



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 11:48 PM UTC

PDB ID : 7OIK / pdb_00007oik
EMDB ID : EMD-12931
Title : Mouse RNF213:UBE2L3 transthiolation intermediate, chemically stabilized
Authors : Grabarczyk, D.; Ahel, J.; Clausen, T.
Deposited on : 2021-05-11
Resolution : 3.50 Å(reported)
Based on initial models : 4Q5E, 6TAX

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

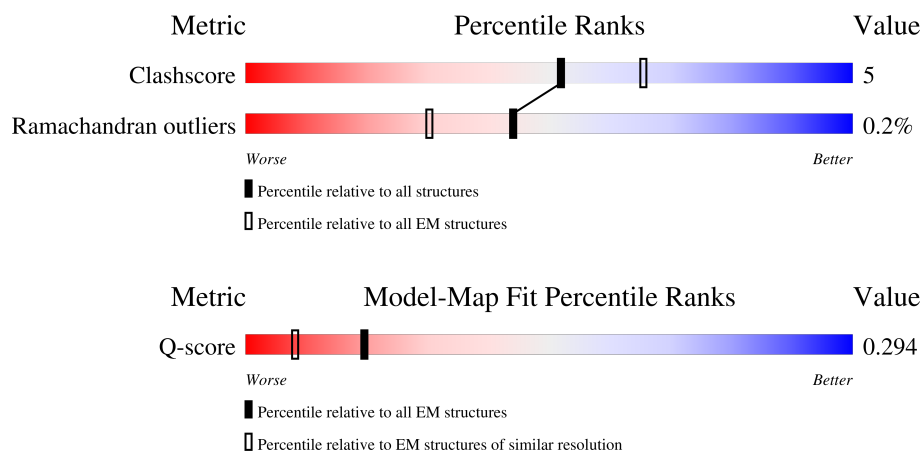
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMD archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	13950 (3.00 - 4.00)

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	5161	 6% 72% 14% 14%
2	B	166	 8% 84% 8% 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 36779 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 RNF213.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4426	Total	C	N	O	S	0	0
			35505	22641	6093	6561	210		

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	VAL	deletion	UNP E9Q555
A	?	-	ARG	deletion	UNP E9Q555
A	?	-	ASN	deletion	UNP E9Q555
A	?	-	ARG	deletion	UNP E9Q555
A	5149	GLY	-	expression tag	UNP E9Q555
A	5150	GLY	-	expression tag	UNP E9Q555
A	5151	GLY	-	expression tag	UNP E9Q555
A	5152	HIS	-	expression tag	UNP E9Q555
A	5153	HIS	-	expression tag	UNP E9Q555
A	5154	HIS	-	expression tag	UNP E9Q555
A	5155	HIS	-	expression tag	UNP E9Q555
A	5156	HIS	-	expression tag	UNP E9Q555
A	5157	HIS	-	expression tag	UNP E9Q555
A	5158	HIS	-	expression tag	UNP E9Q555
A	5159	HIS	-	expression tag	UNP E9Q555
A	5160	HIS	-	expression tag	UNP E9Q555
A	5161	HIS	-	expression tag	UNP E9Q555

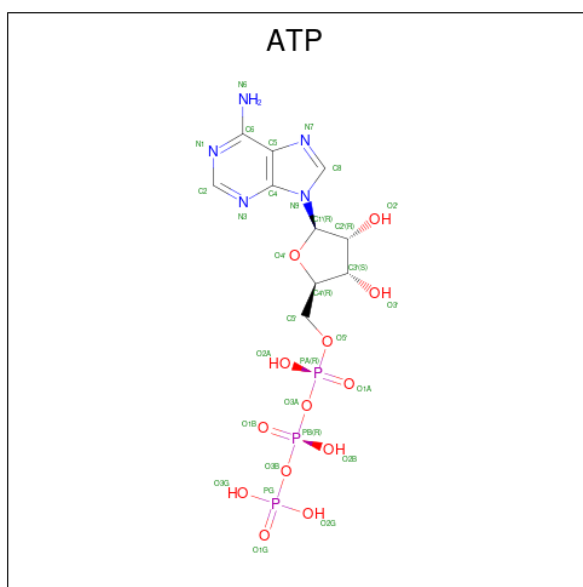
- Molecule 2 is a protein called Ubiquitin-conjugating enzyme E2 L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	153	Total	C	N	O	S	0	0
			1240	792	214	230	4		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	GLY	-	expression tag	UNP P68036
B	-10	TRP	-	expression tag	UNP P68036
B	-9	SER	-	expression tag	UNP P68036
B	-8	HIS	-	expression tag	UNP P68036
B	-7	PRO	-	expression tag	UNP P68036
B	-6	GLN	-	expression tag	UNP P68036
B	-5	PHE	-	expression tag	UNP P68036
B	-4	GLU	-	expression tag	UNP P68036
B	-3	LYS	-	expression tag	UNP P68036
B	-2	PRO	-	expression tag	UNP P68036
B	-1	GLY	-	expression tag	UNP P68036
B	0	SER	-	expression tag	UNP P68036
B	17	SER	CYS	conflict	UNP P68036
B	137	SER	CYS	conflict	UNP P68036

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

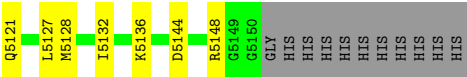
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Mg	0
			1	1	

