	L3642	V3494	GLY	C3334	F3250
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R4443	ASP	T4327	V4001	A4086	L3999	I3906	R3836	L3642	V3494	GLY	C3339	I3270
M4444	ASP	T4327	V4001	A4086	L3999	I3906	R3836	L3642	V3494	GLY	C3340	M3273
R4445	ASP	T4327	V4001	A4086	L3999	I3906	R3836	L3642	V3494	GLY	C3341	E3274
E4446	ASP	T4327	V4001	A4086	L3999	I3906	R3836	L3642	V3494	GLY	C3342	H3275
E4447	ASP	T4327	V4001	A4086	L3999	I3906	R3836	L3642	V3494	GLY	C3343	Q3285
L4448	ASP	T4327	V4001	A4086	L3999	I3906	R3836	L3642	V3494	GLY	C3344	R3286
Q4449	ASP	T4327	V4001	A4086	L3999	I3906	R3836	L3642	V3494	GLY	C3345	N3289
D4450	ASP	T4327	V4001	A4086	L3999	I3906	R3836	L3642	V3494	GLY	C3346	K3290
A4451	ASP	T4327	V4001	A4086	L3999	I3906	R3836	L3642	V3494	GLY	C3347	Q3291
T4452	ASP	T4327	V4001	A4086	L3999	I3906	R3836	L3642	V3494	GLY	C3348	K3292
E4453	ASP	T4327	V4001	A4086	L3999	I3906	R3836	L3642	V3494	GLY	C3349	F3293
E4454	ASP	T4327	V4001	A4086	L3999	I3906	R3836	L3642	V3494	GLY	C3350	K3294
E4455	ASP	T4327	V4001	A4086	L3999	I3906	R3836	L3642	V3494	GLY	C3351	I3295
E4456	ASP	T4327	V4001	A4086	L3999	I3906	R3836	L3642	V3494	GLY	C3352	K3296
T4457	ASP	T4327	V4001	A4086	L3999	I3906	R3836	L3642	V3494	GLY	C3353	N3297
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S4459	ASP	T4327	V4001	A4086	L3999	I3906	R3836	L3642	V3494	GLY	C3355	
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T4462	ASP	T4327	V4001	A4086	L3999	I3906	R3836	L3642	V3494	GLY	C3358	
T4463	ASP	T4327	V4001	A4086	L3999	I3906	R3836	L3642	V3494	GLY	C3359	
D4464	ASP	T4327	V4001	A4086	L3999	I3906	R3836	L3642	V3494	GLY	C3360	
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D4468	ASP	T4327	V4001	A4086	L3999	I3906	R3836	L3642	V3494	GLY	C3364	
E4471	ASP	T4327	V4001	A4086	L3999	I3906	R3836	L3642	V3494	GLY	C3365	
V4472	ASP	T4327	V4001	A4086	L3999	I3906	R3836	L3642	V3494	GLY	C3366	

[illegible]

- Molecule 1: E3 ubiquitin-protein ligase UBR4



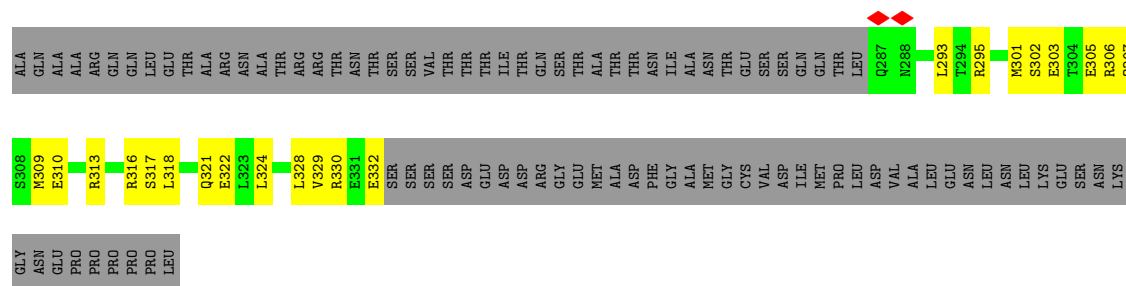
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PHE	PHE	GLU	GLN	ALA	ALA	SER	LYS
ILE	GLN	GLN	VAL	CYS	PHE	ASP	HIS
MET	SER	SER	LYS	LYS	GLU	ASP	ASP
PRO	PRO	THR	THR	VAL	MET	GLY	GLY
ALA	ALA	THR	LEU	LEU	LYS	TYR	TYR
THR	THR	ASP	SER	ILE	GLU	ASP	LYS
VAL	VAL	GLN	ASP	GLU	LEU	LEU	LYS
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ASP	ASP	SER	GLU	SER	GLN	HIS	HIS
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ASN	ASN	ASN	ALA	ASN	ILE	ILE	ASP
GLY	GLY	VAL	SER	PRO	GLU	GLU	ASP
PHE	PHE	PHE	PRO	ASP	SER	SER	ASP
HIS	HIS	ILE	VAL	GLU	GLU	GLU	ASP
SER	SER	ALA	SER	ALA	SER	SER	LYS
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LEU	LEU	SER	LEU	LYS	LYS	TYR	PRO
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GLU	GLU	VAL	SER	GLY	ALA	ALA	PRO
PRO	PRO	CYS	VAL	CYS	LEU	LEU	ALA
ASN	ASN	LEU	PHE	SER	SER	THR	THR
ASN	ASN	ASN	ASN	ARG	ARG	GLY	GLY
PRO	PRO	LEU	PRO	LEU	LEU	HIS	ALA
SER	SER	LEU	ARG	ASP	ASP	TYR	ASP
ARG	ARG	TYR	THR	THR	THR	ILE	THR
LEU	LEU	PHE	VAL	VAL	ARG	THR	THR
GLN	GLN	LEU	ALA	ALA	GLU	THR	PRO
ASP	ASP	ARG	SER	ILE	ILE	THR	GLY
VAL	VAL	TYR	GLN	ILE	ILE	VAL	TRP
THR	THR	ILE	THR	THR	PHE	SER	GLU
VAL	VAL	ASN	ILE	PHE	THR	LEU	VAL
LEU	LEU	ARG	SER	THR	THR	ILE	ALA
SER	SER	PHE	THR	ALA	ALA	PRO	VAL
LEU	LEU	GLN	GLN	MET	ARG	VAL	ARG
SER	SER	ASP	THR	MET	MET	ASN	PRO
CYS	CYS	ALA	LEU	LYS	LYS	GLN	LEU
VAL	VAL	VAL	VAL	SER	SER	LEU	LEU
TRP	TRP	LEU	GLU	ALA	THR	GLN	SER



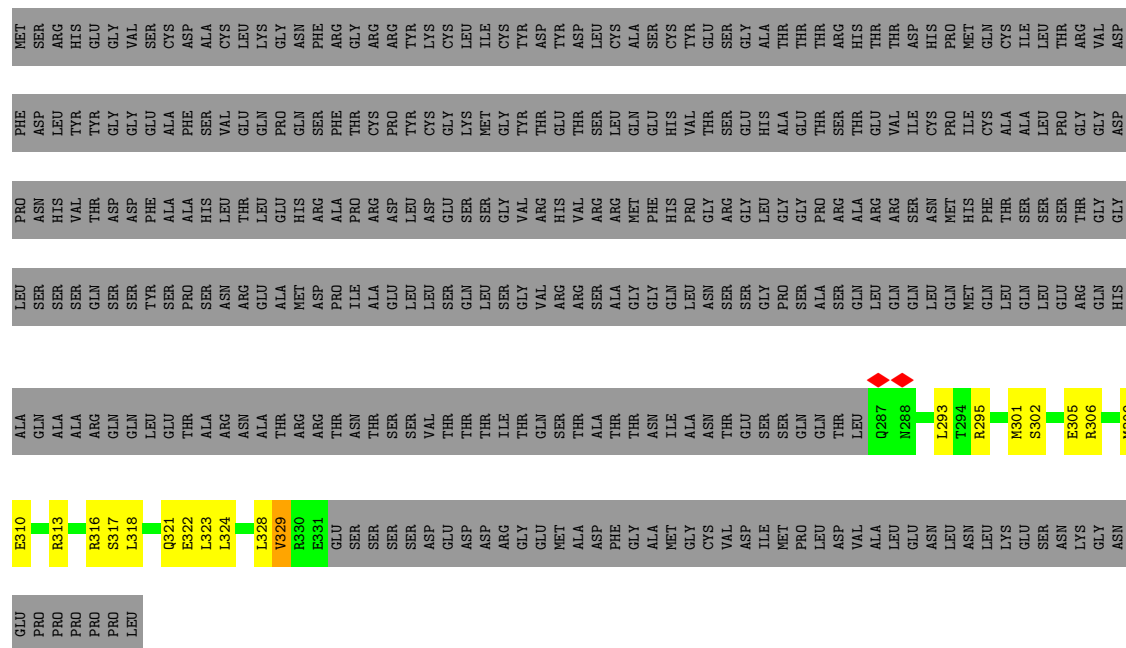




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ARG	CYS	LEU	D4648	I4709	D4648	LEU	D4468	L4408	F4348	C4272	V4132	L3968
PRO	LEU	GLU	E4649	W4710	E4649	LEU	E4471	L4409	F4349	L4273	T4135	Q3969
THR	ALA	GLU	D4650	K4711	D4650	THR	E4474	V4410	F4350	K4274	R4142	Y3970
GLN	VAL	GLY	H4651	S4652	H4651	GLY	K4474	M4411	V4351	L4275	C4146	L3973
LEU	ARG	LEU	G4653	G4653	G4653	D4590	M4475	M4412	T4352	L4276	W4071	I3979
THR	ASP	THR	D4654	D4654	D4654	K4591	M4478	K4413	L4353	V4277	W4059	C3985
CYS	VAL	CYS	D4655	D4655	D4655	D4592	M4479	T4414	F4354	V4278	K4061	W3986
ILE	ASN	ILE	K4656	K4656	K4656	Q4593	W4479	I4415	I4155	R4062	L3987	L3988
ARG	LYS	ARG	V4657	V4657	V4657	L4594	C4482	S4416	R4158	W4071	L3994	
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ASP	ASP	ASP	L4659	L4659	L4659	L4597	G4484	D4418	E4286	L4075	L3996	
ALA	ALA	ALA	D4660	D4660	D4660	L4598	R4491	L4419	L4165	L4075	L3997	
ARG	ARG	ARG				L4599	L4492	P4420	L4166	L4075	L3997	
GLN	GLN	GLN	C4663	C4663	C4663	Q4600	L4496	V4421	Y4169	L4075	L3998	
PRO	THR	PRO	I4665	I4665	I4665	I4601	R4496	A4422	L4170	L4075	L3999	
THR	THR	THR	A4666	A4666	A4666	M4602	G4496	L4423	N4083	L4075	A4000	
VAL	VAL	VAL	A4667	A4667	A4667	S4603	Q4500	V4424	G4084	L4075	V4001	
LEU	LEU	LEU	G4668	G4668	G4668	T4604	Q4500	Y4425	L4173	L4075	M4002	
LYS	LYS	LYS				F4605	L4606	K4426	Y4183	L4075	I4003	
ILE	LYS	ILE	I4669	I4669	I4669	V4606	L4606	G4427	K4089	L4075	V4007	
ARG	ARG	ARG	K4670	K4670	K4670	R4607	F4612	V4428	L4186	L4075	V4008	
TYR	TYR	TYR	M4671	M4671	M4671	S4608	V4512	W4429	Y4187	L4075		
MET	ASP	MET				M4609	V4520	C4430	L4092	L4075	N4011	
LYS	LYS	LYS	M4672	M4672	M4672	P4610	M4621	T4431	R4093	L4075	T4012	
ARG	ARG	ARG	S4673	S4673	S4673	S4611	R4522	T4432	H4094	L4075	T4013	
VAL	VAL	VAL	M4674	M4674	M4674	V4612	Q4523	T4433	L4095	L4075	L4014	
ALA	ALA	ALA	G4675	G4675	G4675	L4616	L4628	M4433	L4096	L4075	M4015	
GLU	GLU	GLU	H4676	H4676	H4676	L4619	L4629	I4434	L4097	L4075	L4017	
MET	GLY	MET	Q4677	Q4677	Q4677	L4620	L4630	C4313	L4228	L4075	R4018	
THR	THR	THR	L4678	L4678	L4678	P4621	L4642	I4314	L4229	L4075	L4019	
LEU	LEU	LEU	D4680	D4680	D4680	Y4622	L4643	E4315	R4104	L4075	L4020	
ASN	ASN	ASN	L4681	L4681	L4681	L4623	L4644	T4316	W4105	L4075	Q4021	
PRO	PRO	PRO	I4682	I4682	I4682	PHE	G4549	K4318	Q4106	L4075	R4022	
GLN	GLN	GLN	Q4684	Q4684	Q4684	GLY	E4549	L4382	Q4107	L4075	L4023	
LYS	LYS	LYS	K4685	K4685	K4685	VAL	G4554	M4383	F4108	L4075	K4025	
GLY	GLY	GLY	G4686	G4686	G4686	GLU	V4556	L4384	L4109	L4075	P4026	
THR	THR	THR	T4687	T4687	T4687	K4630	L4570	R4445	L4244	L4075	P4027	
VAL	VAL	VAL	H4748	H4748	H4748	M4631	D4571	G4446	L4245	L4075	A4028	
ASN	ASN	ASN	L4749	L4749	L4749	Q4632	L4571	L4447	V4251	L4075	S4031	
LYS	LYS	LYS	K4750	K4750	K4750	L4633	D4572	L4448	E4252	L4075	K4035	
THR	THR	THR	L4751	L4751	L4751	L4634	S4573	G4449	I4254	L4075	D4036	
ALA	ALA	ALA	S4752	S4752	S4752	V4635	M4574	D4450	R4255	L4075	VAL	
LEU	LEU	LEU	D4692	D4692	D4692	E4636	A4575	L4390	K4256	L4075	PRO	
ILE	ILE	ILE	D4693	D4693	D4693	R4637	E4576	C4391	H4257	L4075	GLU	
VAL	VAL	VAL	Y4694	Y4694	Y4694	F4638	P4577	Q4392	G4124	L4075	ALA	
GLN	GLN	GLN	K4695	K4695	K4695	K4639	LEU	D4393	N4126	L4075	LEU	
TYR	TYR	TYR				S4639	SER	C4394	E4343	L4075	THR	
			K4696	K4696	K4696	P4640	GLU	C4394	N4344	L4075	T4044	
			K4697	K4697	K4697	Y4641	ASP	D4395	E4345	L4075	Y4045	
			H4698	H4698	H4698	ASP	LYS	D4396	V4263	L4075		
			I4699	I4699	I4699	C4642	GLY	V4397	L4267	L4075		
			P4700	P4700	P4700	M4643		L4398		L4075		
			S4701	S4701	S4701	F4644		L4399		L4075		
			A4702	A4702	A4702	D4645		L4400		L4075		
			K4703	K4703	K4703	K4646		E4401		L4075		
			M4704	M4704	M4704			D4402		L4075		
			L4705	L4705	L4705			D4403		L4075		
			M4706	M4706	M4706			S4404		L4075		
			L4767	L4767	L4767			G4405		L4075		
			L4768	L4768	L4768			M4406		L4075		



- Molecule 3: E3 ubiquitin-protein ligase KCMF1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	87263	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.0	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.493	Depositor
Minimum map value	-0.698	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.146	Depositor
Map size (\AA)	419.19998, 419.19998, 419.19998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.048, 1.048, 1.048	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: ZN, CA

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	0.61	1/13355 (0.0%)	0.90	24/18055 (0.1%)
1	B	0.64	6/13357 (0.0%)	0.91	24/18057 (0.1%)
2	C	1.06	2/1146 (0.2%)	1.31	5/1539 (0.3%)
2	D	1.14	2/1138 (0.2%)	1.34	8/1526 (0.5%)
3	E	0.36	0/382	0.68	0/511
3	F	0.35	0/373	0.77	1/499 (0.2%)
All	All	0.66	11/29751 (0.0%)	0.94	62/40187 (0.2%)

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	2
1	B	0	1
All	All	0	3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	4013	THR	C-O	-6.08	1.17	1.24
1	B	4023	LEU	C-O	-6.06	1.17	1.24
1	A	3968	LEU	C-O	-5.96	1.16	1.24
2	D	14	LYS	CA-C	-5.91	1.45	1.52
2	C	14	LYS	CA-C	-5.89	1.45	1.52
2	D	18	SER	N-CA	-5.53	1.39	1.46
1	B	4020	LEU	C-O	-5.34	1.17	1.24
1	B	4131	GLN	C-O	-5.33	1.18	1.24
2	C	18	SER	N-CA	-5.32	1.40	1.46
1	B	4014	LEU	C-O	-5.28	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	4021	GLN	C-O	-5.13	1.18	1.24

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3792	VAL	CA-C-N	-17.13	96.38	120.71
1	A	3792	VAL	C-N-CA	-17.13	96.38	120.71
1	A	3792	VAL	O-C-N	13.47	136.41	122.54
1	A	3969	GLN	CB-CA-C	-12.40	91.86	110.96
2	C	86	ILE	N-CA-C	-11.11	97.20	111.09
2	D	106	LEU	N-CA-C	-9.97	100.49	111.36
1	A	3969	GLN	CA-C-N	-9.22	107.92	120.28
1	A	3969	GLN	C-N-CA	-9.22	107.92	120.28
1	A	3331	LYS	N-CA-C	-9.13	101.28	111.14
1	B	3331	LYS	N-CA-C	-8.96	101.46	111.14
2	C	139	TYR	N-CA-C	-8.93	101.44	111.71
1	B	4021	GLN	N-CA-C	-8.63	101.83	111.07
1	A	3973	LEU	N-CA-C	-7.65	102.92	111.71
1	A	3851	PHE	N-CA-C	-7.60	102.99	111.28
1	A	4134	PHE	CB-CA-C	7.51	122.86	110.17
1	B	3851	PHE	N-CA-C	-7.50	103.11	111.28
1	A	4133	LEU	CA-C-N	-7.41	111.01	122.49
1	A	4133	LEU	C-N-CA	-7.41	111.01	122.49
2	D	142	PHE	N-CA-C	-6.99	103.74	111.36
2	D	119	ASP	N-CA-C	-6.87	104.76	113.01
2	C	142	PHE	N-CA-C	-6.83	103.83	111.28
1	B	3750	TYR	CB-CA-C	-6.78	99.15	110.68
1	B	4023	LEU	CA-C-O	-6.76	113.66	120.90
1	B	4129	LEU	N-CA-C	-6.52	104.17	111.28
2	C	143	VAL	CB-CA-C	-6.16	104.08	111.97
1	B	4021	GLN	CA-C-O	-6.16	114.35	120.82
2	D	143	VAL	CB-CA-C	-6.06	104.21	111.97
1	A	3296	LYS	N-CA-C	-5.97	105.48	112.89
1	A	3535	CYS	CB-CA-C	-5.94	98.60	110.42
1	B	4131	GLN	CA-C-N	-5.87	113.56	120.72
1	B	4131	GLN	C-N-CA	-5.87	113.56	120.72
1	B	3296	LYS	N-CA-C	-5.78	105.72	112.89
2	D	110	MET	N-CA-C	-5.67	105.10	111.28
1	B	4130	ARG	N-CA-C	-5.66	104.80	110.97
1	A	3968	LEU	N-CA-C	-5.63	105.02	112.34
1	A	3970	TYR	CA-C-N	-5.59	112.23	120.28
1	A	3970	TYR	C-N-CA	-5.59	112.23	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	10	ILE	N-CA-C	-5.56	104.25	112.04
2	C	10	ILE	N-CA-C	-5.55	104.28	112.04
1	A	4744	SER	CA-C-N	5.41	124.66	120.33
1	A	4744	SER	C-N-CA	5.41	124.66	120.33
1	A	3327	LEU	CA-C-O	-5.38	115.16	120.70
1	A	3716	TYR	N-CA-C	-5.38	103.87	110.65
3	F	329	VAL	O-C-N	5.36	128.31	122.63
1	B	4052	ILE	CA-C-N	-5.31	114.74	122.86
1	B	4052	ILE	C-N-CA	-5.31	114.74	122.86
1	B	4012	ILE	CA-C-O	-5.25	115.94	121.41
2	D	74	ALA	N-CA-C	-5.24	105.46	111.07
1	B	3751	HIS	CB-CA-C	5.24	120.73	110.67
1	B	3327	LEU	CA-C-O	-5.21	115.34	120.70
1	B	4014	LEU	N-CA-C	-5.19	105.62	111.28
1	B	4744	SER	CA-C-N	5.18	124.47	120.33
1	B	4744	SER	C-N-CA	5.18	124.47	120.33
1	B	4023	LEU	CA-C-N	5.16	127.52	120.46
1	B	4023	LEU	C-N-CA	5.16	127.52	120.46
1	B	4021	GLN	N-CA-CB	5.12	117.44	110.01
1	B	3854	SER	CA-C-N	-5.05	114.20	122.79
1	B	3854	SER	C-N-CA	-5.05	114.20	122.79
1	A	3866	HIS	CA-CB-CG	5.02	118.82	113.80
2	D	17	PHE	N-CA-C	-5.02	105.81	111.28
1	A	3854	SER	CA-C-N	-5.01	114.27	122.79
1	A	3854	SER	C-N-CA	-5.01	114.27	122.79

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3286	ARG	Sidechain
1	A	4319	ARG	Sidechain
1	B	4112	ARG	Sidechain

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	13132	0	13358	477	0
1	B	13134	0	13352	460	0
2	C	1134	0	1063	91	0
2	D	1127	0	1055	112	0
3	E	380	0	376	30	0
3	F	371	0	370	17	0
4	A	3	0	0	3	0
4	B	3	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
All	All	29288	0	29574	1056	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 18.