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

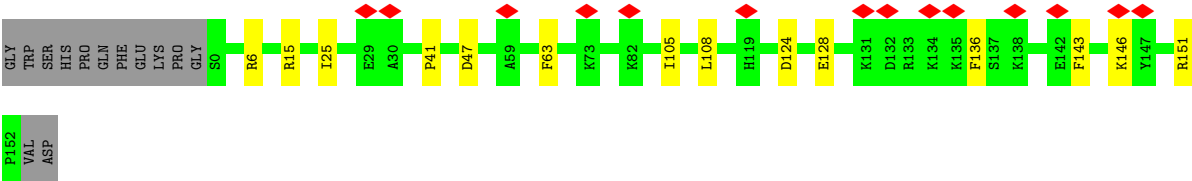
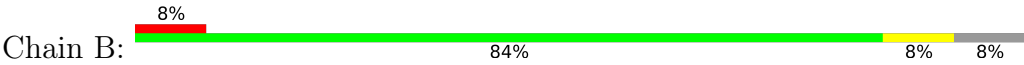
Mol	Chain	Residues	Atoms		AltConf
5	A	2	Total 2	Zn 2	0



N4846	L4611	GLY	P4410	M4270	Q4076	P3957	K3731	A3605	L3201	P3025	D2648
N4863	R4617	LEU	L4411	D4271	Q4076	V3958	F3732	W3606	LYS	E3026	V2686
N4873	L4628	ASN	R4412	R4272	K4086	C3959	L3733	V3607	GLU	I3027	N2852
N4874	L4646	HIS	M4421	V4275	K4086	P3961	Q3734	Q3608	LEU	L3028	M2855
N4876	L4675	THR	M4422	M4278	L4104	D3962	K3735	D3609	ALA	Y3039	L2694
N4876	L4876	GLY	M4423	L4278	Q4106	C3963	L3736	L3610	GLU	R3214	T2701
C4880	Y4662	GLY	H3964	D4285	K4109	H3964	L3737	W3611	GLN	D3219	K2710
Q4881	Y4662	PHE	P3969	D4285	K4109	P3969	D3752	V3626	MET	K3053	V2861
Y4882	Y4662	SER	C3970	C4284	E4115	C3970	K3756	LEU	VAL	D2882	D2882
Q4886	I4678	ASN	I3971	K4295	F4124	I3971	P3762	ASN	ASP	K3057	D2887
L4895	H4679	ASN	Q3972	D4288	A4138	Q3972	Q3769	THR	SER	V3059	C2719
L4896	C4680	GLU	T3973	R4307	A4138	T3973	Q3769	ARG	GLU	Y3068	L2722
L4896	S4681	ALA	W3974	S4308	E4150	W3974	R3772	ASN	ASN	D3073	L2726
K4892	K4682	ASP	I3976	Q4312	E4150	I3976	R3772	SER	LYS	F2912	F2727
L4883	L4683	ARG	T3977	Q4312	Q4164	T3977	F3778	GLU	ALA	G2913	L2728
R4926	Q4500	THR	G3978	Y4322	E4165	G3978	R3779	MET	SER	L2914	K2731
L4971	H4503	TRP	C3979	Y4322	P4166	C3979	R3780	S3637	ASP	Q3077	P2732
L4971	H4503	ARG	Q3979	Y4322	P4166	Q3979	I3781	F3638	PRO	K3086	G2733
T4974	L4512	LEU	M3980	L4328	I4169	M3980	S3790	I3639	ARG	L2920	K2736
A4981	G4512	GLY	H3981	Y4329	A4170	H3981	S3790	M3645	SER	L3090	K2736
D4988	E4515	ASN	C3982	M4333	S4171	C3982	S3793	V3655	CYS	G3091	K2747
C5000	Y4525	VAL	P3983	L4336	R4180	P3983	K3814	P3656	ASP	H3095	E2755
D5001	T4529	TRP	Y3984	L4336	R4180	Y3984	K3814	F3657	CYS	N2946	R2946
Q5002	L4530	TYR	C3985	H4337	L4185	C3985	K3821	R3658	L3283	V3101	F2948
L5003	L4531	THR	L3986	P4338	L4185	L3986	K3821	R3662	L3284	R3106	R2758
L5003	L4532	CYS	T3987	E4339	E4197	T3987	Q3822	Q3496	D3312	L3107	V2801
Q5014	L4535	ARG	D3988	Q4342	E4200	D3988	K3826	L3492	Q3337	I3108	V2802
H5017	L4535	GLY	L3989	L4343	L4201	L3989	K3826	R3493	S3346	K3113	D2805
R5033	A4547	HIS	P3990	E4344	L4201	P3990	Q3834	R3501	L3349	R3122	L2809
K5038	V4550	CYS	D3991	K4351	D4204	D3991	P3842	K3502	L3349	F3123	D2812
E5039	L4551	SER	K3992	K4351	K4205	K3992	P3842	K3503	V3376	L3124	D2812
L5040	L4552	VAL	F3993	E4352	R4206	F3993	S3855	F3697	R3397	I3125	K2816
F5041	L4552	GLY	S3994	E4352	R4207	S3994	S3855	L3698	R3397	L3128	P2817
R5042	Q4557	CYS	P3995	I4355	M4221	P3995	R3860	Q3706	R3406	Y3135	L2818
L5044	L4557	GLY	K4007	L4356	H4224	K4007	E3865	Q3706	E3429	L3139	L2821
L5080	Q4573	ARG	V4020	L4356	R4225	V4020	A3868	L3709	ASP	Q3140	D2827
S5092	L4574	PRO	L4045	R4366	R4225	L4045	L3869	D3716	LYS	P3141	E2831
E5108	T4575	GLN	L4045	Y4369	L4228	L4045	I3891	F3717	PRO	K3142	E2831
L4819	K4576	SER	Q4049	R4379	L4232	Q4049	S3903	L3718	GLU	R3143	P2834
A4825	M4577	THR	K4050	S4380	F4240	K4050	S3903	L3719	GLN	K3144	P2834
L4826	L4591	CYS	L4063	T4388	P4256	L4063	K3907	T3721	GLU	F3157	G2841
V4827	L4596	LEU	ARG	Y4394	R4257	ARG	S3913	V3724	MET	L3190	F2842
M4837	Q4600	CYS	ASP	H4395	R4257	ASP	S3913	S3725	GLU	L3015	L2845
Q4842	V4604	GLY	ALA	V4396	K4264	ALA	K3937	S3726	GLU	Q3017	S2846
		LEU	SER	D4265	D4265	SER	K3937	S3726	THR	E3194	N2847
		PRO	GLN	D4265	D4265	GLN	F3942	E3729	SER	D3200	W2848
		VAL	LYS	H4060	H4266	LYS	F3942	E3729	GLN		
		GLY	R4061	H4061	H4266	R4061	P3956	L3730			
			K4065	K4065		K4065					
			S4066	S4066		S4066					
			L4067	L4067		L4067					
			S4068	S4068		S4068					