All (1056) 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:4032:LYS:CE	3:E:307:GLN:HG3	1.25	1.55
1:A:4307:LYS:CG	1:A:4475:MET:HE1	1.45	1.44
1:A:4307:LYS:HG3	1:A:4475:MET:CE	1.47	1.42
1:A:4032:LYS:CE	3:E:307:GLN:CG	2.11	1.28
1:B:4098:THR:OG1	2:D:113:LEU:HD21	1.18	1.26
1:A:4032:LYS:HE3	3:E:307:GLN:CG	1.66	1.25
1:A:4307:LYS:CG	1:A:4475:MET:CE	2.09	1.24
1:B:3270:ILE:CD1	1:B:3632:PRO:HG2	1.66	1.24
1:A:3270:ILE:CD1	1:A:3632:PRO:HG2	1.66	1.23
1:B:4307:LYS:CG	1:B:4475:MET:HE1	1.67	1.22
1:A:3270:ILE:HD13	1:A:3632:PRO:HG2	1.25	1.14
1:A:4309:PHE:HE1	1:A:4338:ILE:CD1	1.59	1.14
1:B:3328:CYS:SG	1:B:3333:LEU:HD11	1.90	1.12
1:B:4314:ILE:HD11	1:B:4479:MET:SD	1.88	1.11
1:A:3328:CYS:SG	1:A:3333:LEU:HD11	1.89	1.10
1:A:4271:LEU:HD11	1:A:4331:ILE:HD11	1.29	1.10
1:A:4310:MET:SD	1:A:4338:ILE:HG21	1.89	1.10
1:A:4032:LYS:HE2	3:E:307:GLN:HG3	1.13	1.10
1:B:3270:ILE:HD13	1:B:3632:PRO:HG2	1.25	1.09
1:B:4271:LEU:HD11	1:B:4331:ILE:HD11	1.28	1.07
1:A:4309:PHE:HE1	1:A:4338:ILE:HD11	1.19	1.05
2:C:106:LEU:HD22	2:C:126:ILE:HD11	1.38	1.04
1:A:3269:LEU:HB3	1:A:3633:LEU:CD1	1.89	1.03
1:B:4098:THR:OG1	2:D:113:LEU:CD2	2.05	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3791:SER:O	1:B:3521:GLU:N	1.89	1.03
1:B:4307:LYS:HG3	1:B:4475:MET:HE1	1.09	1.03
1:A:4309:PHE:CE1	1:A:4338:ILE:HD11	1.93	1.03
1:A:3532:CYS:HB3	1:A:3869:SER:H	1.25	1.02
1:B:3269:LEU:HB3	1:B:3633:LEU:CD1	1.89	1.02
2:D:103:ALA:HB2	2:D:126:ILE:HG13	1.41	1.01
1:A:3839:ALA:HB1	1:B:4500:GLN:NE2	1.74	1.00
1:A:4500:GLN:NE2	1:B:3839:ALA:HB1	1.78	0.97
1:A:3793:ASN:HA	1:B:3521:GLU:HG3	1.45	0.97
1:B:4309:PHE:CE1	1:B:4338:ILE:HD11	2.00	0.97
2:D:50:GLN:O	2:D:53:ILE:HG22	1.65	0.97
1:B:4648:ASP:HA	1:B:4717:PRO:HD2	1.46	0.96
1:B:4671:ASN:HB2	1:B:4732:GLN:OE1	1.66	0.96
1:A:4671:ASN:HB2	1:A:4732:GLN:OE1	1.66	0.95
1:B:4271:LEU:CD1	1:B:4331:ILE:HD11	1.98	0.94
1:A:4032:LYS:HE2	3:E:307:GLN:CG	1.81	0.94
1:A:3532:CYS:HB3	1:A:3869:SER:N	1.84	0.93
1:A:4309:PHE:CE1	1:A:4338:ILE:CD1	2.50	0.93
2:D:101:ILE:HB	2:D:137:VAL:HB	1.47	0.93
1:A:4271:LEU:CD1	1:A:4331:ILE:HD11	1.98	0.92
1:A:4032:LYS:HE3	3:E:307:GLN:HG3	0.93	0.92
2:C:24:GLY:HA3	2:C:28:ILE:HD12	1.52	0.91
1:A:3328:CYS:SG	1:A:3333:LEU:CD1	2.58	0.90
1:B:3328:CYS:SG	1:B:3333:LEU:CD1	2.58	0.90
1:A:4307:LYS:CG	1:A:4475:MET:HE3	2.02	0.90
2:C:138:ASN:HB3	2:C:140:GLU:HG2	1.53	0.90
1:A:3532:CYS:HG	4:A:5203:ZN:ZN	0.86	0.89
1:A:4307:LYS:CG	1:A:4478:VAL:HG21	2.02	0.89
1:A:3794:ARG:N	1:B:3521:GLU:OE2	2.04	0.89
1:B:3270:ILE:CD1	1:B:3632:PRO:CG	2.51	0.88
1:A:3535:CYS:SG	4:A:5203:ZN:ZN	1.62	0.88
1:A:3270:ILE:CD1	1:A:3632:PRO:CG	2.50	0.87
1:B:4307:LYS:CG	1:B:4475:MET:CE	2.52	0.87
1:A:4307:LYS:HG2	1:A:4478:VAL:HG21	1.58	0.86
2:C:69:PHE:CZ	2:C:73:MET:SD	2.67	0.86
2:C:106:LEU:CD2	2:C:126:ILE:HD11	2.05	0.86
1:B:4296:GLU:HG2	1:B:4334:ARG:HH22	1.40	0.86
1:B:3419:SER:O	1:B:3420:ASN:CG	2.19	0.85
1:B:3327:LEU:O	1:B:3392:CYS:SG	2.34	0.85
1:B:4309:PHE:HE1	1:B:4338:ILE:HD11	1.36	0.85
1:A:3419:SER:O	1:A:3420:ASN:CG	2.19	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3327:LEU:O	1:A:3392:CYS:SG	2.35	0.85
2:C:106:LEU:HD22	2:C:126:ILE:CD1	2.07	0.85
2:C:80:THR:O	2:C:81:ASP:OD1	1.94	0.85
1:B:4444:MET:HE3	1:B:4447:LEU:HD13	1.58	0.84
1:A:4275:LYS:NZ	1:A:4327:THR:HG21	1.93	0.84
1:A:4307:LYS:HG2	1:A:4475:MET:HE3	1.57	0.84
1:A:4444:MET:HE3	1:A:4447:LEU:HD13	1.58	0.84
2:D:106:LEU:HD22	2:D:126:ILE:CD1	2.09	0.83
1:A:3269:LEU:HB3	1:A:3633:LEU:HD11	1.61	0.83
1:A:3419:SER:O	1:A:3420:ASN:OD1	1.96	0.82
1:A:4714:LEU:HD11	1:A:4754:VAL:HG11	1.59	0.82
1:A:4232:LEU:HD13	1:B:3750:TYR:HB2	1.61	0.82
1:B:3419:SER:O	1:B:3420:ASN:OD1	1.96	0.82
1:B:4714:LEU:HD11	1:B:4754:VAL:HG11	1.59	0.82
1:B:3979:ILE:HG21	1:B:4019:ILE:HG23	1.62	0.82
1:B:4275:LYS:NZ	1:B:4327:THR:HG21	1.94	0.82
1:B:4307:LYS:HG2	1:B:4475:MET:HE1	1.60	0.81
1:A:3839:ALA:HB1	1:B:4500:GLN:HE21	1.41	0.81
1:B:3269:LEU:HB3	1:B:3633:LEU:HD11	1.61	0.81
1:B:3516:LEU:HD22	1:B:3799:LEU:HD21	1.63	0.81
1:A:4500:GLN:HE21	1:B:3839:ALA:HB1	1.46	0.81
1:A:3997:PHE:HB2	1:A:4016:CYS:HB3	1.63	0.80
1:B:3270:ILE:HD13	1:B:3632:PRO:CG	2.11	0.80
2:C:49:LEU:C	2:C:49:LEU:HD13	2.06	0.80
1:B:4313:CYS:HB3	1:B:4331:ILE:HG23	1.64	0.79
1:A:3516:LEU:HD22	1:A:3799:LEU:HD21	1.63	0.79
1:A:4632:GLN:HA	1:A:4681:LEU:HD21	1.62	0.79
1:B:3330:SER:HA	1:B:3333:LEU:HB2	1.64	0.79
1:A:4307:LYS:HD2	1:A:4478:VAL:CG2	2.12	0.79
1:A:3793:ASN:ND2	1:B:3519:LEU:O	2.12	0.79
1:B:3588:ARG:HD2	1:B:3646:ASP:OD2	1.83	0.79
2:D:106:LEU:CD2	2:D:126:ILE:HD11	2.12	0.79
1:A:3532:CYS:CB	1:A:3869:SER:H	1.96	0.78
1:A:3330:SER:HA	1:A:3333:LEU:HB2	1.64	0.78
1:A:3532:CYS:SG	4:A:5203:ZN:ZN	1.72	0.78
1:A:3588:ARG:HD2	1:A:3646:ASP:OD2	1.82	0.78
1:A:4029:PRO:O	1:A:4034:ASN:OD1	2.01	0.78
2:D:106:LEU:HD22	2:D:126:ILE:HD11	1.66	0.78
2:D:101:ILE:HD11	2:D:142:PHE:HD1	1.48	0.77
1:B:3315:VAL:HG22	1:B:3633:LEU:HD21	1.66	0.77
1:B:4027:PRO:HB2	3:F:313:ARG:HH21	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3968:LEU:CD1	1:A:4012:ILE:HD11	2.14	0.77
2:D:137:VAL:HG13	2:D:141:GLU:HB2	1.67	0.77
2:D:50:GLN:O	2:D:53:ILE:CG2	2.32	0.77
1:B:4307:LYS:HG2	1:B:4475:MET:CE	2.14	0.76
1:A:3315:VAL:HG22	1:A:3633:LEU:HD21	1.67	0.76
1:A:3793:ASN:HD22	1:B:3519:LEU:C	1.93	0.76
1:B:4108:PHE:CD1	2:D:148:ALA:HB3	2.21	0.76
1:B:4105:TRP:CZ3	2:D:106:LEU:HD11	2.21	0.76
1:A:4108:PHE:CD1	2:C:148:ALA:HB3	2.21	0.76
1:A:3951:VAL:HG13	1:A:4012:ILE:HD13	1.67	0.75
1:B:4296:GLU:HG2	1:B:4334:ARG:NH2	2.01	0.75
2:C:140:GLU:HG3	2:C:141:GLU:HG3	1.68	0.75
1:A:3054:VAL:HA	1:A:3057:ARG:HD2	1.68	0.75
1:A:3532:CYS:HB2	1:A:3868:SER:HA	1.68	0.75
1:A:3955:LEU:HD21	1:A:4012:ILE:HD12	1.67	0.75
1:A:3270:ILE:HD13	1:A:3632:PRO:CG	2.10	0.74
1:A:3240:ILE:HD11	1:A:3275:HIS:HB2	1.70	0.74
1:A:4105:TRP:CD1	2:C:145:MET:HG3	2.22	0.74
1:B:3054:VAL:HA	1:B:3057:ARG:HD2	1.68	0.74
1:A:3965:ALA:HA	1:A:4011:ASN:HD21	1.53	0.74
1:A:4307:LYS:CD	1:A:4475:MET:HE1	2.16	0.74
1:A:4310:MET:HG3	1:A:4335:LEU:HD23	1.70	0.74
1:A:3459:PRO:HA	1:A:3879:VAL:HG21	1.69	0.74
1:B:3459:PRO:HA	1:B:3879:VAL:HG21	1.69	0.74
1:A:3954:ALA:HB3	1:A:3968:LEU:HD11	1.70	0.73
1:B:4105:TRP:CD1	2:D:145:MET:HG3	2.22	0.73
1:B:4127:ASN:HD21	1:B:4165:LEU:HD21	1.53	0.73
2:C:139:TYR:O	2:C:143:VAL:HG23	1.88	0.73
2:C:140:GLU:HG3	2:C:141:GLU:N	2.04	0.73
1:B:3240:ILE:HD11	1:B:3275:HIS:HB2	1.70	0.73
2:C:69:PHE:CE1	2:C:73:MET:SD	2.82	0.72
1:B:4105:TRP:HZ2	2:D:129:ALA:HB2	1.55	0.72
1:A:4310:MET:CG	1:A:4335:LEU:HD23	2.19	0.72
2:C:24:GLY:CA	2:C:28:ILE:HD12	2.20	0.71
1:A:3793:ASN:HA	1:B:3521:GLU:CG	2.21	0.71
1:B:3547:LEU:HD13	1:B:3715:LEU:HD11	1.73	0.71
1:A:3968:LEU:HD12	1:A:4012:ILE:HD11	1.72	0.71
1:A:3791:SER:HB3	1:B:3521:GLU:O	1.91	0.71
2:D:147:THR:O	2:D:148:ALA:C	2.34	0.71
1:A:3518:GLY:HA2	1:B:3770:ALA:HB1	1.73	0.70
1:A:3791:SER:HB3	1:B:3804:CYS:SG	2.31	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3270:ILE:HD12	1:B:3632:PRO:HG2	1.72	0.70
2:C:147:THR:O	2:C:148:ALA:C	2.34	0.70
1:B:4598:LEU:HD12	1:B:4634:LEU:HD22	1.73	0.70
1:A:4011:ASN:O	1:A:4015:MET:HG2	1.90	0.70
2:C:137:VAL:HG13	2:C:141:GLU:HB2	1.73	0.69
2:D:118:THR:O	2:D:122:VAL:HG23	1.90	0.69
1:A:4492:LEU:HD12	1:A:4512:PHE:HE2	1.57	0.69
1:A:3836:ARG:O	1:A:3840:THR:OG1	2.11	0.69
1:B:4492:LEU:HD12	1:B:4512:PHE:HE2	1.57	0.69
1:B:3556:TYR:O	1:B:3606:LYS:HE3	1.93	0.68
1:A:4105:TRP:HZ2	2:C:129:ALA:HB2	1.58	0.68
1:A:3270:ILE:HD12	1:A:3632:PRO:HG2	1.72	0.68
1:B:3836:ARG:O	1:B:3840:THR:OG1	2.11	0.68
1:B:4238:LEU:HG	1:B:4287:THR:HG21	1.74	0.68
1:B:4314:ILE:HG21	1:B:4484:GLY:HA2	1.74	0.68
1:A:4232:LEU:HD12	1:B:3750:TYR:CG	2.29	0.68
1:A:4238:LEU:HG	1:A:4287:THR:HG21	1.74	0.68
1:B:4123:LEU:HD13	1:B:4165:LEU:HD22	1.75	0.68
2:C:140:GLU:HG3	2:C:141:GLU:H	1.59	0.68
1:A:3556:TYR:O	1:A:3606:LYS:HE3	1.93	0.68
1:B:4314:ILE:HD12	1:B:4482:CYS:SG	2.34	0.68
1:A:4037:VAL:HG13	1:A:4038:PRO:HD3	1.76	0.67
1:B:3244:LEU:HB3	1:B:3249:ILE:HB	1.75	0.67
1:B:4643:ASN:HB3	1:B:4646:LYS:HB3	1.77	0.67
2:C:24:GLY:HA3	2:C:28:ILE:CD1	2.24	0.67
1:A:3258:ALA:HB3	1:A:3847:VAL:HG22	1.75	0.67
1:B:3258:ALA:HB3	1:B:3847:VAL:HG22	1.75	0.67
1:A:4232:LEU:HD12	1:B:3750:TYR:CD2	2.30	0.67
1:A:4307:LYS:CD	1:A:4475:MET:CE	2.71	0.67
1:A:3244:LEU:HB3	1:A:3249:ILE:HB	1.76	0.66
1:A:3839:ALA:CB	1:B:4500:GLN:NE2	2.55	0.66
1:A:4094:HIS:O	1:A:4098:THR:HG23	1.96	0.66
1:B:4094:HIS:O	1:B:4098:THR:HG23	1.95	0.66
1:A:4089:LYS:HA	1:A:4092:LEU:HD12	1.77	0.66
1:B:4314:ILE:CD1	1:B:4479:MET:SD	2.77	0.66
1:A:3190:TRP:H	1:A:3190:TRP:CD1	2.12	0.66
1:A:3940:THR:HG21	1:A:3985:CYS:HB3	1.76	0.66
1:B:3241:LYS:O	1:B:3245:GLU:HG2	1.95	0.66
1:B:4309:PHE:CD1	1:B:4338:ILE:HD11	2.30	0.66
1:A:3241:LYS:O	1:A:3245:GLU:HG2	1.95	0.66
1:B:3527:LEU:HD21	1:B:3757:ARG:HD3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3270:ILE:HD12	1:A:3632:PRO:CG	2.26	0.65
1:A:3826:LYS:N	1:B:4228:LEU:CD1	2.55	0.65
1:B:3190:TRP:CD1	1:B:3190:TRP:H	2.12	0.65
1:B:3290:TRP:NE1	1:B:3326:ALA:HB2	2.12	0.65
1:B:3408:LEU:HD12	1:B:3411:PHE:HE2	1.61	0.65
1:A:4495:ILE:HG21	1:A:4505:LEU:HD12	1.78	0.65
1:A:4600:GLN:HB3	1:A:4606:VAL:HG21	1.79	0.65
1:A:3290:TRP:NE1	1:A:3326:ALA:HB2	2.11	0.65
1:A:3408:LEU:HD12	1:A:3411:PHE:HE2	1.62	0.65
1:B:3497:LEU:HD11	1:B:3913:ASN:HD21	1.62	0.65
1:B:4307:LYS:HG2	1:B:4478:VAL:HG21	1.78	0.65
1:A:3447:LEU:HA	1:A:3450:LEU:HD12	1.79	0.64
1:B:3994:LEU:HD23	1:B:4060:LEU:HD21	1.78	0.64
1:B:3270:ILE:HD12	1:B:3632:PRO:CG	2.26	0.64
2:C:137:VAL:HA	2:C:141:GLU:OE1	1.98	0.64
1:A:4228:LEU:CD1	1:B:3826:LYS:N	2.54	0.64
1:B:4495:ILE:HG21	1:B:4505:LEU:HD12	1.78	0.64
1:B:3803:TYR:HA	1:B:3807:CYS:HB2	1.80	0.64
1:A:3211:ARG:HH21	1:A:3228:ARG:HH22	1.45	0.64
1:A:3818:ILE:HD12	1:B:4230:THR:CG2	2.28	0.64
2:C:140:GLU:CG	2:C:141:GLU:H	2.10	0.64
1:A:3791:SER:CB	1:B:3804:CYS:SG	2.86	0.63
1:A:3792:VAL:O	1:A:3793:ASN:C	2.35	0.63
1:A:4309:PHE:HE1	1:A:4338:ILE:HD13	1.58	0.63
1:B:3447:LEU:HA	1:B:3450:LEU:HD12	1.80	0.63
1:B:4258:PHE:HE1	2:D:19:LEU:HD21	1.63	0.63
1:A:3803:TYR:HA	1:A:3807:CYS:HB2	1.80	0.63
1:A:4310:MET:CG	1:A:4335:LEU:CD2	2.77	0.63
1:A:4307:LYS:CD	1:A:4478:VAL:CG2	2.77	0.63
1:A:4500:GLN:NE2	1:B:3839:ALA:O	2.32	0.63
1:B:3211:ARG:HH21	1:B:3228:ARG:HH22	1.44	0.63
1:A:3464:LYS:HE3	1:A:3534:VAL:HG13	1.81	0.63
1:A:3497:LEU:HD11	1:A:3913:ASN:HD21	1.62	0.63
1:A:3905:LEU:HD23	1:A:3932:LEU:HD11	1.81	0.63
1:A:4307:LYS:HD2	1:A:4478:VAL:HG22	1.81	0.63
2:C:140:GLU:CG	2:C:141:GLU:N	2.62	0.62
2:C:143:VAL:O	2:C:144:GLN:C	2.42	0.62
2:D:21:ASP:HA	2:D:28:ILE:HA	1.80	0.62
2:D:106:LEU:CD2	2:D:126:ILE:CD1	2.74	0.62
2:D:143:VAL:O	2:D:144:GLN:C	2.41	0.62
2:D:122:VAL:O	2:D:126:ILE:HG12	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3273:MET:HE1	1:A:3318:VAL:HG21	1.82	0.62
1:A:4228:LEU:HB3	1:B:3822:PHE:CD1	2.35	0.62
1:A:4232:LEU:CD1	1:B:3750:TYR:CG	2.82	0.62
1:B:4295:LEU:HD11	1:B:4309:PHE:HE2	1.64	0.62
1:B:3273:MET:HE1	1:B:3318:VAL:HG21	1.81	0.62
1:B:3850:THR:HG22	1:B:3853:ALA:HB3	1.82	0.62
2:D:29:THR:HG23	2:D:31:LYS:HB2	1.81	0.62
1:A:4230:THR:CG2	1:B:3818:ILE:HD12	2.28	0.62
1:A:3791:SER:O	1:B:3521:GLU:CA	2.47	0.61
1:A:3825:ARG:NH1	1:B:4278:VAL:O	2.33	0.61
1:A:3822:PHE:CD1	1:B:4228:LEU:HB3	2.36	0.61
1:A:3850:THR:HG22	1:A:3853:ALA:HB3	1.82	0.61
1:A:3965:ALA:O	1:A:3969:GLN:HB2	1.99	0.61
1:A:4032:LYS:HE3	3:E:307:GLN:CB	2.29	0.61
1:B:4313:CYS:HB3	1:B:4331:ILE:CG2	2.29	0.61
1:A:3794:ARG:HB3	1:B:3521:GLU:OE2	2.00	0.61
1:A:4500:GLN:NE2	1:B:3839:ALA:CB	2.58	0.61
2:C:33:LEU:CD2	2:C:72:MET:HE1	2.30	0.61
1:A:3332:VAL:HG21	1:A:3434:HIS:NE2	2.15	0.61
1:A:4032:LYS:HB3	1:A:4035:LYS:HD2	1.83	0.61
2:C:49:LEU:C	2:C:49:LEU:CD1	2.74	0.61
1:B:3332:VAL:HG21	1:B:3434:HIS:NE2	2.15	0.60
2:C:33:LEU:HD21	2:C:72:MET:HE1	1.83	0.60
1:B:4022:LYS:O	1:B:4023:LEU:C	2.42	0.60
2:C:10:ILE:HG13	2:C:66:PHE:HZ	1.67	0.60
1:A:4278:VAL:O	1:B:3825:ARG:NH1	2.33	0.60
2:D:50:GLN:C	2:D:53:ILE:HG22	2.26	0.60
1:A:3201:GLN:HA	1:A:3207:ARG:HH21	1.68	0.59
1:A:4130:ARG:HA	1:A:4133:LEU:HB2	1.84	0.59
1:A:4134:PHE:O	1:A:4135:THR:C	2.44	0.59
3:F:302:SER:O	3:F:306:ARG:N	2.34	0.59
1:A:4029:PRO:HB2	1:A:4034:ASN:HA	1.85	0.59
1:B:3894:PRO:O	1:B:3898:HIS:ND1	2.35	0.59
2:C:100:TYR:HB3	2:C:136:GLN:HB3	1.85	0.59
1:A:3240:ILE:HD11	1:A:3275:HIS:CB	2.33	0.59
1:A:3270:ILE:O	1:A:3274:GLU:HG2	2.03	0.59
1:A:3792:VAL:C	1:B:3521:GLU:HG3	2.27	0.59
1:A:4429:TRP:CE2	1:A:4438:MET:HA	2.38	0.59
1:B:4096:TYR:CE1	2:D:48:GLU:HG2	2.38	0.59
1:A:3901:VAL:HG11	1:A:3939:ALA:HB2	1.84	0.59
1:B:4429:TRP:CE2	1:B:4438:MET:HA	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3270:ILE:O	1:B:3274:GLU:HG2	2.03	0.58
2:C:141:GLU:O	2:C:144:GLN:HB3	2.02	0.58
1:A:4643:ASN:HB3	1:A:4646:LYS:HB3	1.85	0.58
2:C:93:PHE:HB3	2:C:101:ILE:HD12	1.85	0.58
1:A:4277:VAL:HG21	1:B:3732:ARG:HH22	1.68	0.58
1:B:3240:ILE:HD11	1:B:3275:HIS:CB	2.33	0.58
1:B:3683:GLN:OE1	1:B:3688:ARG:HD2	2.03	0.58
2:D:106:LEU:HD22	2:D:126:ILE:HD13	1.83	0.58
1:B:3299:SER:O	1:B:3303:PHE:HB3	2.04	0.58
1:B:4105:TRP:HZ3	2:D:106:LEU:HD11	1.67	0.58
1:B:4109:LEU:HD12	1:B:4114:LYS:HB2	1.85	0.58
1:B:4714:LEU:CD1	1:B:4754:VAL:HG11	2.32	0.58
2:D:111:THR:HA	2:D:115:GLU:O	2.04	0.58
1:A:3001:GLN:O	1:A:3005:MET:HG2	2.04	0.58
1:A:3683:GLN:OE1	1:A:3688:ARG:HD2	2.03	0.58
1:A:3469:VAL:HG21	1:A:3882:HIS:HB3	1.86	0.58
1:A:3792:VAL:CG1	1:A:3793:ASN:N	2.66	0.58
1:A:3965:ALA:HA	1:A:4011:ASN:ND2	2.18	0.58
1:A:4271:LEU:HD11	1:A:4331:ILE:CD1	2.19	0.58
2:D:78:LYS:HB3	2:D:80:THR:HG23	1.84	0.58
2:D:106:LEU:HD23	2:D:126:ILE:HD11	1.86	0.58
1:A:4101:TYR:CD2	2:C:89:ALA:HB2	2.39	0.58
1:A:4307:LYS:HG3	1:A:4475:MET:HE1	0.64	0.58
1:A:3732:ARG:HH22	1:B:4277:VAL:HG21	1.68	0.58
1:A:4032:LYS:HE3	3:E:307:GLN:CA	2.34	0.58
1:B:4295:LEU:O	1:B:4299:THR:HG23	2.03	0.58
2:C:49:LEU:HD11	2:C:53:ILE:HD12	1.85	0.58
1:A:3327:LEU:HD12	1:A:3431:LEU:HD11	1.85	0.58
1:B:3679:GLU:CD	1:B:3683:GLN:HE22	2.11	0.58
1:B:3754:MET:O	1:B:3758:PRO:HD3	2.04	0.58
2:D:20:PHE:HB3	2:D:32:GLU:HB3	1.86	0.58
1:A:3839:ALA:O	1:B:4500:GLN:NE2	2.36	0.58
1:A:4307:LYS:HD3	1:A:4475:MET:SD	2.43	0.58
1:A:3679:GLU:CD	1:A:3683:GLN:HE22	2.11	0.57
1:B:4263:VAL:HG12	1:B:4312:VAL:HG11	1.85	0.57
1:A:3792:VAL:HG12	1:A:3793:ASN:N	2.19	0.57
1:A:3299:SER:O	1:A:3303:PHE:HB3	2.04	0.57
1:A:3894:PRO:O	1:A:3898:HIS:ND1	2.35	0.57
1:B:4314:ILE:CD1	1:B:4482:CYS:SG	2.92	0.57
1:B:4355:LYS:HE3	1:B:4365:GLY:O	2.04	0.57
1:B:3034:MET:SD	1:B:3034:MET:N	2.77	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3298:ASP:OD1	1:B:3298:ASP:N	2.38	0.57
1:A:3979:ILE:HG12	1:A:3989:ARG:HB3	1.86	0.57
1:B:3327:LEU:HD12	1:B:3431:LEU:HD11	1.85	0.57
1:A:3964:LEU:HD23	1:A:4011:ASN:HD22	1.70	0.57
1:A:4307:LYS:CB	1:A:4478:VAL:HG21	2.34	0.57
1:B:3469:VAL:HG21	1:B:3882:HIS:HB3	1.86	0.57
1:B:4492:LEU:HD12	1:B:4512:PHE:CE2	2.40	0.57
2:D:101:ILE:HD11	2:D:142:PHE:CD1	2.34	0.57
1:A:3324:SER:O	1:A:3328:CYS:SG	2.62	0.57
1:B:3001:GLN:O	1:B:3005:MET:HG2	2.04	0.57
1:B:3964:LEU:HD23	1:B:4011:ASN:HD22	1.70	0.57
1:B:4314:ILE:HD13	1:B:4484:GLY:HA3	1.86	0.57
1:A:3290:TRP:HE1	1:A:3326:ALA:HB2	1.70	0.57
1:A:4714:LEU:CD1	1:A:4754:VAL:HG11	2.32	0.57
1:A:4355:LYS:HE3	1:A:4365:GLY:O	2.04	0.56
1:B:4419:LEU:HD13	1:B:4459:LEU:HG	1.87	0.56
2:D:59:ASP:HB2	2:D:63:THR:HG21	1.87	0.56
1:A:4492:LEU:HD12	1:A:4512:PHE:CE2	2.40	0.56
1:A:3972:MET:HE2	1:A:4015:MET:HB2	1.86	0.56
1:A:4313:CYS:HB3	1:A:4331:ILE:HG23	1.87	0.56
1:B:4602:ASN:HA	1:B:4607:ARG:HH21	1.71	0.56
1:A:4232:LEU:HD13	1:B:3750:TYR:CB	2.33	0.56
3:E:302:SER:O	3:E:306:ARG:N	2.34	0.56
1:A:4713:PHE:HE1	1:A:4751:LEU:HD21	1.71	0.56
1:B:3324:SER:O	1:B:3328:CYS:SG	2.62	0.56
1:B:4271:LEU:HD11	1:B:4331:ILE:CD1	2.18	0.56
1:A:4423:GLU:HB3	1:A:4459:LEU:HD13	1.88	0.56
2:C:124:GLU:O	2:C:128:GLU:HG2	2.06	0.56
1:A:3187:ASP:OD1	1:A:3190:TRP:NE1	2.39	0.56
1:B:3290:TRP:HE1	1:B:3326:ALA:HB2	1.70	0.56
1:A:4024:ILE:HD11	3:E:324:LEU:HD12	1.88	0.56
1:A:4130:ARG:HB2	1:A:4169:TYR:CE1	2.41	0.56
1:B:3662:ARG:NH2	1:B:3679:GLU:OE2	2.39	0.56
1:B:4307:LYS:HE3	1:B:4475:MET:SD	2.45	0.56
1:B:4105:TRP:CZ3	2:D:106:LEU:CD1	2.87	0.56
1:A:4602:ASN:HA	1:A:4607:ARG:HH21	1.71	0.55
3:E:301:MET:O	3:E:306:ARG:NH1	2.39	0.55
1:B:3409:ILE:HG12	1:B:3450:LEU:HD22	1.88	0.55
1:B:4129:LEU:HD21	1:B:4149:VAL:HG22	1.86	0.55
1:B:4105:TRP:HZ3	2:D:106:LEU:CD1	2.18	0.55
1:B:4131:GLN:O	1:B:4135:THR:HG23	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4258:PHE:CE1	2:D:19:LEU:HD21	2.40	0.55
1:B:4713:PHE:HE1	1:B:4751:LEU:HD21	1.71	0.55
3:F:301:MET:O	3:F:306:ARG:NH1	2.39	0.55
1:A:4105:TRP:CD2	2:C:145:MET:HE2	2.42	0.55
1:B:3201:GLN:HA	1:B:3207:ARG:HH21	1.72	0.55
1:B:4594:LEU:O	1:B:4598:LEU:HG	2.06	0.55
2:D:137:VAL:CG1	2:D:141:GLU:HB2	2.35	0.55
1:A:3662:ARG:NH2	1:A:3679:GLU:OE2	2.39	0.55
1:A:3833:LEU:HD12	1:A:3836:ARG:NH2	2.22	0.55
1:B:3833:LEU:HD12	1:B:3836:ARG:NH2	2.22	0.55
1:A:3292:LYS:O	1:A:3295:ILE:HG22	2.07	0.55
1:B:4045:VAL:HG21	1:B:4075:LEU:HB2	1.89	0.55
1:A:3409:ILE:HG12	1:A:3450:LEU:HD22	1.88	0.55
1:B:4423:GLU:HB3	1:B:4459:LEU:HD13	1.88	0.55
2:D:137:VAL:HG13	2:D:141:GLU:CB	2.36	0.55
1:A:4595:VAL:HG21	1:A:4630:LYS:HA	1.88	0.55
1:B:3292:LYS:O	1:B:3295:ILE:HG22	2.07	0.55
1:B:4105:TRP:CD2	2:D:145:MET:HE2	2.42	0.55
1:A:3954:ALA:CB	1:A:3968:LEU:HD21	2.37	0.54
1:B:3955:LEU:HD21	1:B:4012:ILE:HD12	1.89	0.54
1:B:4017:LEU:HD11	1:B:4132:VAL:HG11	1.88	0.54
2:D:28:ILE:HD12	2:D:33:LEU:HA	1.88	0.54
1:B:3187:ASP:OD1	1:B:3190:TRP:NE1	2.39	0.54
1:A:3521:GLU:HG3	1:B:3793:ASN:HA	1.89	0.54
1:A:4295:LEU:O	1:A:4299:THR:HG23	2.07	0.54
1:A:3298:ASP:N	1:A:3298:ASP:OD1	2.38	0.54
1:A:4263:VAL:HG12	1:A:4312:VAL:HG11	1.89	0.54
1:B:4129:LEU:HD23	1:B:4165:LEU:HD23	1.90	0.54
1:B:4355:LYS:CE	1:B:4365:GLY:O	2.56	0.54
1:A:3757:ARG:HB3	1:A:3758:PRO:HD3	1.88	0.54
1:B:4107:GLN:O	1:B:4111:ARG:HG2	2.07	0.54
1:B:4647:TYR:HD1	1:B:4717:PRO:HB2	1.72	0.54
1:A:3034:MET:SD	1:A:3034:MET:N	2.77	0.54
1:A:4105:TRP:CZ2	2:C:129:ALA:HB2	2.42	0.54
1:A:4107:GLN:O	1:A:4111:ARG:HG2	2.07	0.54
1:B:3706:CYS:O	1:B:3710:ARG:NH1	2.41	0.54
1:B:4595:VAL:HG21	1:B:4630:LYS:HB3	1.90	0.54
1:B:3881:GLU:HG2	1:B:3921:MET:HG3	1.88	0.54
1:B:4642:CYS:HA	1:B:4659:LEU:HD13	1.90	0.54
1:A:3706:CYS:O	1:A:3710:ARG:NH1	2.41	0.54
1:A:4032:LYS:HE3	3:E:307:GLN:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4355:LYS:CE	1:A:4365:GLY:O	2.56	0.54
1:A:3881:GLU:HG2	1:A:3921:MET:HG3	1.89	0.53
1:A:4123:LEU:HD13	1:A:4165:LEU:HD22	1.90	0.53
1:B:4309:PHE:CD1	1:B:4338:ILE:CD1	2.91	0.53
2:C:33:LEU:CD1	2:C:72:MET:HE1	2.38	0.53
1:A:3513:TYR:CZ	1:A:3525:TYR:HB3	2.44	0.53
1:A:3818:ILE:HD12	1:B:4230:THR:HG21	1.90	0.53
1:A:4307:LYS:CG	1:A:4478:VAL:CG2	2.84	0.53
1:A:4309:PHE:CE1	1:A:4338:ILE:HD13	2.38	0.53
1:B:4314:ILE:HG22	1:B:4318:LYS:HE3	1.91	0.53
2:D:109:VAL:O	2:D:113:LEU:HG	2.07	0.53
1:B:4423:GLU:CB	1:B:4459:LEU:HD13	2.38	0.53
2:D:117:LEU:HB3	2:D:121:GLU:HB2	1.91	0.53
1:A:3512:ILE:O	1:A:3516:LEU:HG	2.08	0.53
1:A:4228:LEU:HB3	1:B:3822:PHE:CE1	2.42	0.53
1:A:4230:THR:HG21	1:B:3818:ILE:HD12	1.90	0.53
1:A:3793:ASN:CA	1:B:3521:GLU:HG3	2.30	0.53
1:A:3822:PHE:CE1	1:B:4228:LEU:HB3	2.44	0.53
1:B:3512:ILE:O	1:B:3516:LEU:HG	2.08	0.53
1:B:4547:GLU:HG2	1:B:4605:PHE:CE2	2.44	0.53
2:C:59:ASP:HB3	2:C:63:THR:HB	1.89	0.53
1:A:3547:LEU:O	1:A:3551:LYS:HG3	2.09	0.53
1:A:4307:LYS:HB3	1:A:4478:VAL:HG21	1.91	0.53
1:B:4129:LEU:HB3	1:B:4169:TYR:HE2	1.74	0.53
1:B:4314:ILE:CG2	1:B:4484:GLY:HA2	2.39	0.53
1:A:4245:LEU:HD23	1:A:4294:MET:HE1	1.90	0.53
1:B:3408:LEU:HD12	1:B:3411:PHE:CE2	2.44	0.53
1:B:3404:ASP:N	1:B:3404:ASP:OD1	2.41	0.53
1:B:3419:SER:HB3	1:B:3425:ARG:HG3	1.91	0.53
1:B:3751:HIS:O	1:B:3755:GLY:N	2.42	0.53
2:C:30:THR:HB	2:C:53:ILE:HG12	1.90	0.53
1:A:4105:TRP:CE2	2:C:145:MET:HE2	2.44	0.52
1:B:4306:THR:HG22	1:B:4338:ILE:CG2	2.40	0.52
2:D:138:ASN:CG	2:D:139:TYR:H	2.17	0.52
1:A:4096:TYR:CE1	2:C:48:GLU:HG2	2.44	0.52
1:B:3547:LEU:O	1:B:3551:LYS:HG3	2.09	0.52
1:A:4032:LYS:CE	3:E:307:GLN:HG2	2.28	0.52
1:B:3199:MET:HE1	1:B:3232:THR:HA	1.90	0.52
1:B:3763:LEU:O	1:B:3767:VAL:HG23	2.10	0.52
1:B:4245:LEU:HD23	1:B:4294:MET:HE1	1.90	0.52
1:A:3535:CYS:SG	1:A:3872:CYS:SG	3.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3513:TYR:CZ	1:B:3525:TYR:HB3	2.44	0.52
1:B:4017:LEU:CD1	1:B:4132:VAL:HG11	2.40	0.52
1:B:4195:HIS:CD2	2:D:35:THR:HG21	2.45	0.52
2:C:78:LYS:HB2	2:C:80:THR:HG23	1.90	0.52
2:D:105:GLU:HA	2:D:108:HIS:HB2	1.91	0.52
1:B:3309:PHE:HE1	1:B:3411:PHE:HB3	1.74	0.52
1:B:4309:PHE:CE1	1:B:4338:ILE:CD1	2.85	0.52
1:A:3324:SER:OG	1:A:3333:LEU:HD11	2.10	0.52
1:A:3771:ALA:HB1	1:B:3919:ALA:HB2	1.91	0.52
1:B:3749:VAL:O	1:B:3750:TYR:C	2.52	0.52
2:C:49:LEU:HD13	2:C:49:LEU:O	2.09	0.52
3:F:324:LEU:O	3:F:328:LEU:HG	2.10	0.52
1:A:3727:GLU:H	1:A:3731:ASP:HB2	1.75	0.52
1:A:4195:HIS:CD2	2:C:35:THR:HG21	2.44	0.52
1:A:4310:MET:HG2	1:A:4335:LEU:CD2	2.40	0.52
1:B:3324:SER:OG	1:B:3333:LEU:HD11	2.10	0.52
1:B:4048:TYR:HD1	1:B:4048:TYR:H	1.58	0.52
1:B:4647:TYR:OH	1:B:4656:LYS:HA	2.09	0.52
2:D:145:MET:SD	2:D:146:MET:N	2.83	0.52
1:A:3309:PHE:HE1	1:A:3411:PHE:HB3	1.74	0.52
1:B:4306:THR:HG22	1:B:4338:ILE:HG23	1.92	0.52
2:D:117:LEU:O	2:D:118:THR:C	2.53	0.52
1:A:3419:SER:HB3	1:A:3425:ARG:HG3	1.92	0.51
1:B:3936:ASN:HB3	1:B:3939:ALA:HB3	1.93	0.51
1:B:4105:TRP:CE2	2:D:145:MET:HE2	2.44	0.51
1:B:4155:ILE:HB	1:B:4158:ARG:HD2	1.92	0.51
1:A:3522:PHE:H	1:A:3522:PHE:HD1	1.57	0.51
1:A:4423:GLU:CB	1:A:4459:LEU:HD13	2.39	0.51
1:B:3097:TYR:O	1:B:3101:VAL:HG12	2.10	0.51
1:B:3850:THR:CG2	1:B:3853:ALA:HB3	2.39	0.51
1:B:3965:ALA:HA	1:B:4011:ASN:ND2	2.24	0.51
2:C:49:LEU:HD11	2:C:53:ILE:CD1	2.40	0.51
1:A:3200:ILE:HG22	1:A:3202:GLN:H	1.75	0.51
1:A:4128:TRP:HA	1:A:4131:GLN:HG2	1.93	0.51
2:C:33:LEU:HD11	2:C:72:MET:HE1	1.91	0.51
2:C:145:MET:SD	2:C:146:MET:N	2.83	0.51
2:D:18:SER:O	2:D:21:ASP:N	2.41	0.51
1:A:3850:THR:CG2	1:A:3853:ALA:HB3	2.40	0.51
1:B:3405:LYS:HB2	1:B:3450:LEU:HD21	1.93	0.51
1:B:3458:LEU:HD11	1:B:3465:ALA:HB1	1.93	0.51
1:B:4282:LYS:O	1:B:4286:GLU:HG2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3097:TYR:O	1:A:3101:VAL:HG12	2.10	0.51
1:A:3968:LEU:N	1:A:3968:LEU:HD23	2.25	0.51
1:A:3998:LEU:O	1:A:4001:VAL:HG12	2.10	0.51
1:B:3200:ILE:HG22	1:B:3202:GLN:H	1.76	0.51
1:B:4129:LEU:HB3	1:B:4169:TYR:CE2	2.46	0.51
2:D:10:ILE:HA	2:D:13:PHE:CD2	2.46	0.51
1:B:3095:VAL:HG12	1:B:3190:TRP:CZ3	2.46	0.51
1:B:3226:GLN:HA	1:B:3289:ASN:ND2	2.26	0.51
2:C:106:LEU:CD2	2:C:126:ILE:CD1	2.80	0.51
1:A:3053:LEU:HA	1:A:3056:MET:HE2	1.93	0.51
1:A:3536:ASN:O	1:A:3538:PRO:HD3	2.11	0.51
1:A:4130:ARG:HB2	1:A:4169:TYR:CZ	2.46	0.51
1:B:3440:SER:OG	1:B:3443:GLN:OE1	2.20	0.51
1:B:3519:LEU:HD13	1:B:3767:VAL:HG11	1.93	0.51
1:B:4643:ASN:O	1:B:4647:TYR:HB2	2.10	0.51
1:B:3053:LEU:HA	1:B:3056:MET:HE2	1.93	0.51
1:B:3954:ALA:HB3	1:B:3968:LEU:HD11	1.93	0.51
1:A:3818:ILE:HD12	1:B:4230:THR:HG23	1.92	0.51
1:A:4230:THR:HG23	1:B:3818:ILE:HD12	1.92	0.51
2:C:10:ILE:HA	2:C:13:PHE:CD2	2.46	0.51
2:D:100:TYR:CD1	2:D:136:GLN:HB2	2.46	0.50
3:E:324:LEU:O	3:E:328:LEU:HG	2.10	0.50
1:A:3405:LYS:HB2	1:A:3450:LEU:HD21	1.93	0.50
1:A:4155:ILE:HB	1:A:4158:ARG:HD2	1.92	0.50
1:B:3273:MET:HE3	1:B:3273:MET:O	2.11	0.50
1:B:4035:LYS:O	1:B:4036:ASP:C	2.54	0.50
1:B:4599:ASP:HA	1:B:4602:ASN:HD22	1.76	0.50
1:A:3307:VAL:O	1:A:3311:VAL:HG13	2.12	0.50
1:A:3458:LEU:HD11	1:A:3465:ALA:HB1	1.92	0.50
1:A:4282:LYS:O	1:A:4286:GLU:HG2	2.11	0.50
1:B:3307:VAL:O	1:B:3311:VAL:HG13	2.12	0.50
2:D:118:THR:OG1	2:D:120:GLU:HB2	2.12	0.50
1:A:4077:ILE:HG13	1:A:4079:GLY:H	1.76	0.50
1:B:4306:THR:CG2	1:B:4338:ILE:HG23	2.42	0.50
2:C:7:GLU:HA	2:C:10:ILE:HG22	1.93	0.50
1:A:3095:VAL:HG12	1:A:3190:TRP:CZ3	2.46	0.50
1:A:3212:LYS:HA	1:A:3215:LEU:HG	1.94	0.50
1:A:4108:PHE:O	1:A:4112:ARG:HG3	2.12	0.50
1:A:4307:LYS:CD	1:A:4478:VAL:HG21	2.40	0.50
1:A:4438:MET:HE3	1:A:4440:ILE:HD11	1.94	0.50
1:A:4492:LEU:CD1	1:A:4512:PHE:CE2	2.95	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4089:LYS:HA	1:B:4092:LEU:HD12	1.92	0.50
1:B:4307:LYS:HA	1:B:4310:MET:HE2	1.93	0.50
1:B:4492:LEU:CD1	1:B:4512:PHE:CE2	2.95	0.50
2:D:14:LYS:HD3	2:D:66:PHE:CD2	2.46	0.50
1:B:4310:MET:HE1	1:B:4478:VAL:HG21	1.94	0.49
2:C:44:PRO:HB2	2:C:48:GLU:HB2	1.94	0.49
2:D:87:ARG:HG3	2:D:139:TYR:HE1	1.77	0.49
1:A:3273:MET:HE3	1:A:3273:MET:O	2.11	0.49
1:A:3404:ASP:OD1	1:A:3404:ASP:N	2.41	0.49
1:A:3968:LEU:HD13	1:A:4012:ILE:HD11	1.92	0.49
1:B:3588:ARG:HG3	1:B:3648:TYR:CZ	2.47	0.49
1:A:4310:MET:HE1	1:A:4475:MET:HE3	1.94	0.49
1:B:4505:LEU:HD22	1:B:4558:VAL:HG11	1.93	0.49
2:C:65:ASP:H	2:C:68:GLU:HB3	1.78	0.49
3:E:309:MET:O	3:E:313:ARG:HG2	2.12	0.49
1:A:3726:ILE:HD12	1:A:3828:LEU:HA	1.94	0.49
1:A:4275:LYS:HZ2	1:A:4327:THR:HG21	1.72	0.49
1:A:4355:LYS:NZ	1:A:4363:LEU:O	2.40	0.49
1:B:3940:THR:HG21	1:B:3985:CYS:HB3	1.93	0.49
1:B:4523:GLN:NE2	1:B:4576:GLU:OE1	2.46	0.49
1:A:3408:LEU:HD12	1:A:3411:PHE:CE2	2.44	0.49
1:A:4098:THR:HA	2:C:93:PHE:CE2	2.47	0.49
1:B:4438:MET:HE3	1:B:4440:ILE:HD11	1.94	0.49
2:D:124:GLU:O	2:D:128:GLU:HG2	2.12	0.49
1:A:3324:SER:HG	1:A:3333:LEU:HD11	1.78	0.49
1:A:3548:SER:HA	1:A:3551:LYS:HE2	1.95	0.49
1:A:4001:VAL:C	1:A:4003:ILE:N	2.69	0.49
3:F:301:MET:SD	3:F:306:ARG:HG3	2.53	0.49
1:A:3262:SER:HA	1:A:3833:LEU:HD23	1.95	0.49
1:A:4310:MET:HG2	1:A:4335:LEU:HD23	1.92	0.49
1:A:4608:SER:O	1:A:4610:PRO:HD3	2.13	0.49
1:A:3412:LEU:HD22	1:A:3454:ILE:HD12	1.95	0.49
1:A:3850:THR:O	1:A:3851:PHE:C	2.56	0.49
1:A:4505:LEU:HD22	1:A:4558:VAL:HG11	1.93	0.49
1:B:3412:LEU:HD22	1:B:3454:ILE:HD12	1.95	0.49
1:A:3988:LEU:HD12	1:A:3988:LEU:H	1.77	0.48
3:E:301:MET:SD	3:E:306:ARG:HG3	2.53	0.48
1:A:4032:LYS:HE2	3:E:307:GLN:CD	2.38	0.48
1:B:3968:LEU:CD1	1:B:4012:ILE:HD11	2.43	0.48
1:B:4071:TRP:O	1:B:4075:LEU:HD12	2.13	0.48
1:A:3309:PHE:CE1	1:A:3411:PHE:HB3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3955:LEU:HD21	1:A:4012:ILE:CD1	2.41	0.48
1:B:4252:GLU:O	1:B:4256:ARG:HG3	2.13	0.48
2:D:105:GLU:O	2:D:109:VAL:HG23	2.14	0.48
2:D:145:MET:SD	2:D:146:MET:SD	3.12	0.48
1:A:3308:SER:HA	1:A:3319:LEU:HD13	1.95	0.48
1:A:4424:VAL:HA	1:A:4459:LEU:HD21	1.95	0.48
1:B:3292:LYS:HA	1:B:3295:ILE:HG22	1.96	0.48
2:C:132:ASP:OD1	2:C:133:GLY:N	2.47	0.48
2:D:103:ALA:HB2	2:D:126:ILE:CG1	2.30	0.48
1:A:4071:TRP:O	1:A:4075:LEU:HD12	2.13	0.48
1:B:4108:PHE:CE2	2:D:146:MET:O	2.66	0.48
3:F:309:MET:O	3:F:313:ARG:HG2	2.12	0.48
1:A:4252:GLU:O	1:A:4256:ARG:HG3	2.13	0.48
1:A:4310:MET:HE1	1:A:4475:MET:CE	2.44	0.48
1:B:3262:SER:HA	1:B:3833:LEU:HD23	1.95	0.48
1:B:3749:VAL:HA	1:B:3752:GLN:HG3	1.95	0.48
1:B:4021:GLN:HE21	1:B:4025:LYS:HE2	1.78	0.48
2:C:52:MET:O	2:C:56:VAL:HG22	2.13	0.48
2:D:7:GLU:HA	2:D:10:ILE:HG22	1.94	0.48
1:A:4159:LYS:HZ3	1:A:4196:TRP:CD1	2.31	0.48
1:A:3418:GLU:HG2	1:A:3461:TYR:CE1	2.49	0.48
1:A:4310:MET:HG3	1:A:4335:LEU:CD2	2.41	0.48
1:B:3169:TYR:HD1	1:B:3213:LEU:HD13	1.79	0.48
1:B:3226:GLN:OE1	1:B:3227:LEU:HD22	2.14	0.48
1:B:3309:PHE:CE1	1:B:3411:PHE:HB3	2.48	0.48
1:B:3964:LEU:HD22	1:B:4007:VAL:HG12	1.95	0.48
1:B:4053:HIS:CE1	1:B:4118:PRO:HB3	2.49	0.48
2:D:33:LEU:HD13	2:D:64:ILE:HG21	1.95	0.48
1:A:4299:THR:HG22	1:A:4309:PHE:CE2	2.49	0.48
1:B:4135:THR:O	1:B:4142:ARG:NH1	2.36	0.48
1:A:3169:TYR:HD1	1:A:3213:LEU:HD13	1.79	0.48
1:A:4108:PHE:CE2	2:C:146:MET:O	2.67	0.48
1:B:3955:LEU:HD12	1:B:3999:MET:HE3	1.96	0.48
1:B:4651:HIS:HD2	1:B:4656:LYS:HB2	1.78	0.48
2:C:100:TYR:CB	2:C:136:GLN:HB3	2.44	0.48
1:A:3071:LYS:HB3	1:A:3074:ILE:HB	1.95	0.47
1:A:4134:PHE:CD2	1:A:4172:GLU:HG2	2.49	0.47
1:B:4071:TRP:CE2	1:B:4075:LEU:HD11	2.49	0.47
1:A:3884:ILE:HD11	1:A:3913:ASN:HD22	1.79	0.47
1:A:3954:ALA:HB3	1:A:3968:LEU:HD21	1.96	0.47
1:A:4230:THR:CG2	1:B:3818:ILE:HG23	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3212:LYS:HA	1:B:3215:LEU:HG	1.95	0.47
1:B:3872:CYS:O	1:B:3873:TYR:C	2.57	0.47
1:B:3850:THR:O	1:B:3851:PHE:C	2.56	0.47
1:B:3884:ILE:HD11	1:B:3913:ASN:HD22	1.80	0.47
2:C:145:MET:SD	2:C:146:MET:SD	3.12	0.47
1:A:3533:LEU:HD12	1:A:3533:LEU:H	1.80	0.47
1:A:3588:ARG:HG3	1:A:3648:TYR:CZ	2.49	0.47
2:C:49:LEU:CD1	2:C:53:ILE:HD12	2.44	0.47
2:D:20:PHE:HE1	2:D:35:THR:CG2	2.26	0.47
1:A:3292:LYS:HA	1:A:3295:ILE:HG22	1.96	0.47
1:A:3872:CYS:O	1:A:3873:TYR:C	2.57	0.47
1:A:4071:TRP:CE2	1:A:4075:LEU:HD11	2.49	0.47
1:A:4129:LEU:HD11	1:A:4149:VAL:HG21	1.95	0.47
1:A:4695:MET:HE1	1:A:4748:LEU:HD21	1.96	0.47
1:B:3308:SER:HA	1:B:3319:LEU:HD13	1.96	0.47
1:B:3548:SER:HA	1:B:3551:LYS:HE2	1.95	0.47
1:B:4101:TYR:HB3	2:D:146:MET:SD	2.55	0.47
2:C:19:LEU:HD23	2:C:19:LEU:HA	1.77	0.47
1:A:4101:TYR:HB3	2:C:146:MET:SD	2.55	0.47
1:A:4119:LEU:HD23	3:E:329:VAL:HG21	1.96	0.47
1:A:4413:LYS:HD3	1:A:4456:ILE:HD11	1.96	0.47
1:B:3455:TRP:CZ3	1:B:3458:LEU:HD22	2.50	0.47
1:B:4275:LYS:HZ2	1:B:4327:THR:HG21	1.72	0.47
1:B:4642:CYS:SG	1:B:4643:ASN:N	2.88	0.47
1:B:4644:PHE:HB3	1:B:4694:TYR:CD2	2.49	0.47
2:C:66:PHE:HB3	2:C:67:PRO:HD3	1.97	0.47
1:A:3226:GLN:HA	1:A:3289:ASN:ND2	2.28	0.47
1:A:3456:PRO:HA	1:A:3496:ILE:HD11	1.96	0.47
1:A:4006:PRO:HG2	1:B:3507:HIS:O	2.14	0.47
1:A:4419:LEU:HD13	1:A:4459:LEU:HG	1.96	0.47
1:B:3417:LEU:HD13	1:B:3461:TYR:CD2	2.49	0.47
1:B:3515:THR:O	1:B:3519:LEU:HG	2.15	0.47
1:B:4109:LEU:HG	1:B:4115:ARG:HB2	1.97	0.47
1:B:4119:LEU:HD11	3:F:329:VAL:HG11	1.97	0.47
1:B:4311:ALA:O	1:B:4315:GLU:HG2	2.15	0.47
1:B:4413:LYS:HD3	1:B:4456:ILE:HD11	1.96	0.47
2:C:131:ILE:HD11	2:C:144:GLN:HG2	1.96	0.47
1:A:3005:MET:O	1:A:3008:THR:OG1	2.33	0.47
1:A:3571:ILE:HG12	1:A:3717:ALA:HB2	1.97	0.47
1:B:3194:LEU:HD13	1:B:3214:LEU:HD21	1.97	0.47
1:B:3324:SER:HG	1:B:3333:LEU:HD11	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3727:GLU:H	1:B:3731:ASP:HB2	1.80	0.47
1:B:3969:GLN:O	1:B:3973:LEU:HG	2.15	0.47
1:B:4307:LYS:HG2	1:B:4475:MET:HE3	1.96	0.47
2:D:102:SER:HB2	2:D:105:GLU:OE1	2.15	0.47
1:A:3298:ASP:HB3	1:A:3398:GLN:CD	2.39	0.47
1:B:3298:ASP:HB3	1:B:3398:GLN:CD	2.39	0.47
1:B:3456:PRO:HA	1:B:3496:ILE:HD11	1.96	0.47
1:A:3515:THR:O	1:A:3519:LEU:HG	2.15	0.47
1:A:3750:TYR:HB2	1:B:4232:LEU:HD13	1.22	0.47
2:C:28:ILE:HG22	2:C:32:GLU:HG2	1.96	0.47
2:D:103:ALA:CB	2:D:126:ILE:HG13	2.28	0.47
1:A:3226:GLN:OE1	1:A:3227:LEU:HD22	2.14	0.46
1:A:3417:LEU:HD13	1:A:3461:TYR:CD2	2.49	0.46
1:A:3732:ARG:NH2	1:B:4277:VAL:HG21	2.30	0.46
1:B:3004:LEU:O	1:B:3008:THR:HG23	2.16	0.46
1:B:3418:GLU:HG2	1:B:3461:TYR:CE1	2.49	0.46
1:A:3527:LEU:HD21	1:A:3757:ARG:HD3	1.98	0.46
1:B:3005:MET:O	1:B:3008:THR:OG1	2.33	0.46
2:D:119:ASP:HA	2:D:122:VAL:HG23	1.96	0.46
1:A:3090:LEU:HD11	1:A:3184:PRO:HB3	1.97	0.46
1:A:3419:SER:HB3	1:A:3425:ARG:CG	2.46	0.46
1:A:3793:ASN:ND2	1:B:3519:LEU:C	2.68	0.46
1:A:3848:GLN:C	1:A:3850:THR:H	2.24	0.46
1:B:3071:LYS:HB3	1:B:3074:ILE:HB	1.96	0.46
1:B:3301:LEU:HD23	1:B:3301:LEU:HA	1.76	0.46
1:B:3419:SER:HB3	1:B:3425:ARG:CG	2.45	0.46
1:B:3905:LEU:HD23	1:B:3932:LEU:HD11	1.96	0.46
1:A:3455:TRP:CZ3	1:A:3458:LEU:HD22	2.50	0.46
1:A:4001:VAL:C	1:A:4003:ILE:H	2.22	0.46
1:A:4101:TYR:HA	1:A:4104:ARG:HB2	1.97	0.46
1:A:4232:LEU:HD13	1:B:3750:TYR:CG	2.50	0.46
1:B:4639:LYS:HB2	1:B:4640:PRO:HD3	1.97	0.46
2:C:12:GLU:O	2:C:15:GLU:HB3	2.16	0.46
2:D:70:LEU:HA	2:D:73:MET:HG2	1.97	0.46
1:A:3887:LEU:HD13	1:A:3905:LEU:HD21	1.98	0.46
1:A:4419:LEU:HD22	1:A:4459:LEU:HD12	1.97	0.46
1:B:4634:LEU:HA	1:B:4637:ARG:HD2	1.98	0.46
1:B:4640:PRO:O	1:B:4643:ASN:ND2	2.48	0.46
2:D:42:GLN:OE1	2:D:77:MET:HG3	2.16	0.46
2:D:69:PHE:HA	2:D:72:MET:HE2	1.98	0.46
1:A:4281:THR:HG22	1:A:4283:LEU:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4640:PRO:C	1:A:4642:CYS:H	2.24	0.46
1:B:3305:LEU:HB2	1:B:3323:LEU:HD21	1.96	0.46
1:A:3301:LEU:HD23	1:A:3301:LEU:HA	1.76	0.46
1:A:3305:LEU:HB2	1:A:3323:LEU:HD21	1.96	0.46
1:A:3478:LYS:HD2	1:A:3478:LYS:HA	1.83	0.46
1:A:4195:HIS:NE2	2:C:35:THR:HG21	2.30	0.46
1:A:4631:MET:O	1:A:4634:LEU:HG	2.15	0.46
1:B:3909:LEU:HD22	1:B:3925:VAL:HG13	1.98	0.46
1:B:4310:MET:HE1	1:B:4478:VAL:CG2	2.45	0.46
1:B:4646:LYS:HE2	1:B:4651:HIS:HA	1.96	0.46
2:D:93:PHE:HB2	2:D:109:VAL:HG21	1.97	0.46
1:A:3226:GLN:HA	1:A:3289:ASN:HD22	1.81	0.46
1:A:4277:VAL:HG21	1:B:3732:ARG:NH2	2.30	0.46
1:A:4467:GLU:HB3	1:A:4472:VAL:HG21	1.98	0.46
1:B:3848:GLN:C	1:B:3850:THR:H	2.24	0.46
2:D:20:PHE:HD1	2:D:32:GLU:HB3	1.80	0.46
1:A:4310:MET:SD	1:A:4338:ILE:HD13	2.55	0.46
1:B:3190:TRP:CD1	1:B:3190:TRP:N	2.83	0.46
1:B:3910:PHE:HB2	1:B:3929:MET:HE1	1.97	0.46
1:B:4101:TYR:HA	1:B:4104:ARG:HB2	1.97	0.46
1:B:4281:THR:HG22	1:B:4283:LEU:H	1.81	0.46
1:B:4695:MET:HE1	1:B:4748:LEU:HD21	1.96	0.46
2:C:73:MET:O	2:C:77:MET:N	2.48	0.46
2:D:12:GLU:O	2:D:15:GLU:HB3	2.16	0.46
1:A:3234:ASP:O	1:A:3238:ARG:HG2	2.16	0.46
1:A:3791:SER:O	1:B:3521:GLU:HB2	2.16	0.46
1:A:3818:ILE:HG23	1:B:4230:THR:CG2	2.45	0.46
1:B:3757:ARG:HB3	1:B:3758:PRO:HD3	1.98	0.46
1:B:3840:THR:HG22	1:B:3843:SER:HB2	1.97	0.46
2:D:52:MET:CE	2:D:76:LYS:HB2	2.46	0.46
3:E:302:SER:OG	3:E:305:GLU:HB3	2.16	0.46