● Molecule 2: Ubiquitin-conjugating enzyme E2 L3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	98000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	-800	Depositor
Maximum defocus (nm)	-2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.031	Depositor
Minimum map value	-0.011	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	377.344, 377.344, 377.344	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.072, 1.072, 1.072	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, 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	0.27	0/36242	0.72	34/49026 (0.1%)
2	B	0.26	0/1271	0.71	0/1719
All	All	0.27	0/37513	0.71	34/50745 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	721	MET	CA-CB-CG	8.79	131.68	114.10
1	A	1135	GLU	N-CA-CB	7.99	122.67	110.28
1	A	2012	MET	CA-CB-CG	7.82	129.74	114.10
1	A	5121	GLN	CA-CB-CG	7.54	129.19	114.10
1	A	3000	ARG	CA-C-N	7.00	134.92	121.54
1	A	3000	ARG	C-N-CA	7.00	134.92	121.54
1	A	2831	GLU	CA-CB-CG	6.82	127.73	114.10
1	A	2747	MET	CA-CB-CG	6.50	127.10	114.10
1	A	3826	LYS	N-CA-C	6.34	123.82	109.81
1	A	2816	MET	CA-CB-CG	6.31	126.72	114.10
1	A	878	LEU	CA-CB-CG	6.20	138.01	116.30
1	A	2216	MET	N-CA-CB	6.14	119.80	110.28
1	A	1013	HIS	CA-C-N	5.96	133.11	123.93
1	A	1013	HIS	C-N-CA	5.96	133.11	123.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1302	ARG	CB-CG-CD	5.79	124.61	111.30
1	A	675	MET	CG-SD-CE	5.68	113.39	100.90
1	A	3645	MET	CB-CA-C	5.62	120.06	110.56
1	A	1028	LEU	CA-CB-CG	5.62	135.95	116.30
1	A	5127	LEU	CA-CB-CG	5.60	135.89	116.30
1	A	3526	GLU	CB-CG-CD	5.51	121.97	112.60
1	A	2216	MET	CA-CB-CG	5.30	124.70	114.10
1	A	1688	LEU	CA-CB-CG	5.27	134.75	116.30
1	A	1975	LEU	CA-CB-CG	5.25	134.67	116.30
1	A	1101	ARG	CA-CB-CG	5.22	124.55	114.10
1	A	4076	GLN	CA-C-N	5.22	134.53	121.80
1	A	4076	GLN	C-N-CA	5.22	134.53	121.80
1	A	4295	LYS	CA-CB-CG	5.21	124.52	114.10
1	A	783	MET	CB-CG-SD	5.21	128.33	112.70
1	A	2216	MET	CB-CG-SD	5.21	128.32	112.70
1	A	3122	VAL	CA-CB-CG1	5.14	119.14	110.40
1	A	3526	GLU	N-CA-CB	5.14	118.21	110.30
1	A	675	MET	CA-CB-CG	5.11	124.32	114.10
1	A	1646	LEU	CA-CB-CG	5.09	134.11	116.30
1	A	4423	ASN	CA-CB-CG	5.01	117.61	112.60

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1016	GLU	Peptide
1	A	1170	GLU	Peptide
1	A	1373	ILE	Peptide
1	A	1845	THR	Peptide
1	A	3122	VAL	Peptide
1	A	4165	GLU	Peptide
1	A	688	PRO	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	35505	0	35641	392	0
2	B	1240	0	1240	9	0
3	A	31	0	12	1	0
4	A	1	0	0	0	0
5	A	2	0	0	0	0
All	All	36779	0	36893	399	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 5.