3:F:302:SER:OG	3:F:305:GLU:HB3	2.16	0.46
1:A:3825:ARG:HH21	1:B:4230:THR:HB	1.82	0.45
2:C:9:GLN:O	2:C:13:PHE:CG	2.70	0.45
1:A:3004:LEU:O	1:A:3008:THR:HG23	2.15	0.45
1:A:4128:TRP:HA	1:A:4131:GLN:CG	2.47	0.45
1:A:4639:LYS:HB3	1:A:4640:PRO:HD3	1.98	0.45
1:A:3909:LEU:HD22	1:A:3925:VAL:HG13	1.98	0.45
1:A:3910:PHE:HB2	1:A:3929:MET:HE1	1.97	0.45
1:B:3090:LEU:HD11	1:B:3184:PRO:HB3	1.97	0.45
1:B:3571:ILE:HG12	1:B:3717:ALA:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3714:MET:HE3	1:B:3714:MET:HB3	1.78	0.45
1:B:4047:PRO:O	1:B:4048:TYR:C	2.60	0.45
2:D:51:ASP:HA	2:D:54:ASN:HD22	1.81	0.45
1:A:3251:LEU:HD12	1:A:3303:PHE:CD2	2.52	0.45
1:A:3791:SER:C	1:B:3521:GLU:HB2	2.41	0.45
1:B:3328:CYS:O	1:B:3332:VAL:HG12	2.16	0.45
1:B:3965:ALA:HA	1:B:4011:ASN:HD21	1.81	0.45
1:B:4130:ARG:O	1:B:4131:GLN:C	2.60	0.45
1:B:4316:THR:HA	1:B:4319:ARG:HD2	1.97	0.45
2:D:121:GLU:O	2:D:125:MET:HG2	2.16	0.45
1:A:3194:LEU:HD13	1:A:3214:LEU:HD21	1.97	0.45
1:A:3195:SER:HG	1:A:3231:HIS:CE1	2.32	0.45
1:A:3328:CYS:O	1:A:3332:VAL:HG12	2.16	0.45
1:A:3626:GLU:OE1	1:A:3628:LYS:HE3	2.17	0.45
1:A:3880:THR:O	1:A:3884:ILE:HG12	2.16	0.45
1:A:4307:LYS:HD3	1:A:4475:MET:CE	2.46	0.45
1:B:3626:GLU:OE1	1:B:3628:LYS:HE3	2.17	0.45
1:B:4011:ASN:O	1:B:4015:MET:HG2	2.16	0.45
1:A:3840:THR:HG22	1:A:3843:SER:HB2	1.98	0.45
1:B:3766:LYS:HB3	1:B:3795:TYR:CD2	2.52	0.45
1:B:3887:LEU:HD13	1:B:3905:LEU:HD21	1.98	0.45
2:D:39:SER:C	2:D:41:GLY:H	2.25	0.45
1:A:3826:LYS:N	1:B:4228:LEU:HD12	2.31	0.45
1:A:4170:LEU:O	1:A:4173:LEU:HB3	2.17	0.45
1:B:4170:LEU:O	1:B:4173:LEU:HB3	2.17	0.45
2:C:138:ASN:C	2:C:140:GLU:N	2.71	0.45
2:D:120:GLU:O	2:D:123:ASP:HB2	2.17	0.45
1:A:3324:SER:OG	1:A:3328:CYS:SG	2.56	0.45
1:A:4098:THR:HB	2:C:109:VAL:HG13	1.99	0.45
1:A:4299:THR:HG21	1:A:4334:ARG:HH21	1.81	0.45
1:A:4360:GLU:CD	1:A:4366:ARG:HH21	2.24	0.45
1:A:4606:VAL:HG13	1:A:4612:VAL:HG12	1.98	0.45
1:B:3051:VAL:O	1:B:3055:VAL:HG23	2.17	0.45
1:B:4413:LYS:CD	1:B:4456:ILE:HD11	2.47	0.45
1:A:3051:VAL:O	1:A:3055:VAL:HG23	2.17	0.44
1:A:3440:SER:OG	1:A:3443:GLN:OE1	2.20	0.44
1:A:3532:CYS:CB	1:A:3868:SER:HA	2.43	0.44
1:A:4047:PRO:HA	1:A:4075:LEU:HD23	1.99	0.44
1:A:4310:MET:SD	1:A:4338:ILE:CG2	2.82	0.44
1:B:3273:MET:HG3	1:B:3633:LEU:CD2	2.48	0.44
1:B:3286:ARG:HH21	1:B:3286:ARG:HG3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3642:ILE:HD13	1:B:3713:PHE:CE1	2.52	0.44
1:B:3880:THR:O	1:B:3884:ILE:HG12	2.16	0.44
1:B:3922:ARG:NH1	1:B:3970:TYR:OH	2.50	0.44
2:D:18:SER:O	2:D:19:LEU:C	2.60	0.44
2:D:101:ILE:N	2:D:137:VAL:O	2.46	0.44
1:A:3642:ILE:HD13	1:A:3713:PHE:CE1	2.52	0.44
1:A:3951:VAL:CG1	1:A:4012:ILE:HD13	2.44	0.44
1:B:4360:GLU:CD	1:B:4366:ARG:HH21	2.24	0.44
2:C:89:ALA:HB3	2:C:142:PHE:HE2	1.81	0.44
1:A:4101:TYR:CE2	2:C:89:ALA:HB2	2.52	0.44
1:A:4598:LEU:HD12	1:A:4634:LEU:HD22	1.99	0.44
1:B:3234:ASP:O	1:B:3238:ARG:HG2	2.16	0.44
1:B:3889:ALA:HB2	3:F:293:LEU:HD13	1.99	0.44
1:B:4093:ARG:NH2	2:D:51:ASP:OD2	2.51	0.44
2:D:9:GLN:O	2:D:13:PHE:CG	2.70	0.44
1:A:4228:LEU:HD12	1:B:3826:LYS:N	2.30	0.44
1:B:3461:TYR:O	1:B:3534:VAL:HG11	2.17	0.44
1:B:3950:LYS:O	1:B:3953:THR:HG22	2.18	0.44
2:D:56:VAL:HG13	2:D:72:MET:SD	2.57	0.44
1:A:3412:LEU:O	1:A:3416:LEU:HB2	2.18	0.44
1:A:4230:THR:HB	1:B:3825:ARG:HH21	1.82	0.44
1:A:4281:THR:HB	1:A:4284:ILE:HG12	2.00	0.44
1:B:4651:HIS:CD2	1:B:4656:LYS:HB2	2.53	0.44
2:D:13:PHE:N	2:D:13:PHE:CD1	2.83	0.44
3:E:317:SER:O	3:E:321:GLN:HG3	2.17	0.44
1:A:4017:LEU:HD11	1:A:4132:VAL:HG11	1.98	0.44
1:A:4413:LYS:CD	1:A:4456:ILE:HD11	2.47	0.44
1:B:3323:LEU:O	1:B:3327:LEU:HB2	2.18	0.44
1:B:4125:HIS:HA	1:B:4165:LEU:HD12	1.99	0.44
1:B:4295:LEU:HD11	1:B:4309:PHE:CE2	2.48	0.44
1:A:3273:MET:HG3	1:A:3633:LEU:CD2	2.48	0.44
1:A:3520:VAL:HG11	1:A:3799:LEU:HD22	2.00	0.44
1:A:3957:GLY:O	1:A:3958:HIS:C	2.61	0.44
2:D:81:ASP:O	2:D:85:GLU:N	2.51	0.44
3:F:301:MET:HE1	3:F:305:GLU:HG2	2.00	0.44
1:A:3490:SER:O	1:A:3494:VAL:HG23	2.18	0.44
1:A:4115:ARG:NH2	2:C:125:MET:SD	2.91	0.44
1:B:3251:LEU:HD12	1:B:3303:PHE:CD2	2.52	0.44
1:B:4631:MET:O	1:B:4634:LEU:HG	2.18	0.44
2:D:132:ASP:OD1	2:D:132:ASP:N	2.50	0.44
3:E:301:MET:HE1	3:E:305:GLU:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4275:LYS:HZ1	1:A:4327:THR:HG21	1.79	0.43
1:A:4278:VAL:O	1:B:3825:ARG:HD3	2.18	0.43
1:A:4621:PRO:HB3	1:A:4668:GLY:HA3	2.00	0.43
1:B:3412:LEU:O	1:B:3416:LEU:HB2	2.18	0.43
1:B:3899:ILE:O	1:B:3903:GLN:HG2	2.18	0.43
1:B:4414:ILE:HD11	1:B:4451:ALA:HB1	2.00	0.43
1:B:4671:ASN:CB	1:B:4732:GLN:OE1	2.54	0.43
2:C:85:GLU:HA	2:C:88:GLU:HB2	2.00	0.43
2:C:145:MET:O	2:C:147:THR:N	2.51	0.43
2:D:42:GLN:HE22	2:D:76:LYS:HG3	1.82	0.43
2:D:90:PHE:HB2	2:D:142:PHE:CD2	2.53	0.43
1:B:3951:VAL:HA	1:B:3968:LEU:HD21	2.00	0.43
1:B:4590:ASP:OD1	1:B:4593:GLN:HG3	2.18	0.43
1:A:3294:CYS:HB3	1:A:3301:LEU:HG	1.99	0.43
1:A:3889:ALA:HB2	3:E:293:LEU:HD13	2.00	0.43
1:A:3899:ILE:O	1:A:3903:GLN:HG2	2.19	0.43
1:A:4146:CYS:HA	1:A:4186:LEU:HD22	2.00	0.43
1:B:3490:SER:O	1:B:3494:VAL:HG23	2.18	0.43
1:B:4281:THR:HB	1:B:4284:ILE:HG12	2.00	0.43
1:B:4372:TYR:HD1	1:B:4376:GLU:OE2	2.02	0.43
1:B:4600:GLN:O	1:B:4603:SER:HB3	2.18	0.43
1:B:4643:ASN:O	1:B:4644:PHE:C	2.61	0.43
2:C:54:ASN:C	2:C:56:VAL:N	2.77	0.43
1:B:3998:LEU:O	1:B:4001:VAL:HG12	2.18	0.43
1:B:4003:ILE:HB	1:B:4008:VAL:HG11	2.00	0.43
1:B:4273:LEU:HD12	1:B:4291:LEU:HD12	2.00	0.43
1:B:4310:MET:HE2	1:B:4310:MET:HB2	1.85	0.43
1:B:4646:LYS:HG2	1:B:4650:ASP:O	2.17	0.43
2:C:27:THR:HA	2:C:61:ASN:HA	2.00	0.43
2:C:138:ASN:HB3	2:C:140:GLU:CG	2.36	0.43
2:D:10:ILE:O	2:D:13:PHE:HB2	2.19	0.43
1:A:3940:THR:HG21	1:A:3985:CYS:CB	2.46	0.43
1:A:3986:TRP:CZ2	3:E:316:ARG:HG2	2.54	0.43
1:A:4299:THR:HG21	1:A:4334:ARG:HE	1.84	0.43
1:A:4599:ASP:HA	1:A:4602:ASN:HD22	1.84	0.43
1:B:2993:GLY:O	1:B:2997:ILE:HG13	2.18	0.43
1:B:3295:ILE:HD12	1:B:3295:ILE:HA	1.91	0.43
1:B:3595:ASN:HD21	1:B:3605:LEU:HD13	1.83	0.43
1:B:4109:LEU:CD1	1:B:4114:LYS:HB2	2.47	0.43
1:B:4146:CYS:HA	1:B:4186:LEU:HD22	2.01	0.43
1:A:3207:ARG:O	1:A:3211:ARG:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3595:ASN:HD21	1:A:3605:LEU:HD13	1.83	0.43
1:A:3967:SER:C	1:A:3969:GLN:N	2.72	0.43
1:A:4007:VAL:HG22	1:B:3511:ASN:HB2	2.00	0.43
1:A:4313:CYS:HB3	1:A:4331:ILE:CG2	2.47	0.43
1:A:4414:ILE:HD11	1:A:4451:ALA:HB1	2.00	0.43
1:B:3760:LEU:HD13	1:B:3760:LEU:HA	1.90	0.43
3:F:317:SER:O	3:F:321:GLN:HG3	2.18	0.43
1:A:4372:TYR:HD1	1:A:4376:GLU:OE2	2.02	0.43
3:E:295:ARG:O	3:E:295:ARG:HG2	2.19	0.43
1:A:3974:LEU:O	1:A:3975:LEU:C	2.57	0.43
1:A:4363:LEU:HD21	1:A:4444:MET:HG3	2.01	0.43
1:B:3207:ARG:O	1:B:3211:ARG:HG3	2.18	0.43
1:B:4638:PHE:HA	1:B:4641:TYR:CD2	2.54	0.43
2:D:38:ARG:HD2	2:D:43:ASN:HA	2.00	0.43
1:A:3323:LEU:O	1:A:3327:LEU:HB2	2.19	0.43
1:A:3525:TYR:HE2	1:A:3874:GLY:HA2	1.83	0.43
1:A:3699:LEU:HD23	1:A:3706:CYS:HB2	2.01	0.43
1:B:3764:LEU:HD23	1:B:3764:LEU:HA	1.70	0.43
1:B:3855:GLN:C	1:B:3855:GLN:CD	2.87	0.43
2:C:34:GLY:HA2	2:C:37:MET:HE2	2.01	0.43
2:D:73:MET:HE3	2:D:73:MET:HB2	1.67	0.43
1:A:3544:TYR:HB3	1:A:3714:MET:CE	2.48	0.43
1:A:3727:GLU:H	1:A:3731:ASP:CB	2.31	0.43
1:A:3884:ILE:HD11	1:A:3913:ASN:ND2	2.34	0.43
1:A:4029:PRO:HB3	3:E:310:GLU:OE1	2.19	0.43
1:A:4273:LEU:HD12	1:A:4291:LEU:HD12	2.00	0.43
1:B:3294:CYS:HB3	1:B:3301:LEU:HG	1.99	0.43
1:B:3396:VAL:HG11	1:B:3438:ASN:CB	2.49	0.43
1:B:4258:PHE:HE1	2:D:19:LEU:CD2	2.31	0.43
2:D:145:MET:O	2:D:147:THR:N	2.52	0.43
1:A:2993:GLY:O	1:A:2997:ILE:HG13	2.18	0.42
1:A:3997:PHE:HB2	1:A:4016:CYS:CB	2.42	0.42
2:C:13:PHE:N	2:C:13:PHE:CD1	2.83	0.42
1:A:3967:SER:O	1:A:3968:LEU:C	2.63	0.42
1:A:4003:ILE:HB	1:A:4008:VAL:HG11	2.01	0.42
1:A:4031:SER:HB3	3:E:303:GLU:OE1	2.17	0.42
1:B:3525:TYR:HE2	1:B:3874:GLY:HA2	1.84	0.42
1:B:4621:PRO:HB3	1:B:4668:GLY:HA3	2.00	0.42
2:D:28:ILE:H	2:D:28:ILE:HG12	1.48	0.42
1:A:3525:TYR:CE2	1:A:3874:GLY:HA2	2.54	0.42
1:A:3801:GLN:HA	1:B:3788:THR:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4199:TYR:HE1	2:C:39:SER:HA	1.84	0.42
1:B:3986:TRP:CZ2	3:F:316:ARG:HG2	2.54	0.42
1:B:4597:LEU:HD22	1:B:4616:LEU:HD11	2.00	0.42
1:A:3979:ILE:HD12	1:A:4019:ILE:HG21	2.01	0.42
1:A:4159:LYS:HE2	1:A:4159:LYS:HB3	1.84	0.42
1:B:3794:ARG:O	1:B:3798:GLN:HG3	2.19	0.42
1:B:4129:LEU:O	1:B:4130:ARG:C	2.62	0.42
1:B:4632:GLN:HG2	1:B:4681:LEU:HD21	2.01	0.42
1:A:3825:ARG:HD3	1:B:4278:VAL:O	2.19	0.42
1:B:3269:LEU:HB3	1:B:3633:LEU:HD12	1.92	0.42
1:B:3647:PHE:HB2	1:B:3649:GLU:HG3	2.00	0.42
2:D:16:ALA:O	2:D:20:PHE:HD2	2.02	0.42
2:D:45:THR:OG1	2:D:48:GLU:HG3	2.19	0.42
1:A:4128:TRP:O	1:A:4129:LEU:C	2.62	0.42
1:B:3029:ILE:O	1:B:3034:MET:HE1	2.19	0.42
1:B:3525:TYR:CE2	1:B:3874:GLY:HA2	2.54	0.42
1:B:3884:ILE:HD11	1:B:3913:ASN:ND2	2.34	0.42
2:D:52:MET:O	2:D:55:GLU:HB3	2.20	0.42
1:A:3233:LEU:HD13	1:A:3290:TRP:HE3	1.85	0.42
1:A:3791:SER:O	1:B:3521:GLU:CB	2.68	0.42
1:A:3963:ASP:C	1:A:3965:ALA:N	2.77	0.42
1:B:3699:LEU:HD23	1:B:3706:CYS:HB2	2.01	0.42
1:B:3753:LEU:HD12	1:B:3753:LEU:HA	1.81	0.42
2:C:140:GLU:O	2:C:143:VAL:HB	2.18	0.42
3:F:318:LEU:O	3:F:322:GLU:HG2	2.20	0.42
1:A:3311:VAL:HG23	1:A:3312:ASP:O	2.20	0.42
1:A:3396:VAL:HG11	1:A:3438:ASN:CB	2.49	0.42
1:A:3453:SER:O	1:A:3456:PRO:HD2	2.20	0.42
1:B:3922:ARG:O	1:B:3926:ARG:HG3	2.20	0.42
1:B:4125:HIS:HA	1:B:4165:LEU:CD1	2.50	0.42
1:B:4637:ARG:O	1:B:4640:PRO:HD2	2.20	0.42
3:E:330:ARG:HE	3:E:332:GLU:HG3	1.85	0.42
1:B:3298:ASP:HB3	1:B:3398:GLN:OE1	2.20	0.42
1:B:3387:GLN:HG2	1:B:3388:GLU:N	2.35	0.42
1:A:3855:GLN:CD	1:A:3855:GLN:C	2.87	0.42
1:A:3954:ALA:CB	1:A:3968:LEU:HD11	2.47	0.42
1:A:4547:GLU:HG2	1:A:4605:PHE:CE2	2.55	0.42
1:B:3954:ALA:O	1:B:3964:LEU:HD12	2.19	0.42
1:B:4299:THR:HG21	1:B:4334:ARG:HH21	1.83	0.42
1:B:4355:LYS:NZ	1:B:4363:LEU:O	2.40	0.42
1:A:3101:VAL:O	1:A:3105:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3955:LEU:HD22	1:A:4003:ILE:HD12	2.02	0.41
1:B:4267:LEU:HD12	1:B:4267:LEU:HA	1.91	0.41
1:B:4363:LEU:HD21	1:B:4444:MET:HG3	2.00	0.41
2:C:10:ILE:O	2:C:13:PHE:HB2	2.19	0.41
2:D:130:ASP:OD2	2:D:135:GLY:N	2.48	0.41
2:D:141:GLU:O	2:D:144:GLN:HB3	2.20	0.41
1:A:3029:ILE:O	1:A:3034:MET:HE1	2.19	0.41
1:A:3522:PHE:HD2	1:A:3803:TYR:CE1	2.39	0.41
1:A:4108:PHE:HA	1:A:4111:ARG:CG	2.50	0.41
1:A:4419:LEU:HD21	1:A:4458:SER:HA	2.01	0.41
1:B:3101:VAL:O	1:B:3105:LEU:HG	2.20	0.41
1:B:3409:ILE:HD13	1:B:3454:ILE:HD11	2.01	0.41
1:B:3964:LEU:CD2	1:B:4011:ASN:HD22	2.32	0.41
2:C:18:SER:O	2:C:19:LEU:C	2.63	0.41
1:A:3269:LEU:HB3	1:A:3633:LEU:HD13	1.91	0.41
1:A:3320:LEU:HD12	1:A:3424:VAL:HG13	2.03	0.41
1:A:3991:ARG:HA	1:A:4059:TRP:CZ3	2.55	0.41
1:B:3951:VAL:HG13	1:B:4012:ILE:HD13	2.02	0.41
3:E:318:LEU:O	3:E:322:GLU:HG2	2.20	0.41
3:F:295:ARG:O	3:F:295:ARG:HG2	2.19	0.41
1:A:3332:VAL:HG11	1:A:3434:HIS:CE1	2.56	0.41
1:B:3928:LEU:O	1:B:3932:LEU:HG	2.20	0.41
1:B:4633:ILE:O	1:B:4637:ARG:HG3	2.20	0.41
2:D:121:GLU:O	2:D:122:VAL:C	2.60	0.41
2:D:139:TYR:O	2:D:143:VAL:HG23	2.21	0.41
1:B:3948:ILE:HA	1:B:3996:LEU:HD21	2.02	0.41
1:B:4128:TRP:O	1:B:4129:LEU:C	2.63	0.41
2:C:10:ILE:HG13	2:C:66:PHE:CZ	2.51	0.41
1:A:3095:VAL:HG12	1:A:3190:TRP:HZ3	1.85	0.41
1:A:3298:ASP:HB3	1:A:3398:GLN:OE1	2.20	0.41
1:A:3450:LEU:O	1:A:3454:ILE:HG13	2.21	0.41
1:A:4303:GLU:HB2	1:A:4475:MET:SD	2.61	0.41
1:A:4679:LYS:NZ	1:A:4731:ILE:O	2.54	0.41
1:B:3233:LEU:HD13	1:B:3290:TRP:HE3	1.85	0.41
1:B:3396:VAL:HG11	1:B:3438:ASN:HB3	2.03	0.41
1:B:3470:ASP:OD1	3:F:293:LEU:HG	2.20	0.41
1:B:4187:TYR:O	1:B:4191:ILE:HG12	2.21	0.41
1:B:4199:TYR:HA	2:D:20:PHE:HZ	1.85	0.41
1:B:4307:LYS:CG	1:B:4478:VAL:HG21	2.46	0.41
1:A:3190:TRP:H	1:A:3190:TRP:HD1	1.63	0.41
1:A:3306:GLN:O	1:A:3309:PHE:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3906:ILE:HD11	1:A:3939:ALA:HB1	2.02	0.41
1:A:3981:LYS:HA	1:A:3981:LYS:HD3	1.85	0.41
1:B:3320:LEU:HD23	1:B:3320:LEU:HA	1.92	0.41
1:B:3453:SER:O	1:B:3456:PRO:HD2	2.20	0.41
1:B:3505:THR:OG1	1:B:3916:ARG:NH1	2.37	0.41
1:B:4022:LYS:HE2	1:B:4022:LYS:HB3	1.79	0.41
1:B:3236:HIS:O	1:B:3240:ILE:HG12	2.21	0.41
1:B:3269:LEU:HB3	1:B:3633:LEU:HD13	1.90	0.41
1:B:3515:THR:HG21	1:B:3764:LEU:HD22	2.02	0.41
1:B:3988:LEU:H	1:B:3988:LEU:HD12	1.85	0.41
1:B:4108:PHE:HA	1:B:4111:ARG:CG	2.50	0.41
2:C:7:GLU:O	2:C:8:GLU:C	2.63	0.41
2:C:123:ASP:O	2:C:127:ARG:HG2	2.20	0.41
1:A:3190:TRP:CD1	1:A:3190:TRP:N	2.83	0.41
1:A:3236:HIS:O	1:A:3240:ILE:HG12	2.21	0.41
1:A:3470:ASP:OD1	3:E:293:LEU:HG	2.21	0.41
1:A:3556:TYR:O	1:A:3606:LYS:CE	2.67	0.41
1:A:3963:ASP:O	1:A:3964:LEU:C	2.64	0.41
1:A:4077:ILE:HG22	2:C:114:GLY:O	2.21	0.41
1:A:4216:GLU:HG2	1:A:4238:LEU:HB2	2.03	0.41
1:B:3071:LYS:HD2	1:B:3074:ILE:HB	2.03	0.41
1:B:3311:VAL:HG23	1:B:3312:ASP:O	2.20	0.41
1:B:3320:LEU:HD12	1:B:3424:VAL:HG13	2.03	0.41
1:B:3324:SER:OG	1:B:3328:CYS:SG	2.57	0.41
1:B:3443:GLN:H	1:B:3443:GLN:CD	2.29	0.41
1:B:3556:TYR:O	1:B:3606:LYS:CE	2.67	0.41
1:B:4059:TRP:CE3	3:F:323:LEU:HD21	2.56	0.41
1:B:4244:LEU:O	1:B:4248:PHE:HD1	2.03	0.41
2:D:7:GLU:O	2:D:8:GLU:C	2.64	0.41
2:D:66:PHE:HB3	2:D:67:PRO:HD3	2.02	0.41
2:D:119:ASP:HA	2:D:122:VAL:CG2	2.50	0.41
2:D:145:MET:HE3	2:D:145:MET:HB3	1.86	0.41
1:A:3409:ILE:HD13	1:A:3454:ILE:HD11	2.01	0.41
1:A:3519:LEU:HD11	1:A:3767:VAL:HG11	2.03	0.41
1:A:3937:PRO:O	1:A:3938:GLU:C	2.64	0.41
1:A:4638:PHE:HA	1:A:4641:TYR:CD2	2.56	0.41
1:B:3223:LYS:O	1:B:3227:LEU:HD23	2.21	0.41
1:B:3855:GLN:O	1:B:3855:GLN:NE2	2.54	0.41
1:B:4637:ARG:C	1:B:4640:PRO:HD2	2.46	0.41
2:C:95:LYS:HE3	2:C:109:VAL:HG23	2.03	0.41
2:D:119:ASP:OD1	2:D:119:ASP:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4129:LEU:HG	1:A:4165:LEU:HD23	2.02	0.40
1:A:4201:ALA:HA	1:A:4205:VAL:HG12	2.03	0.40
1:A:4251:VAL:HB	1:A:4254:ILE:HD12	2.02	0.40
1:A:4299:THR:HG22	1:A:4309:PHE:CZ	2.57	0.40
1:B:3053:LEU:HA	1:B:3056:MET:CE	2.50	0.40
1:B:3450:LEU:O	1:B:3454:ILE:HG13	2.21	0.40
1:B:4023:LEU:HD23	1:B:4023:LEU:HA	1.84	0.40
1:B:4679:LYS:NZ	1:B:4731:ILE:O	2.54	0.40
1:A:3742:LEU:HD13	1:A:3820:LYS:HG2	2.04	0.40
1:A:3855:GLN:O	1:A:3855:GLN:NE2	2.54	0.40
1:A:4187:TYR:O	1:A:4191:ILE:HG12	2.21	0.40
1:A:4195:HIS:NE2	2:C:35:THR:CG2	2.85	0.40
1:B:4031:SER:HB3	3:F:310:GLU:OE2	2.21	0.40
1:B:4166:LEU:O	1:B:4183:TYR:OH	2.38	0.40
1:B:4251:VAL:HB	1:B:4254:ILE:HD12	2.02	0.40
2:C:20:PHE:HE1	2:C:35:THR:CG2	2.34	0.40
2:D:29:THR:O	2:D:61:ASN:ND2	2.54	0.40
1:A:3053:LEU:HA	1:A:3056:MET:CE	2.50	0.40
1:A:3196:GLU:HA	1:A:3199:MET:HG2	2.02	0.40
1:A:3270:ILE:HD12	1:A:3632:PRO:HG3	2.03	0.40
1:A:3387:GLN:HG2	1:A:3388:GLU:N	2.35	0.40
1:A:3893:ASN:HB3	1:A:3896:LEU:HB2	2.03	0.40
1:A:3922:ARG:O	1:A:3926:ARG:HG3	2.20	0.40
1:A:3950:LYS:O	1:A:3953:THR:HG22	2.21	0.40
1:A:4027:PRO:HG2	3:E:313:ARG:HH21	1.86	0.40
1:A:4244:LEU:O	1:A:4248:PHE:HD1	2.03	0.40
1:A:4280:ARG:NH1	1:A:4285:ASP:OD2	2.52	0.40
2:D:68:GLU:O	2:D:72:MET:HG3	2.22	0.40
1:A:3289:ASN:HA	1:A:3292:LYS:NZ	2.36	0.40
1:A:3396:VAL:HG11	1:A:3438:ASN:HB3	2.03	0.40
1:A:3413:ARG:NH1	1:A:3457:GLU:OE1	2.41	0.40
1:A:3546:LYS:HG2	1:A:3714:MET:SD	2.61	0.40
1:A:4129:LEU:HD21	1:A:4149:VAL:HG22	2.03	0.40
1:B:3195:SER:HG	1:B:3231:HIS:CG	2.37	0.40
1:B:3478:LYS:HA	1:B:3478:LYS:HD2	1.83	0.40
1:B:4062:ARG:HB2	1:B:4062:ARG:NH1	2.37	0.40
1:B:4098:THR:HB	2:D:109:VAL:CG1	2.52	0.40
1:B:4159:LYS:HE2	1:B:4159:LYS:HB3	1.84	0.40
1:B:4299:THR:HG22	1:B:4309:PHE:CZ	2.56	0.40
2:D:17:PHE:HD1	2:D:69:PHE:CD2	2.40	0.40
1:A:3772:PRO:HG2	1:B:3918:ALA:HA	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4544:LEU:HD23	1:A:4605:PHE:HE1	1.87	0.40
1:B:3099:LEU:HD11	1:B:3193:PHE:CE1	2.57	0.40
1:B:3306:GLN:O	1:B:3309:PHE:HB2	2.21	0.40
1:B:3332:VAL:HG11	1:B:3434:HIS:CE1	2.56	0.40
1:B:4694:TYR:OH	1:B:4716:ARG:HD3	2.22	0.40
2:D:79:ASP:O	2:D:83:GLU:HG2	2.21	0.40
2:D:118:THR:C	2:D:120:GLU:N	2.74	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1644/5205 (32%)	1590 (97%)	54 (3%)	0	100	100
1	B	1644/5205 (32%)	1599 (97%)	45 (3%)	0	100	100
2	C	142/149 (95%)	131 (92%)	11 (8%)	0	100	100
2	D	139/149 (93%)	127 (91%)	12 (9%)	0	100	100
3	E	44/381 (12%)	44 (100%)	0	0	100	100
3	F	43/381 (11%)	43 (100%)	0	0	100	100
All	All	3656/11470 (32%)	3534 (97%)	122 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	1471/4542 (32%)	1439 (98%)	32 (2%)	47	73
1	B	1471/4542 (32%)	1443 (98%)	28 (2%)	52	76
2	C	123/127 (97%)	118 (96%)	5 (4%)	26	59
2	D	122/127 (96%)	114 (93%)	8 (7%)	14	45
3	E	45/330 (14%)	45 (100%)	0	100	100
3	F	44/330 (13%)	44 (100%)	0	100	100
All	All	3276/9998 (33%)	3203 (98%)	73 (2%)	47	73