All (399) 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:731:PHE:HB3	1:A:760:ARG:HH21	1.49	0.77
1:A:4328:LEU:HD21	1:A:4337:HIS:H	1.55	0.72
1:A:893:MET:HE2	1:A:937:ARG:HG2	1.73	0.71
1:A:1811:MET:HE1	1:A:1921:ILE:HA	1.72	0.70
1:A:4270:MET:HE2	1:A:4646:ILE:HG23	1.77	0.66
1:A:4783:ARG:HB2	1:A:4799:CYS:HB2	1.79	0.64
1:A:2218:LEU:HD21	1:A:2303:LYS:HE2	1.79	0.64
1:A:2385:CYS:SG	1:A:2387:LYS:NZ	2.71	0.63
1:A:2801:VAL:HG12	1:A:2841:GLY:HA3	1.80	0.63
1:A:2291:VAL:HB	1:A:2307:MET:HB3	1.81	0.63
1:A:1318:SER:HB2	1:A:1378:GLN:HE21	1.64	0.62
2:B:15:ARG:NH2	2:B:25:ILE:O	2.33	0.62
1:A:1567:ASN:HA	1:A:1570:VAL:HG12	1.81	0.61
1:A:728:GLU:O	1:A:760:ARG:NH2	2.34	0.61
1:A:4065:LYS:NZ	1:A:4068:SER:O	2.33	0.61
1:A:1721:GLU:HA	1:A:1724:LYS:HE2	1.81	0.61
1:A:3639:ILE:HA	1:A:4926:ARG:HH21	1.66	0.61
1:A:5108:GLU:OE2	2:B:6:ARG:NH1	2.34	0.61
1:A:943:PRO:HD3	1:A:3207:ARG:HH21	1.65	0.61
1:A:3501:ARG:HH12	1:A:3593:GLY:HA2	1.65	0.61
1:A:994:ASP:HB3	1:A:997:LYS:HE2	1.82	0.61
1:A:5040:LEU:HD21	1:A:5136:LYS:HE2	1.83	0.61
1:A:4396:VAL:HG11	1:A:4535:LEU:HD13	1.83	0.60
1:A:3605:ALA:O	1:A:3609:ASP:HB2	2.00	0.59
1:A:4185:LEU:HD21	1:A:4228:LEU:HA	1.84	0.59
1:A:2216:MET:HA	1:A:2219:MET:HG2	1.84	0.59
1:A:3122:VAL:HG23	1:A:3125:ILE:HB	1.83	0.59
1:A:3258:PHE:O	1:A:3262:HIS:HB2	2.02	0.59
1:A:4512:GLY:HA2	1:A:4781:ALA:HA	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4086:LYS:NZ	1:A:4880:CYS:SG	2.76	0.59
2:B:41:PRO:O	2:B:151:ARG:NH2	2.35	0.59
1:A:1829:PRO:HD3	1:A:1861:GLN:HB3	1.84	0.59
1:A:2648:MET:HE1	1:A:2686:VAL:HA	1.85	0.59
1:A:4272:ARG:HH12	1:A:4388:THR:HG22	1.67	0.58
1:A:758:PRO:HB2	1:A:805:ILE:HA	1.85	0.58
1:A:2731:LYS:O	1:A:2736:LYS:NZ	2.34	0.58
1:A:3937:LYS:HG3	1:A:3942:PHE:HA	1.86	0.58
1:A:1956:ALA:HB3	1:A:2534:PRO:HB2	1.86	0.58
1:A:2716:MET:HA	1:A:2726:LEU:HD21	1.86	0.58
1:A:4200:GLU:HA	1:A:4206:ARG:HH21	1.67	0.58
1:A:4328:LEU:HD11	1:A:4337:HIS:HB3	1.85	0.58
1:A:2042:MET:HG2	1:A:2048:ILE:HG12	1.86	0.58
1:A:787:VAL:HA	1:A:790:VAL:HG22	1.86	0.58
1:A:2382:GLU:O	1:A:2387:LYS:NZ	2.38	0.57
1:A:2040:TYR:HA	1:A:2049:TRP:O	2.04	0.57
1:A:3610:LEU:HD23	1:A:3656:PRO:HD2	1.87	0.57
1:A:3718:LEU:HD21	1:A:3737:LEU:HD22	1.87	0.57
1:A:3534:LEU:HD22	1:A:3581:ILE:HG23	1.86	0.57
1:A:4339:GLU:HA	1:A:4343:LEU:HD22	1.87	0.57
1:A:2887:ASP:OD1	1:A:2890:ARG:NH1	2.38	0.57
1:A:1183:ARG:NH1	1:A:1188:CYS:SG	2.78	0.57
1:A:3003:LEU:HB2	1:A:3128:LEU:HB3	1.86	0.57
1:A:887:SER:O	1:A:890:LYS:NZ	2.36	0.56
1:A:2358:THR:HA	1:A:2361:MET:HE2	1.85	0.56
1:A:953:SER:O	1:A:956:ARG:NH2	2.37	0.56
1:A:3891:ILE:HD13	1:A:4007:LYS:HD2	1.87	0.56
1:A:717:MET:HE1	1:A:738:VAL:HG22	1.86	0.56
1:A:1140:GLN:HG3	1:A:1204:LYS:HZ2	1.69	0.56
1:A:4525:VAL:HG13	1:A:4628:LEU:HD12	1.86	0.56
1:A:1300:SER:HA	1:A:1303:VAL:HG12	1.88	0.56
1:A:1077:THR:HA	1:A:1168:LEU:HD22	1.88	0.56
1:A:2364:ILE:HG23	1:A:2394:LEU:HD13	1.87	0.56
1:A:2992:ARG:NH2	1:A:2995:ASP:OD1	2.39	0.56
1:A:4515:GLU:HG2	1:A:4530:ARG:HH12	1.70	0.55
1:A:3139:LEU:O	1:A:3144:LYS:NZ	2.38	0.55
1:A:735:LEU:O	1:A:771:ARG:NH2	2.39	0.55
1:A:3479:ARG:NH2	1:A:5000:CYS:SG	2.80	0.55
1:A:4842:GLN:HA	1:A:4846:ASN:HB2	1.88	0.55
1:A:1049:ASP:O	1:A:1056:ARG:NH2	2.39	0.55
1:A:1548:LEU:HA	1:A:1551:LEU:HG	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1675:SER:HB3	1:A:1764:LEU:HD11	1.89	0.55
1:A:3000:ARG:O	1:A:3077:GLN:NE2	2.40	0.55
1:A:1133:TYR:HB3	1:A:1197:ALA:HB1	1.87	0.55
1:A:1547:GLU:HA	1:A:1550:GLU:HG3	1.89	0.55
1:A:2965:PRO:HA	1:A:2968:ARG:HH11	1.72	0.55
1:A:2523:ARG:HG3	1:A:2851:ASP:HB3	1.87	0.55
1:A:2847:ASN:HD22	1:A:3123:PRO:HG3	1.71	0.55
1:A:2115:MET:HA	3:A:5201:ATP:HN62	1.71	0.54
1:A:940:GLN:NE2	1:A:3241:GLN:OE1	2.40	0.54
1:A:2374:GLY:O	1:A:2466:ARG:NH2	2.40	0.54
1:A:2852:PRO:HA	1:A:2855:MET:HG2	1.88	0.54
1:A:5033:ARG:NH2	1:A:5039:GLU:O	2.40	0.54
1:A:1617:PHE:HB3	1:A:1619:LEU:HD13	1.89	0.54
1:A:2733:GLY:HA3	1:A:2914:LEU:HB2	1.89	0.54
1:A:2916:ASP:OD1	1:A:3000:ARG:NH1	2.33	0.54
1:A:3015:LEU:HD23	1:A:3019:PHE:HD2	1.72	0.54
1:A:831:ASN:O	1:A:832:HIS:ND1	2.41	0.54
1:A:1541:ARG:NH1	1:A:1542:THR:O	2.41	0.54
1:A:3277:ILE:HB	1:A:3376:VAL:HG12	1.90	0.54
1:A:4503:HIS:HB3	1:A:4552:ILE:HG23	1.89	0.54
1:A:1129:GLN:HA	1:A:1132:ARG:HG2	1.88	0.53
1:A:646:ARG:HG3	1:A:675:MET:HE3	1.89	0.53
1:A:4204:ASP:OD1	1:A:4207:ARG:NH2	2.41	0.53
1:A:3778:PHE:HA	1:A:3781:ILE:HG12	1.90	0.53
1:A:4873:ASN:HA	1:A:4876:ILE:HG12	1.90	0.53
1:A:882:ARG:NH2	1:A:3230:SER:O	2.42	0.53
1:A:3724:VAL:HG21	1:A:3730:LEU:HD13	1.91	0.53
1:A:3693:PRO:HA	1:A:3696:VAL:HG22	1.89	0.53
1:A:4687:ARG:NH2	1:A:4882:TYR:OH	2.42	0.53
1:A:995:LEU:HD11	1:A:1047:ILE:HG13	1.91	0.53
1:A:4050:LYS:HD2	1:A:4061:ARG:HH11	1.73	0.53
1:A:4713:HIS:ND1	1:A:4837:MET:SD	2.81	0.53
1:A:5116:SER:HA	1:A:5119:GLU:HG3	1.90	0.53
1:A:1984:ILE:HD13	1:A:2017:HIS:HB3	1.90	0.52
1:A:4338:PRO:HA	1:A:4342:GLN:HB2	1.89	0.52
1:A:4708:VAL:HB	1:A:4896:LEU:HD13	1.91	0.52
1:A:4138:ALA:HB2	1:A:4874:PRO:HG3	1.90	0.52
1:A:1544:SER:N	1:A:1547:GLU:OE2	2.39	0.52
1:A:2337:ARG:HA	1:A:2340:LEU:HG	1.91	0.52
1:A:1613:ILE:HD11	1:A:1635:LEU:HD22	1.92	0.52
1:A:3211:GLU:OE2	1:A:3214:ARG:NH1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4221:ASN:O	1:A:4224:HIS:ND1	2.38	0.52
1:A:2035:LEU:HD11	1:A:2057:TYR:HE2	1.75	0.52
1:A:1322:ILE:HA	1:A:1325:VAL:HG12	1.92	0.52
1:A:1383:GLU:OE2	1:A:1386:ARG:NH2	2.43	0.52
1:A:4971:ILE:HA	1:A:4974:THR:HG22	1.90	0.52
1:A:2507:ARG:NH1	1:A:2809:LEU:O	2.43	0.52
1:A:1391:VAL:HA	1:A:1394:LEU:HG	1.91	0.52
1:A:4762:ASP:N	1:A:4762:ASP:OD1	2.42	0.52
1:A:3658:SER:HB3	1:A:3720:LEU:HD11	1.93	0.51
1:A:1503:ILE:HD12	1:A:1528:LEU:HD21	1.93	0.51
1:A:2061:ILE:HD12	1:A:2062:PRO:HD2	1.93	0.51
1:A:665:LEU:HB3	1:A:734:TRP:HE1	1.75	0.51
1:A:1021:VAL:HG12	1:A:1065:VAL:HG22	1.92	0.51
1:A:3718:LEU:HD13	1:A:3733:LEU:HD23	1.93	0.51
1:A:1147:LEU:O	1:A:1229:GLU:N	2.44	0.51
1:A:2513:THR:OG1	1:A:2812:ASP:OD2	2.28	0.51
1:A:2556:GLN:O	1:A:2560:GLN:NE2	2.43	0.51
1:A:2548:ASP:O	1:A:2552:LYS:NZ	2.37	0.51
1:A:896:ILE:HD11	1:A:899:ALA:HA	1.92	0.51
1:A:2250:LEU:HD22	1:A:2488:TYR:HB3	1.93	0.51
1:A:4338:PRO:O	1:A:4343:LEU:N	2.43	0.51
1:A:1549:LYS:HA	1:A:1552:LEU:HG	1.93	0.50
1:A:4407:ILE:HB	1:A:4604:VAL:HG11	1.93	0.50
1:A:4678:ILE:HD12	1:A:4683:ILE:HD13	1.94	0.50