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3237	VAL
1	A	3285	GLN
1	A	3286	ARG
1	A	3458	LEU
1	A	3520	VAL
1	A	3522	PHE
1	A	3532	CYS
1	A	3536	ASN
1	A	3581	LEU
1	A	3793	ASN
1	A	3847	VAL
1	A	3850	THR
1	A	3866	HIS
1	A	3964	LEU
1	A	3994	LEU
1	A	3999	MET
1	A	4007	VAL
1	A	4037	VAL
1	A	4127	ASN
1	A	4129	LEU
1	A	4230	THR
1	A	4277	VAL
1	A	4309	PHE
1	A	4310	MET
1	A	4400	LEU
1	A	4447	LEU
1	A	4492	LEU
1	A	4505	LEU

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Mol	Chain	Res	Type
1	A	4520	VAL
1	A	4542	LEU
1	A	4597	LEU
1	A	4616	LEU
1	B	3286	ARG
1	B	3458	LEU
1	B	3532	CYS
1	B	3535	CYS
1	B	3543	CYS
1	B	3581	LEU
1	B	3754	MET
1	B	3765	CYS
1	B	3847	VAL
1	B	3850	THR
1	B	3866	HIS
1	B	3953	THR
1	B	3968	LEU
1	B	4045	VAL
1	B	4051	GLU
1	B	4053	HIS
1	B	4129	LEU
1	B	4277	VAL
1	B	4303	GLU
1	B	4310	MET
1	B	4400	LEU
1	B	4447	LEU
1	B	4492	LEU
1	B	4505	LEU
1	B	4520	VAL
1	B	4542	LEU
1	B	4616	LEU
1	B	4649	GLU
2	C	33	LEU
2	C	49	LEU
2	C	77	MET
2	C	79	ASP
2	C	101	ILE
2	D	21	ASP
2	D	28	ILE
2	D	33	LEU
2	D	49	LEU
2	D	63	THR