1:A:4104:LEU:HD13	1:A:4124:PHE:HE2	1.76	0.50
1:A:777:LYS:NZ	1:A:778:ILE:O	2.33	0.50
1:A:3135:MET:HE1	1:A:3190:LEU:HD22	1.92	0.50
1:A:1379:ARG:HH12	1:A:1383:GLU:HG2	1.76	0.50
1:A:1578:SER:HA	1:A:1581:GLN:HG2	1.94	0.50
1:A:3284:LEU:HB2	1:A:3337:GLN:HE22	1.76	0.50
1:A:3855:SER:O	1:A:3860:ARG:NH1	2.44	0.50
1:A:4164:GLN:HG3	1:A:4169:ILE:HG22	1.93	0.50
1:A:1820:THR:OG1	1:A:1822:ASP:OD1	2.24	0.50
1:A:1980:VAL:HA	1:A:2012:MET:HE1	1.93	0.50
1:A:2369:MET:SD	1:A:2372:ARG:NH2	2.85	0.49
1:A:3662:ARG:HH21	1:A:3721:THR:HG22	1.75	0.49
1:A:1031:TRP:HE1	1:A:1033:ASP:HB2	1.77	0.49
1:A:2459:ILE:HA	1:A:2462:ILE:HD12	1.93	0.49
1:A:638:VAL:HG23	1:A:639:LEU:HG	1.93	0.49
1:A:3982:CYS:HB3	1:A:3987:THR:H	1.76	0.49
1:A:5033:ARG:HH12	1:A:5042:ARG:HH21	1.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3868:ALA:HB1	1:A:3913:SER:HB3	1.95	0.49
1:A:1994:GLU:HB3	1:A:2041:LEU:HD12	1.95	0.49
1:A:1649:TRP:HA	1:A:1652:VAL:HG12	1.95	0.49
1:A:3091:GLY:HA2	1:A:3095:HIS:O	2.12	0.49
1:A:3732:PHE:HA	1:A:3735:MET:HG2	1.95	0.49
1:A:1005:VAL:O	1:A:1009:SER:HB3	2.13	0.49
1:A:2226:PRO:HG2	1:A:2538:PRO:HA	1.95	0.49
1:A:758:PRO:HG3	1:A:804:ARG:HH11	1.78	0.49
1:A:1156:GLU:HG2	1:A:1157:ILE:HG12	1.94	0.49
1:A:760:ARG:NH1	1:A:763:ASP:OD2	2.46	0.48
1:A:875:GLN:HA	1:A:878:LEU:HD23	1.94	0.48
1:A:1625:LEU:HB3	1:A:1736:LEU:HD11	1.95	0.48
1:A:4329:TYR:OH	1:A:4369:VAL:O	2.31	0.48
1:A:4810:GLU:HB2	1:A:4819:LEU:HD23	1.94	0.48
1:A:1931:VAL:HG13	1:A:1935:LEU:HD23	1.95	0.48
1:A:3017:GLN:HB3	1:A:3194:GLU:HG3	1.95	0.48
1:A:4312:GLN:NE2	1:A:4600:GLN:OE1	2.47	0.48
1:A:1782:PRO:HG2	1:A:1812:GLN:HB3	1.94	0.48
1:A:3086:LYS:HG3	1:A:3101:VAL:HB	1.96	0.48
2:B:128:GLU:HG2	2:B:136:PHE:HB2	1.94	0.48
1:A:1740:LEU:HB3	1:A:1744:MET:HE2	1.96	0.48
1:A:1981:PRO:HB2	1:A:2014:VAL:HG13	1.95	0.48
1:A:3610:LEU:HD13	1:A:3698:LEU:HD21	1.95	0.48
1:A:4427:PRO:HA	1:A:4617:ARG:HD2	1.96	0.48
1:A:2920:LEU:HD22	1:A:2948:PHE:HE2	1.79	0.48
1:A:3834:GLN:HE22	1:A:4846:ASN:HB3	1.79	0.48
1:A:2961:THR:O	1:A:2968:ARG:NH1	2.47	0.48
1:A:3257:ASP:OD1	1:A:3406:ARG:NH2	2.47	0.48
1:A:4574:LEU:HA	1:A:4577:MET:HG2	1.96	0.48
1:A:1704:VAL:HA	1:A:1707:THR:HG22	1.96	0.47
1:A:1751:MET:SD	1:A:1751:MET:N	2.87	0.47
1:A:2728:LEU:HD23	1:A:2861:VAL:HB	1.95	0.47
1:A:3492:LEU:O	1:A:3493:ARG:NH1	2.39	0.47
1:A:1031:TRP:NE1	1:A:1033:ASP:HB2	2.30	0.47
1:A:1301:GLU:OE2	1:A:1302:ARG:NH1	2.46	0.47
1:A:2600:ARG:NH2	1:A:2856:ASN:O	2.47	0.47
1:A:4499:THR:OG1	1:A:4500:GLN:N	2.46	0.47
1:A:912:TRP:HZ3	1:A:930:LEU:HD22	1.79	0.47
1:A:1722:VAL:HA	1:A:1725:LYS:HG2	1.96	0.47
1:A:2701:THR:HG22	1:A:2994:LEU:HD22	1.97	0.47
1:A:1885:ASP:O	1:A:1887:GLN:NE2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1804:PRO:HD3	1:A:2084:PHE:HE1	1.78	0.47
1:A:3253:ASN:ND2	1:A:3257:ASP:OD2	2.48	0.47
1:A:4045:LEU:O	1:A:4065:LYS:NZ	2.39	0.47
1:A:4164:GLN:HG2	1:A:4171:SER:H	1.78	0.47
1:A:1200:LEU:HB3	1:A:1204:LYS:HE3	1.97	0.47
1:A:4759:HIS:HB2	1:A:4765:ARG:HG2	1.96	0.47
1:A:777:LYS:HE2	1:A:830:ALA:H	1.79	0.47
1:A:2564:ASP:HB3	1:A:2610:ARG:HH12	1.80	0.47
1:A:2495:MET:HA	1:A:2498:ARG:HG2	1.96	0.47
1:A:1627:GLU:HB2	1:A:1736:LEU:HD23	1.97	0.47