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Mol	Chain	Res	Type
2	D	70	LEU
2	D	78	LYS
2	D	93	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3170	GLN
1	A	3397	ASN
1	A	3438	ASN
1	A	3491	GLN
1	A	3591	ASN
1	A	3639	ASN
1	A	3683	GLN
1	A	3768	ASN
1	A	3855	GLN
1	A	3866	HIS
1	A	4011	ASN
1	A	4127	ASN
1	A	4161	GLN
1	A	4233	GLN
1	A	4500	GLN
1	A	4602	ASN
1	A	4643	ASN
1	B	3397	ASN
1	B	3438	ASN
1	B	3491	GLN
1	B	3591	ASN
1	B	3639	ASN
1	B	3650	ASN
1	B	3683	GLN
1	B	3768	ASN
1	B	3855	GLN
1	B	3866	HIS
1	B	3958	HIS
1	B	4002	ASN
1	B	4011	ASN
1	B	4021	GLN
1	B	4053	HIS
1	B	4500	GLN
1	B	4523	GLN
1	B	4602	ASN

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Mol	Chain	Res	Type
1	B	4651	HIS
2	C	9	GLN
2	C	43	ASN
2	C	54	ASN
2	D	9	GLN
2	D	54	ASN
2	D	61	ASN
2	D	108	HIS
2	D	112	ASN
2	D	144	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

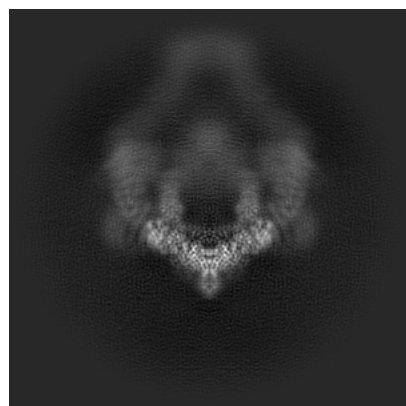
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49876. These allow visual inspection of the internal detail of the map and identification of artifacts.