1:A:3960:LEU:HB2	1:A:3964:HIS:HB2	1.98	0.46
1:A:4322:TYR:CE2	1:A:4394:VAL:HG21	2.50	0.46
1:A:4573:GLN:HA	1:A:4576:LYS:HG2	1.96	0.46
1:A:815:LEU:HB3	1:A:873:THR:HG21	1.97	0.46
1:A:1083:LEU:HD23	1:A:1124:LEU:HD13	1.97	0.46
1:A:627:SER:HA	1:A:726:VAL:HG12	1.98	0.46
1:A:1118:LYS:HG2	1:A:1121:ARG:HH22	1.79	0.46
1:A:1279:GLU:O	1:A:1283:ASP:HB2	2.15	0.46
1:A:1771:LEU:HA	1:A:1774:MET:HE2	1.97	0.46
1:A:4404:HIS:O	1:A:4404:HIS:ND1	2.48	0.46
1:A:1368:GLN:HA	1:A:1371:GLN:HG2	1.96	0.46
1:A:4201:LEU:HB3	1:A:4205:LYS:HB2	1.96	0.46
1:A:4257:ARG:HH11	1:A:4258:LYS:HB2	1.80	0.46
1:A:1277:TYR:CE2	1:A:1307:LYS:HG2	2.50	0.46
1:A:1553:ASN:ND2	1:A:3039:TYR:OH	2.35	0.46
1:A:1800:SER:OG	1:A:1801:GLU:OE1	2.30	0.46
1:A:2818:LEU:HD22	1:A:2821:LEU:HD22	1.98	0.46
1:A:3975:LEU:HD23	1:A:3993:PHE:HD2	1.81	0.46
1:A:3140:GLN:OE1	1:A:3142:TRP:NE1	2.46	0.46
1:A:3958:VAL:HG11	1:A:3971:ILE:HG21	1.97	0.46
1:A:4257:ARG:HH22	1:A:4670:PRO:HG2	1.81	0.46
1:A:4275:VAL:HG11	1:A:4591:LEU:HA	1.98	0.46
1:A:1091:SER:HA	1:A:1094:LEU:HG	1.98	0.46
1:A:1619:LEU:HD23	1:A:1621:LEU:HD21	1.98	0.46
1:A:2611:TRP:HB2	1:A:2722:LEU:HD21	1.97	0.46
1:A:3486:GLN:HE21	1:A:3510:LEU:HD11	1.81	0.46
1:A:4532:LEU:HA	1:A:4535:LEU:HG	1.97	0.46
1:A:4708:VAL:HG22	1:A:4711:LEU:HB2	1.97	0.46
1:A:1630:ASP:OD1	1:A:1630:ASP:N	2.49	0.46
1:A:4020:VAL:HG12	1:A:4067:LEU:HD23	1.98	0.46
1:A:518:ASP:OD2	1:A:640:ARG:NE	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4680:CYS:SG	1:A:4681:SER:N	2.90	0.45
1:A:1052:THR:HG1	1:A:1055:GLY:H	1.61	0.45
1:A:2491:HIS:ND1	1:A:2495:MET:SD	2.90	0.45
1:A:4115:GLU:HG2	1:A:4886:GLN:HE22	1.82	0.45
1:A:886:ARG:HD3	1:A:3236:SER:HB3	1.98	0.45
1:A:1495:SER:HG	1:A:1498:SER:H	1.58	0.45
1:A:2209:LYS:HA	1:A:2212:VAL:HB	1.98	0.45
1:A:3005:LEU:HD23	1:A:3113:LYS:HA	1.98	0.45
1:A:4431:GLU:O	1:A:4788:THR:OG1	2.33	0.45
1:A:987:LEU:HA	1:A:990:LEU:HD13	1.98	0.45
1:A:876:GLU:HG3	1:A:3544:ARG:HD2	1.98	0.45
1:A:1968:HIS:CE1	1:A:1982:LEU:HB2	2.52	0.45
1:A:2576:ILE:HG12	1:A:2646:LEU:HD13	1.98	0.45
1:A:3068:TYR:HE2	1:A:3124:LEU:HB2	1.81	0.45
1:A:3903:SER:OG	1:A:3907:LYS:NZ	2.50	0.45
1:A:4408:LEU:HD21	1:A:4596:LEU:HD21	1.98	0.45
1:A:5002:GLN:HG2	1:A:5003:THR:H	1.82	0.45
1:A:1200:LEU:O	1:A:1204:LYS:HG2	2.16	0.45
1:A:3655:VAL:HG12	1:A:3716:ASP:OD1	2.17	0.45
1:A:3974:TRP:O	1:A:3979:GLN:NE2	2.47	0.45
1:A:1509:TYR:HB3	1:A:1580:MET:HE2	1.99	0.44
1:A:1981:PRO:HD2	1:A:2014:VAL:HG22	1.98	0.44
1:A:2080:PRO:HB2	1:A:2081:LEU:H	1.66	0.44
1:A:5080:ILE:HD13	1:A:5132:ILE:HG22	1.99	0.44
1:A:1421:ASP:HA	1:A:1424:ARG:HE	1.82	0.44
1:A:3026:GLU:HB2	1:A:3057:LYS:HE2	1.99	0.44
1:A:5092:SER:OG	2:B:63:PHE:O	2.35	0.44
1:A:646:ARG:HD2	1:A:646:ARG:HA	1.80	0.44
1:A:982:SER:HA	1:A:3201:LEU:HD21	2.00	0.44
1:A:2100:ILE:HD13	1:A:2159:LEU:HD23	2.00	0.44
1:A:506:LEU:HD23	1:A:509:ILE:HD11	1.98	0.44
1:A:852:SER:OG	1:A:866:TYR:OH	2.35	0.44
1:A:1987:LEU:HD13	1:A:2018:ILE:HG23	1.99	0.44
1:A:3686:VAL:HG22	1:A:3762:PRO:HG2	1.99	0.44
1:A:1687:ALA:HA	1:A:1690:MET:HG2	1.99	0.44
1:A:2580:LEU:HD13	1:A:2602:VAL:HG13	2.00	0.44
1:A:3073:ASP:HA	1:A:3076:ASN:HD22	1.82	0.44