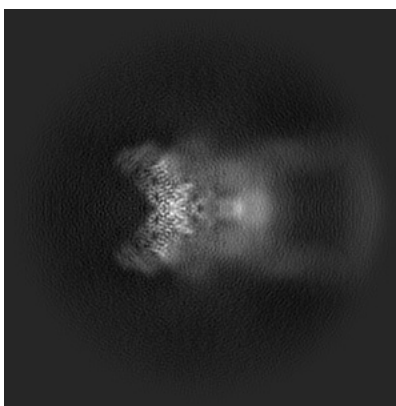
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

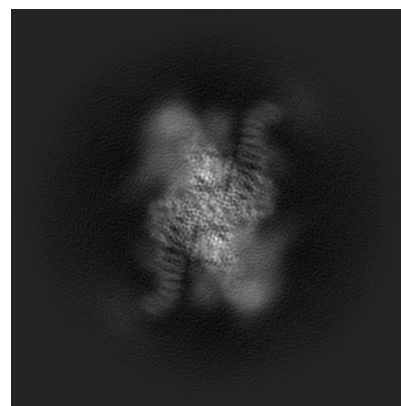
6.1.1 Primary map



X

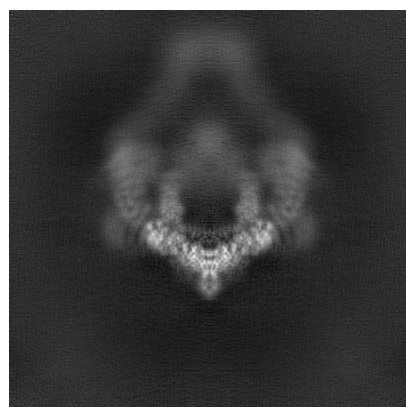


Y

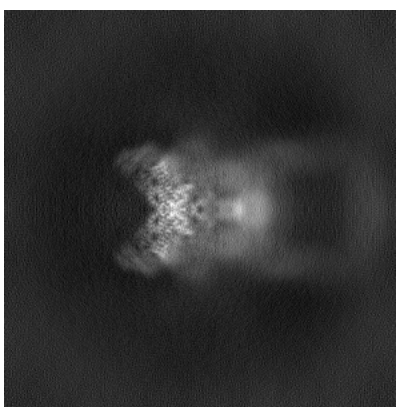


Z

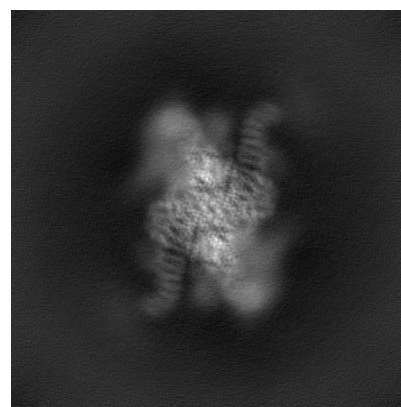
6.1.2 Raw map



X



Y

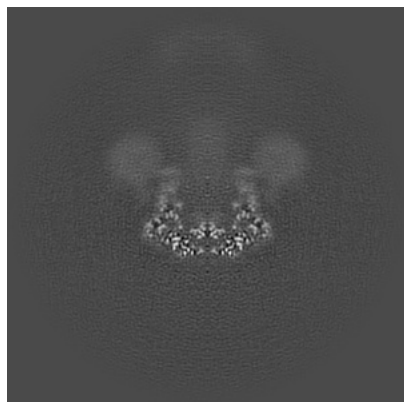


Z

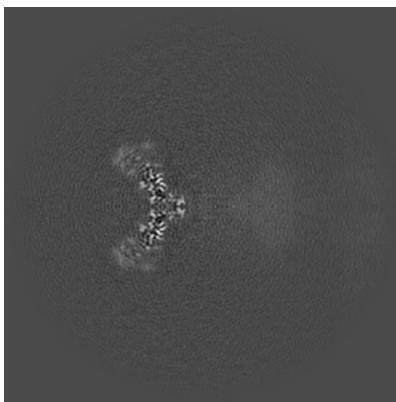
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

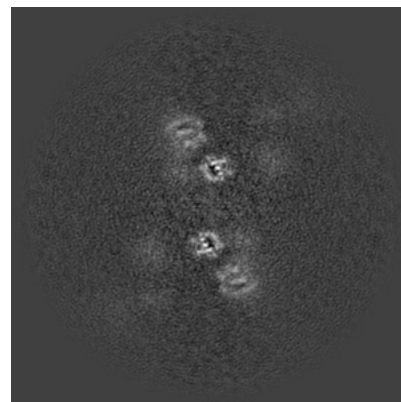
6.2.1 Primary map



X Index: 200

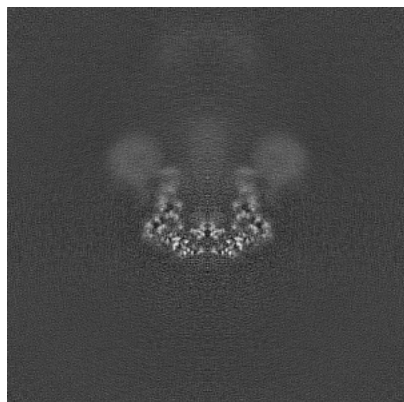


Y Index: 200

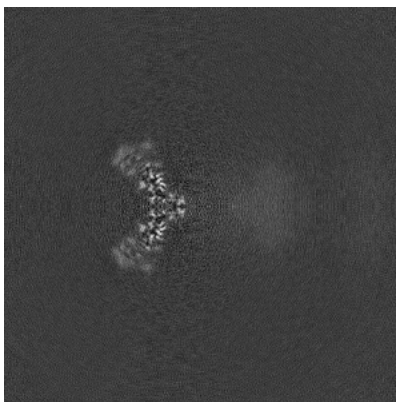


Z Index: 200

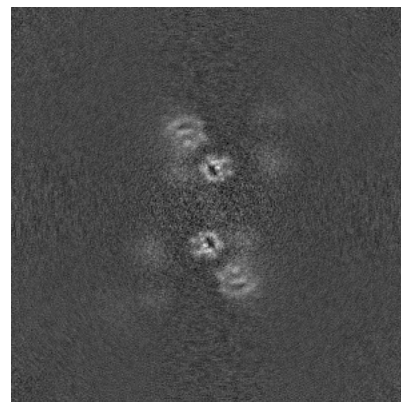
6.2.2 Raw map



X Index: 200



Y Index: 200

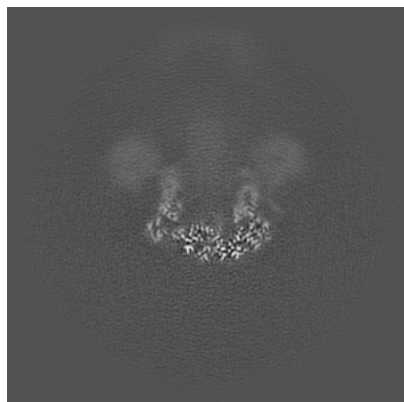


Z Index: 200

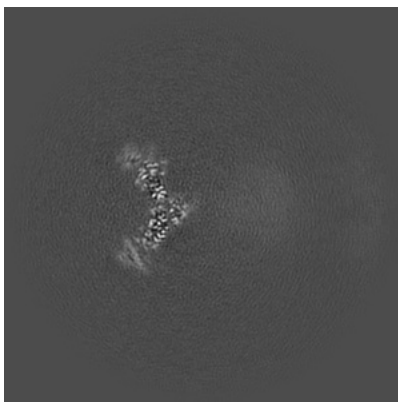
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

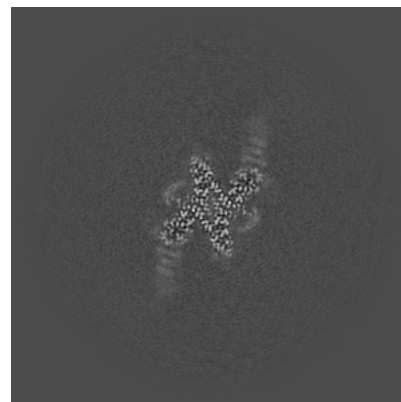
6.3.1 Primary map



X Index: 195

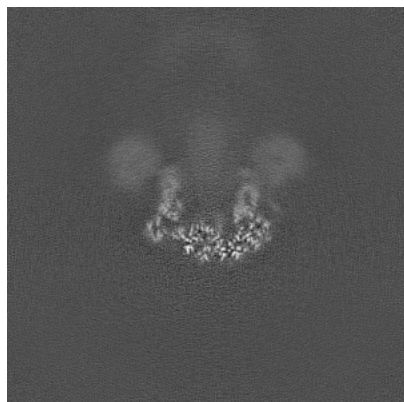


Y Index: 194

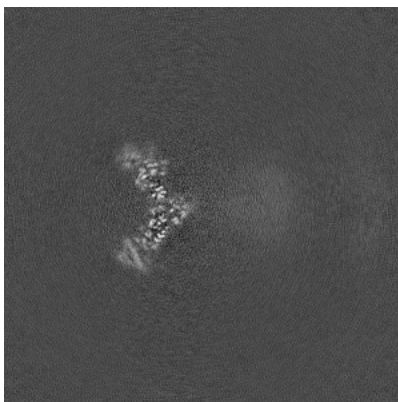


Z Index: 158

6.3.2 Raw map



X Index: 195



Y Index: 194

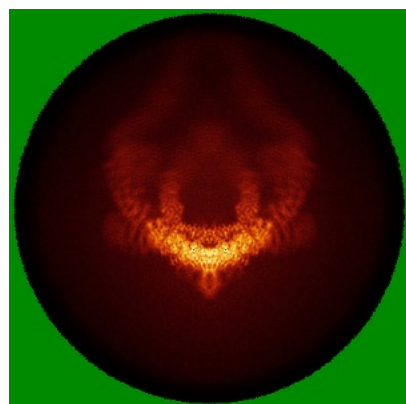


Z Index: 158

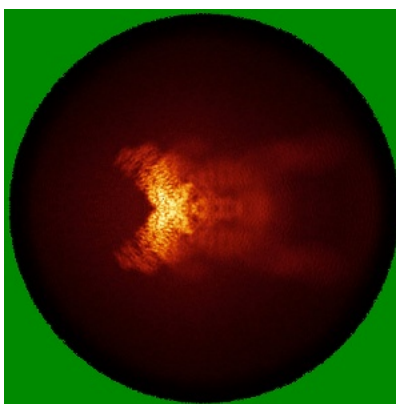
The images above show the largest variance slices of the map in three orthogonal directions.

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

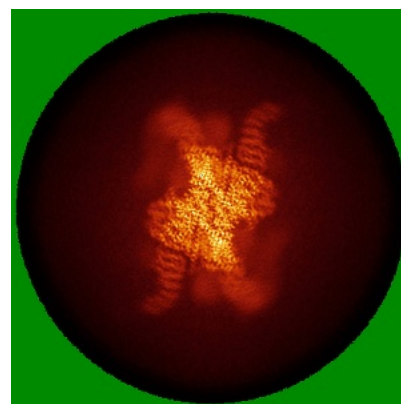
6.4.1 Primary map



X



Y

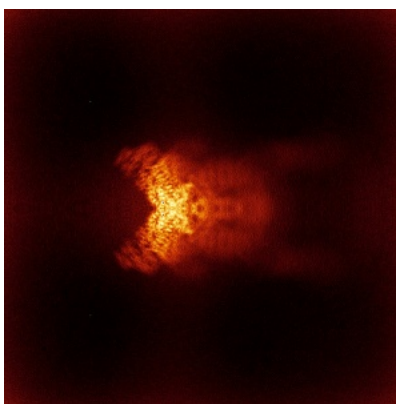


Z

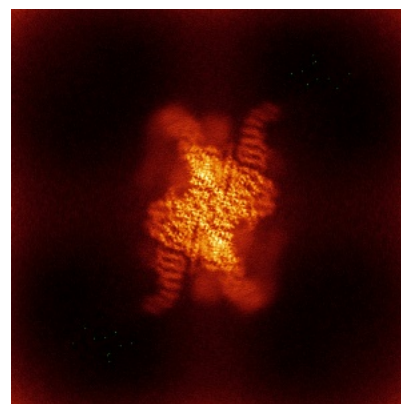
6.4.2 Raw map



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.

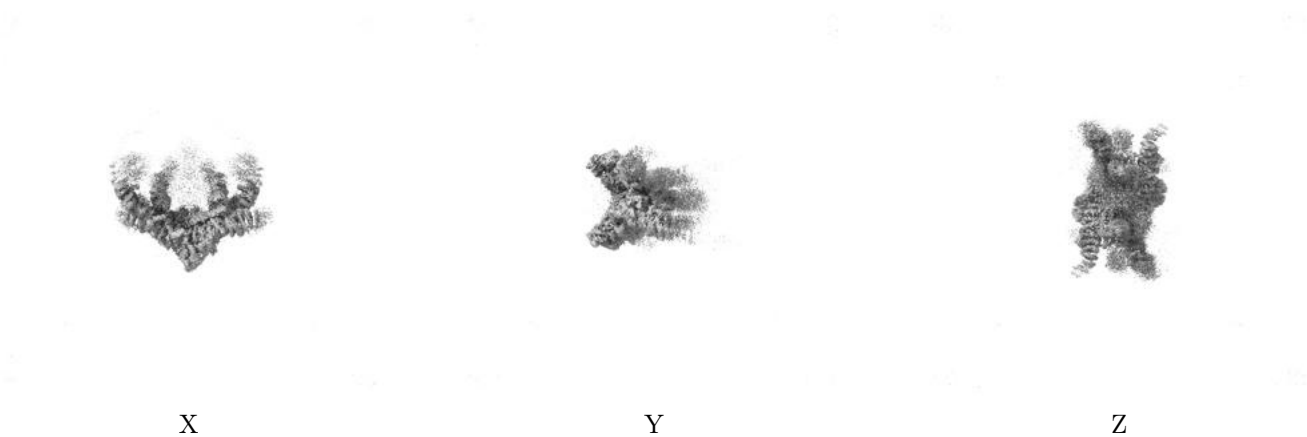
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.146. 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.

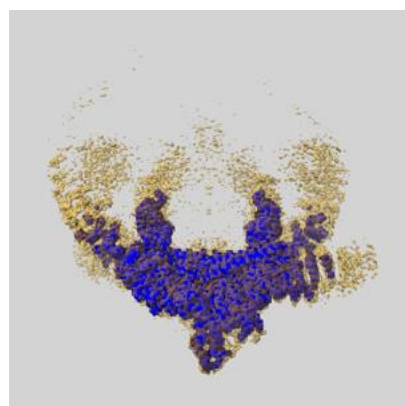
6.6 Mask visualisation [i](#)

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

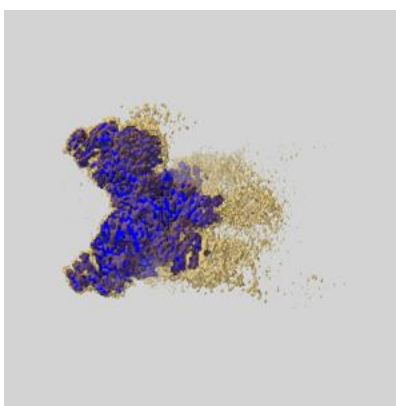
A mask typically either:

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

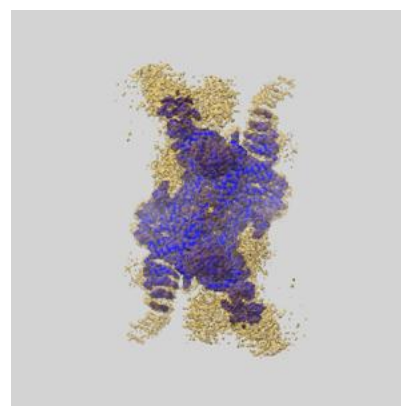
6.6.1 emd_49876_msk_1.map [i](#)



X



Y

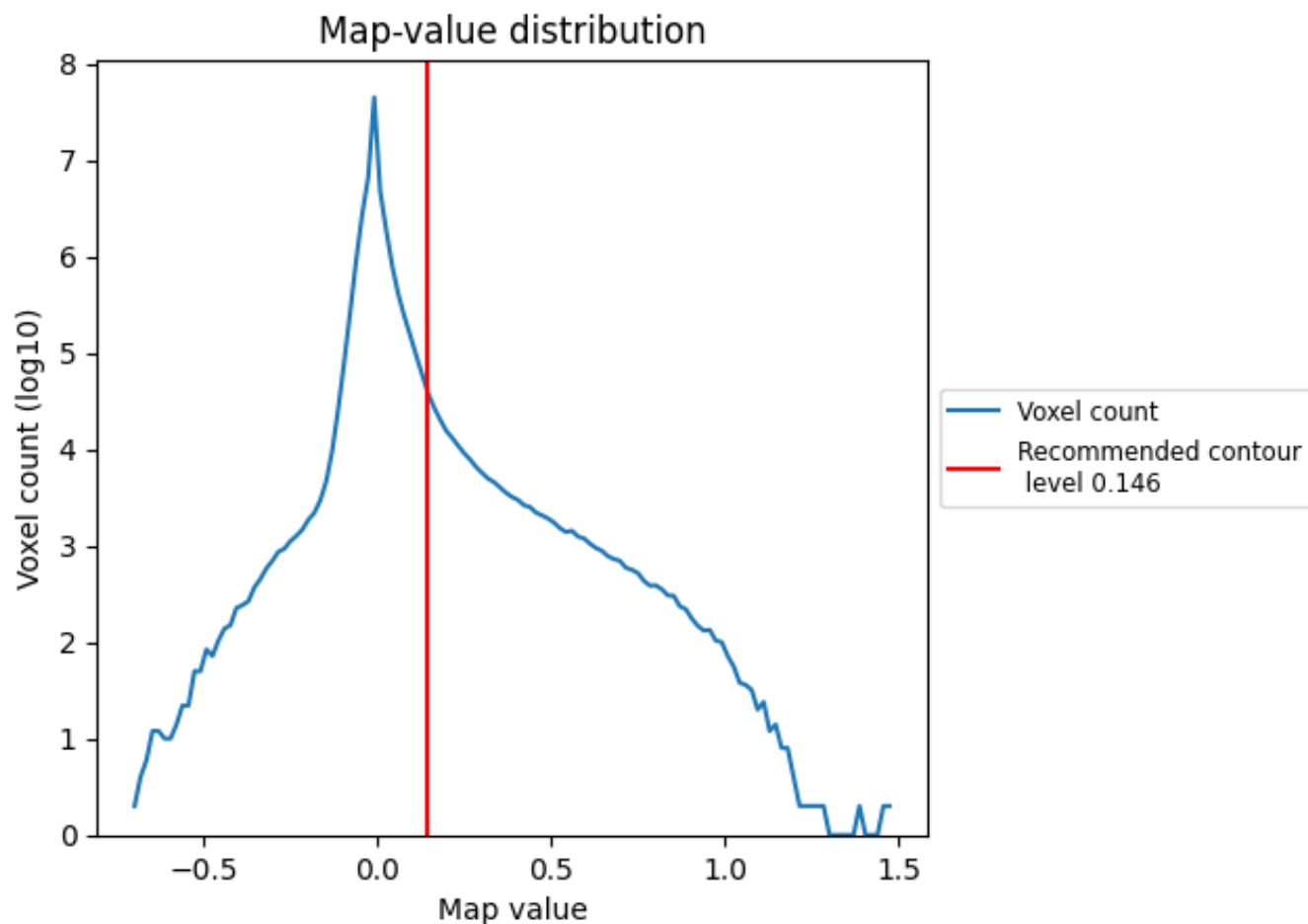


Z

7 Map analysis [i](#)

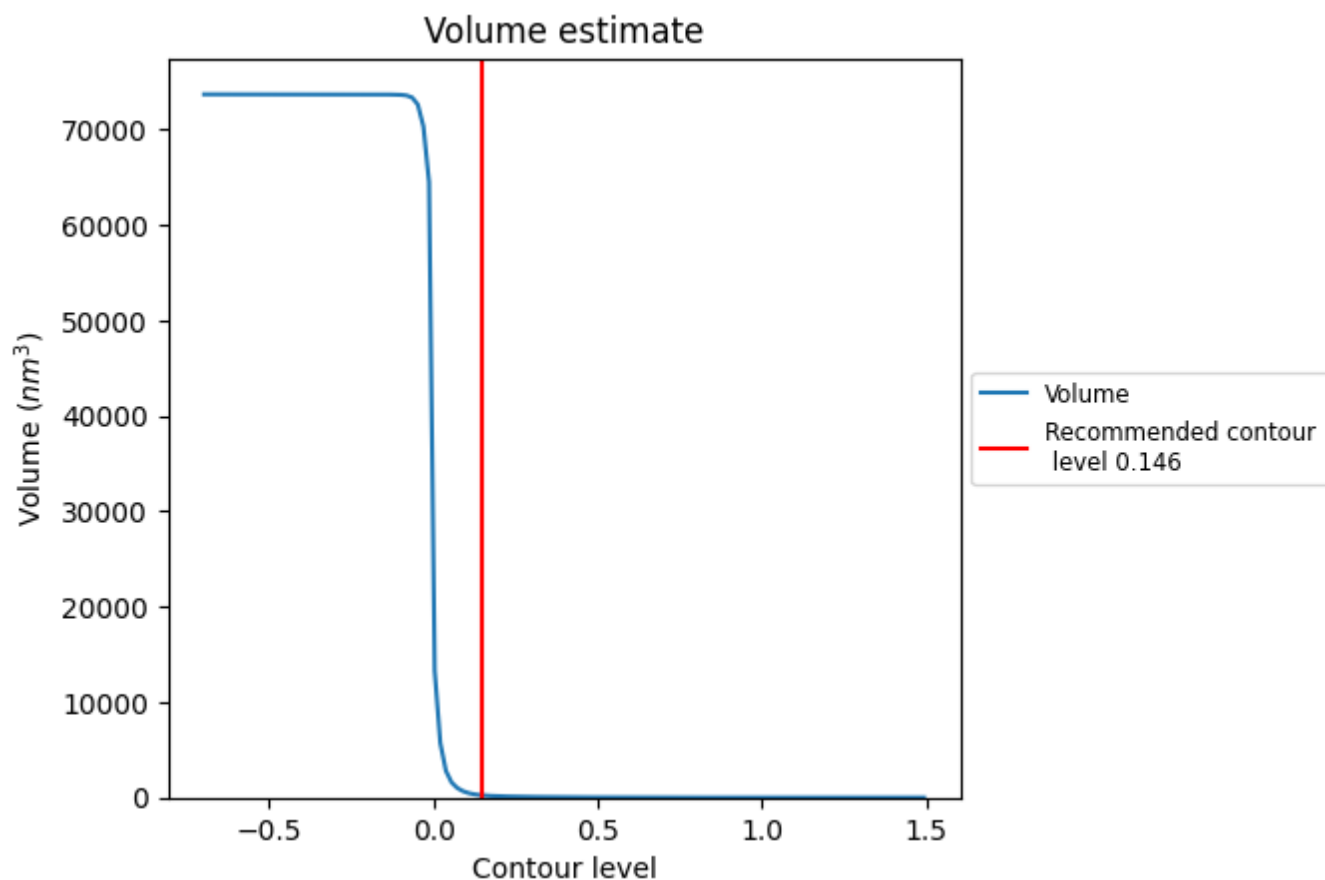
This section contains the results of statistical analysis of the map.

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.

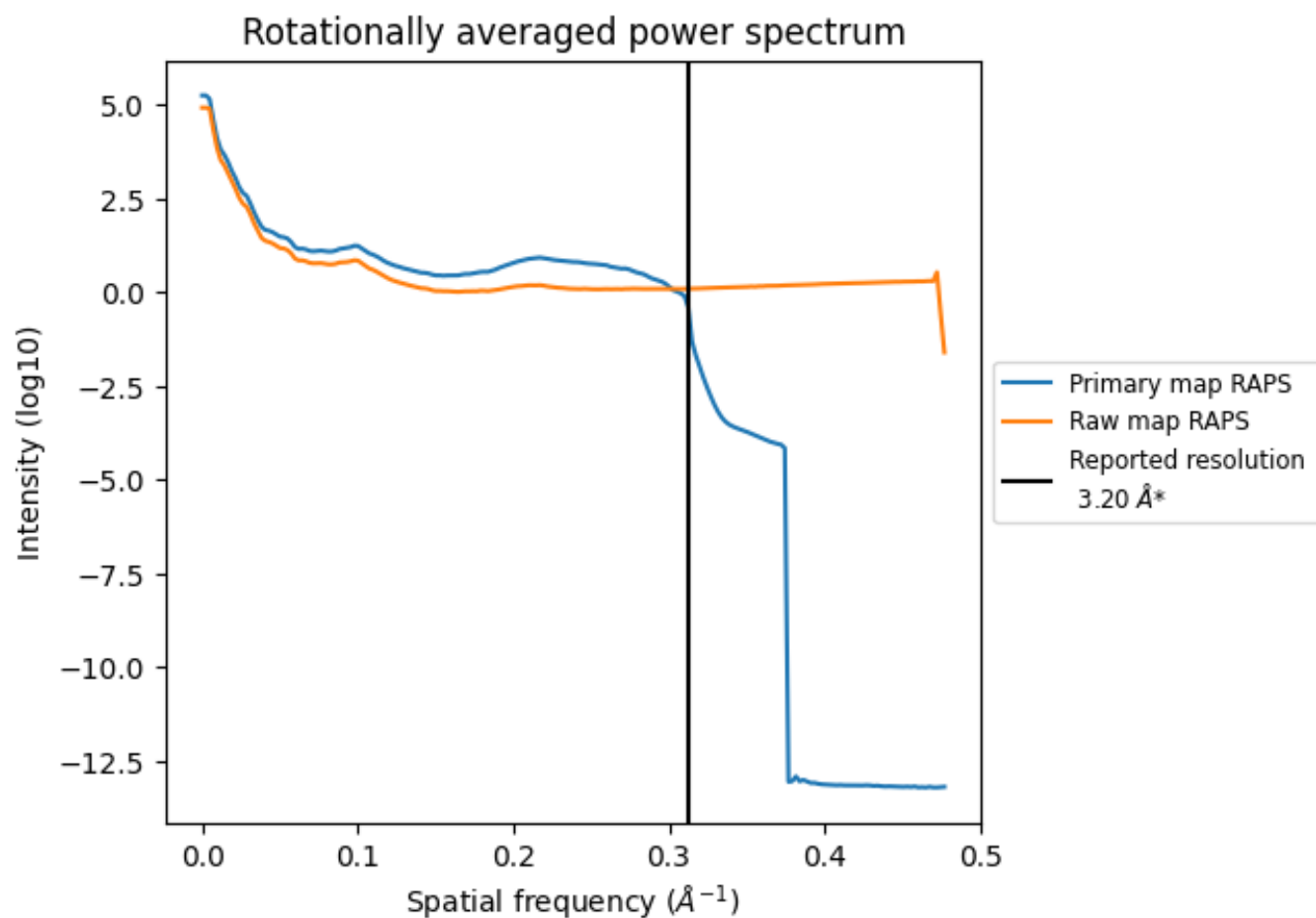
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 247 nm^3 ; this corresponds to an approximate mass of 223 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 ⓘ

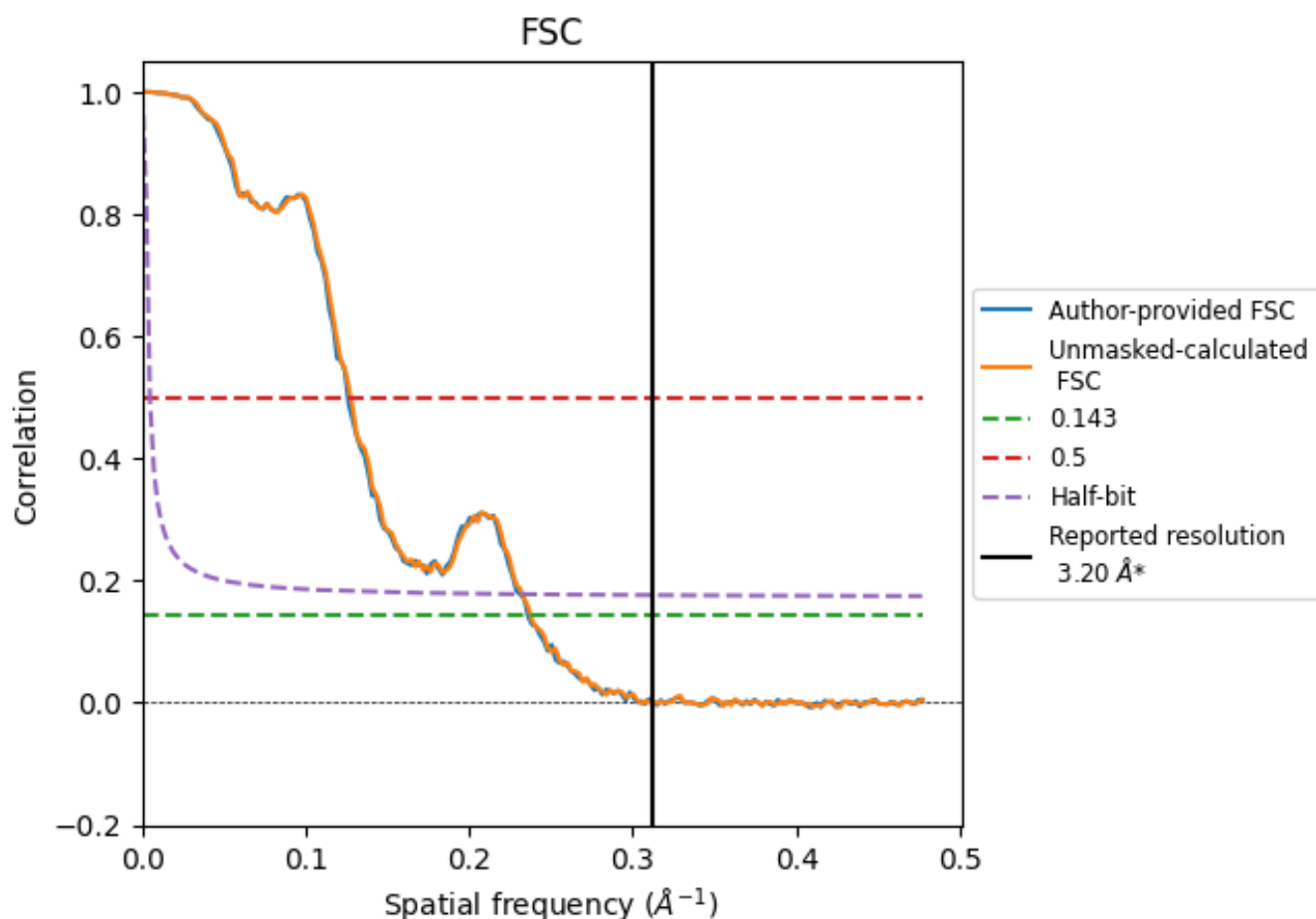


*Reported resolution corresponds to spatial frequency of 0.312 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 \AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	4.24	7.94	4.33
Unmasked-calculated*	4.21	7.84	4.30

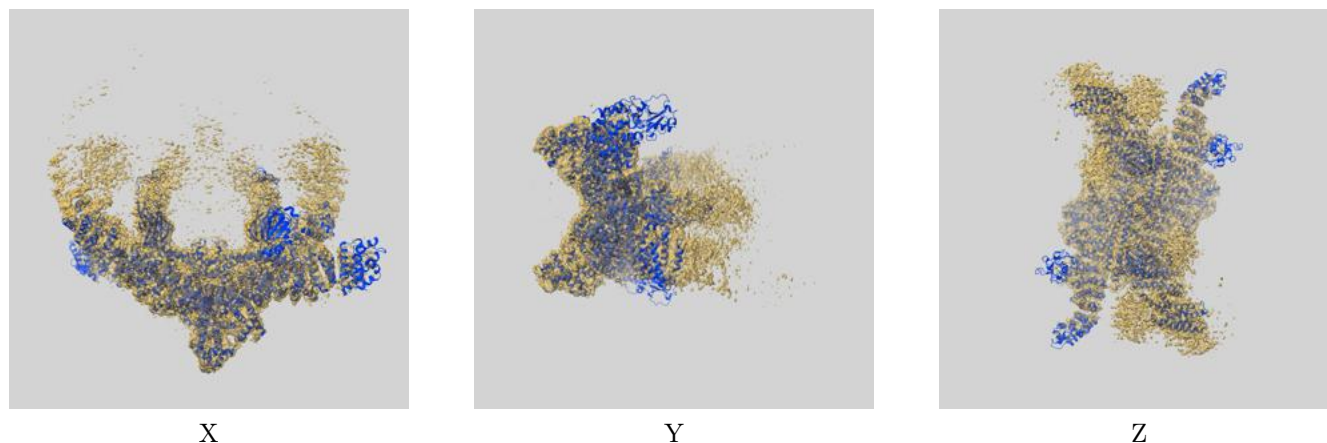
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.24 differs from the reported value 3.2 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.21 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

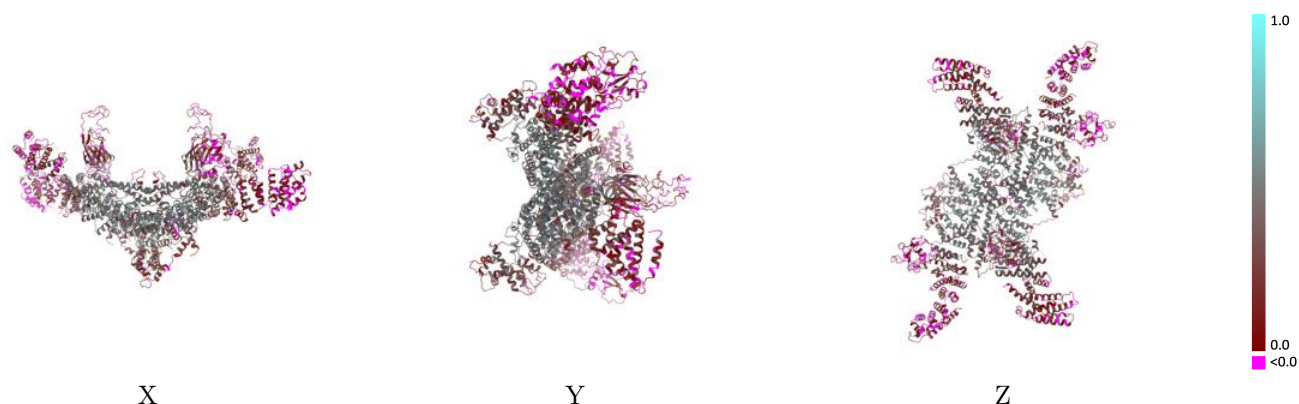
This section contains information regarding the fit between EMDB map EMD-49876 and PDB model 9NWE. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



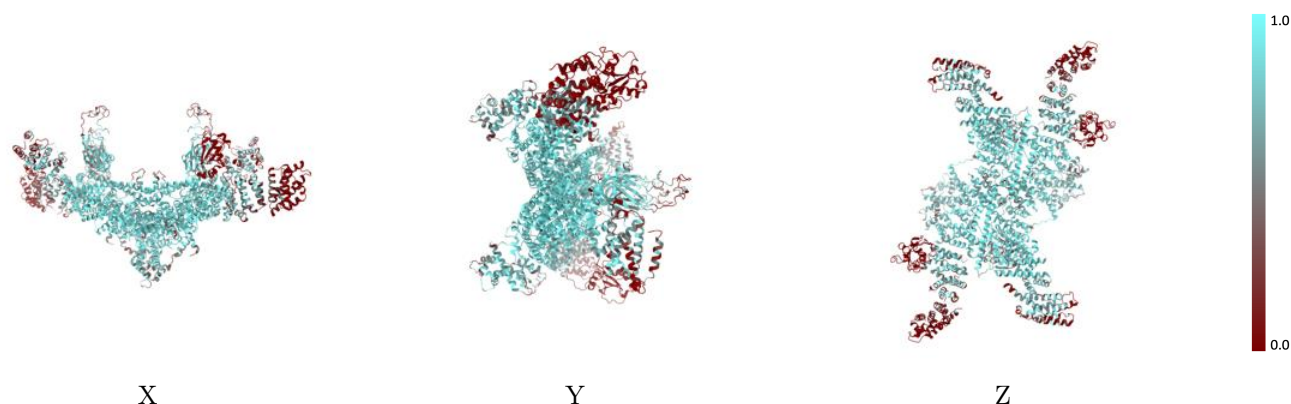
The images above show the 3D surface view of the map at the recommended contour level 0.146 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



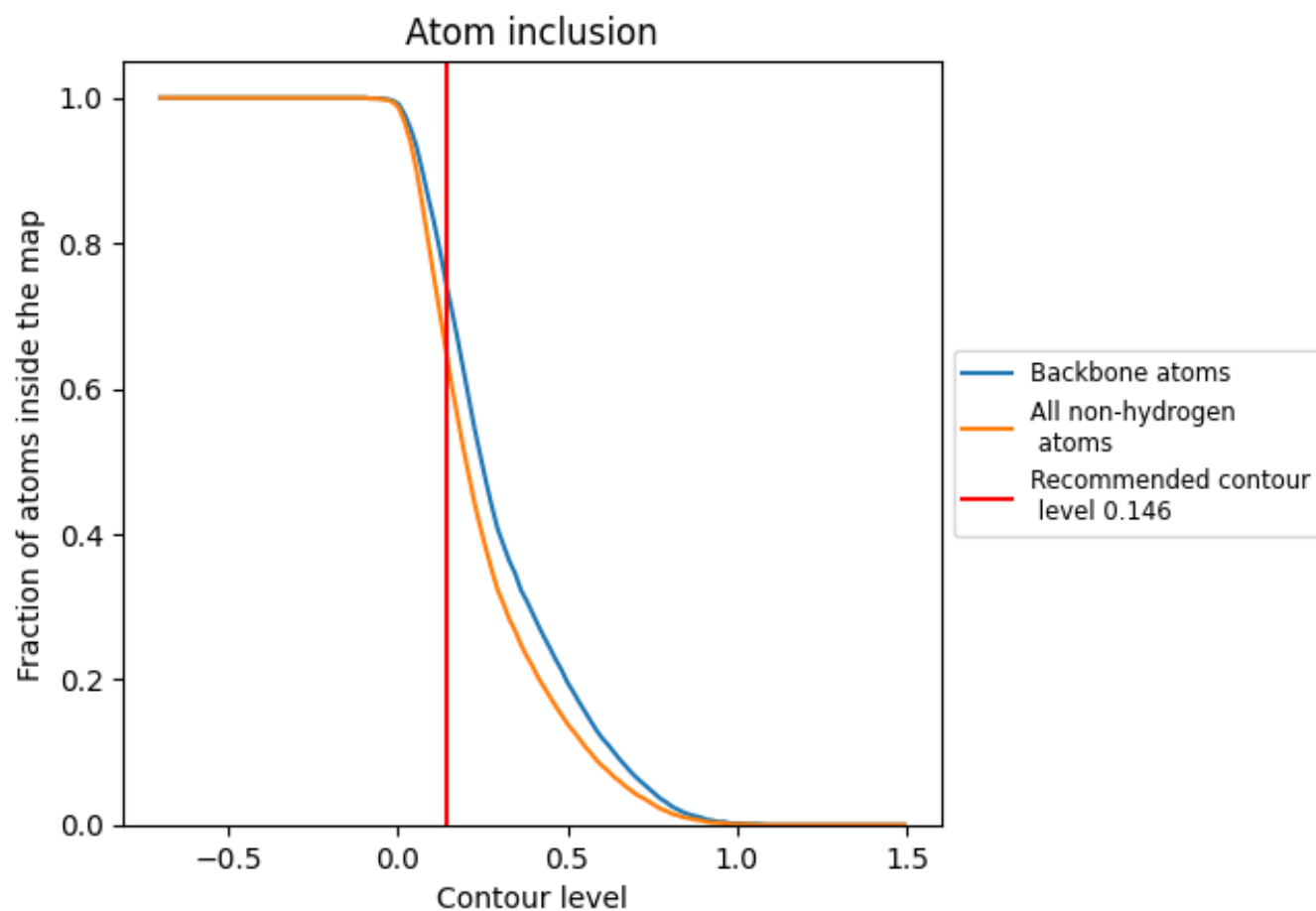
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.146).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 64% 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 (0.146) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6410	<div></div> 0.2850
A	<div></div> 0.6370	<div></div> 0.2880
B	<div></div> 0.6360	<div></div> 0.2870
C	<div></div> 0.6210	<div></div> 0.2260
D	<div></div> 0.6390	<div></div> 0.2360
E	<div></div> 0.8160	<div></div> 0.3900
F	<div></div> 0.8230	<div></div> 0.3850

1.0

0.0

<0.0