1:A:4150:GLU:OE2	1:A:4180:ARG:NH1	2.51	0.44
1:A:4257:ARG:NH1	1:A:4258:LYS:HB2	2.31	0.44
1:A:1377:ARG:HG3	1:A:1459:TRP:CZ3	2.52	0.44
1:A:2719:CYS:HB2	1:A:2726:LEU:HD23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1986:ARG:HD3	1:A:2019:ASP:HB2	1.99	0.44
1:A:2272:ASP:OD1	1:A:2272:ASP:N	2.49	0.44
1:A:2389:ARG:HA	1:A:2392:LYS:HG2	1.99	0.44
1:A:2509:SER:HB3	1:A:2512:GLU:HG3	1.99	0.44
1:A:2907:GLN:HE22	1:A:2912:PHE:H	1.66	0.44
1:A:5014:GLN:H	1:A:5017:HIS:HD2	1.66	0.44
1:A:1253:TYR:HD1	1:A:1287:MET:HE3	1.83	0.44
1:A:1875:GLN:HB2	1:A:5148:ARG:HH22	1.83	0.44
1:A:4529:THR:HA	1:A:4532:LEU:HG	2.00	0.44
1:A:839:ALA:HB1	1:A:914:ARG:HH21	1.83	0.43
1:A:1044:ASN:HB3	1:A:1046:LYS:HG2	2.00	0.43
1:A:1456:GLN:OE1	1:A:1460:ARG:NH1	2.50	0.43
1:A:1781:ARG:NH2	1:A:1817:PRO:O	2.48	0.43
1:A:2424:LYS:HA	1:A:2427:GLU:HG2	2.00	0.43
1:A:3281:SER:OG	1:A:3282:ARG:N	2.51	0.43
1:A:1601:TRP:HZ2	1:A:1615:MET:HE2	1.83	0.43
1:A:3503:MET:HE1	1:A:4981:ALA:HB1	2.01	0.43
1:A:3790:SER:O	1:A:3793:SER:OG	2.26	0.43
1:A:1394:LEU:HD13	1:A:1439:LEU:HD13	1.99	0.43
1:A:2802:VAL:HG23	1:A:2842:PHE:HD1	1.83	0.43
1:A:3028:ILE:HD13	1:A:3059:VAL:HG13	2.00	0.43
1:A:3662:ARG:HD2	1:A:3720:LEU:HD13	2.00	0.43
1:A:4646:ILE:HG22	1:A:4662:TYR:HE2	1.83	0.43
1:A:1031:TRP:HD1	1:A:1034:VAL:HG23	1.84	0.43
1:A:1621:LEU:HD23	1:A:1621:LEU:H	1.82	0.43
1:A:2455:ALA:O	1:A:2458:CYS:HB2	2.17	0.43
1:A:3053:MET:HE2	1:A:3090:LEU:HD11	2.00	0.43
1:A:3706:GLN:HA	1:A:3709:LEU:HG	2.00	0.43
1:A:892:ARG:NH2	1:A:941:GLU:OE1	2.52	0.43
1:A:1556:MET:HG3	1:A:3047:ASN:HB2	2.01	0.43
1:A:3346:SER:HA	1:A:3349:LEU:HD23	2.01	0.43
2:B:124:ASP:N	2:B:124:ASP:OD1	2.52	0.43
1:A:2423:SER:HA	1:A:2426:LYS:HE2	1.99	0.43
1:A:3200:ASP:N	1:A:3200:ASP:OD1	2.51	0.43
1:A:2213:VAL:HA	1:A:2216:MET:HE2	2.01	0.43
1:A:1451:PHE:HA	1:A:1454:HIS:CD2	2.53	0.43
1:A:2457:SER:O	1:A:2460:LYS:HB3	2.19	0.43
1:A:3219:ASP:OD2	1:A:3397:ARG:NH2	2.52	0.43
2:B:143:PHE:HA	2:B:146:LYS:HG2	2.01	0.43
1:A:1013:HIS:HB3	1:A:1017:PRO:HG2	2.00	0.43
1:A:4604:VAL:HG12	1:A:4607:PHE:HE1	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1319:ALA:HA	1:A:1322:ILE:HG22	2.00	0.42
1:A:1860:ASP:O	1:A:1896:ARG:NH1	2.50	0.42
1:A:3312:ASP:OD1	1:A:3312:ASP:N	2.50	0.42
1:A:1054:GLU:OE2	1:A:1057:GLN:NE2	2.49	0.42
1:A:1276:LYS:NZ	1:A:2882:ASP:OD1	2.52	0.42
1:A:882:ARG:HA	1:A:885:LEU:HG	2.01	0.42
1:A:2846:SER:OG	1:A:2848:TRP:O	2.33	0.42
1:A:3025:PRO:HB3	1:A:3058:MET:HB2	2.02	0.42
1:A:4225:ARG:HH11	1:A:4256:PRO:HA	1.83	0.42
2:B:47:ASP:O	2:B:151:ARG:NE	2.52	0.42
2:B:105:ILE:HA	2:B:108:LEU:HG	2.01	0.42
1:A:1643:GLU:HA	1:A:1646:LEU:HG	2.02	0.42
1:A:2295:ASN:HD21	1:A:2300:LYS:HD3	1.84	0.42
1:A:2430:ARG:HA	1:A:2430:ARG:NH1	2.33	0.42
1:A:3002:LEU:HB2	1:A:3108:ILE:HG12	2.02	0.42
1:A:4264:LYS:HG3	1:A:4266:HIS:H	1.85	0.42
1:A:4792:ILE:HD12	1:A:4825:ALA:HA	2.00	0.42
1:A:4258:LYS:HE3	1:A:4669:LEU:HD23	2.02	0.42
1:A:4724:VAL:HG12	1:A:4863:VAL:HB	2.01	0.42
1:A:1963:TYR:CZ	1:A:2091:VAL:HG11	2.54	0.42
1:A:2222:ASP:OD2	1:A:2264:HIS:ND1	2.43	0.42
1:A:4295:LYS:NZ	1:A:4298:ASP:HB3	2.34	0.42
1:A:3516:ASP:OD1	1:A:3516:ASP:N	2.53	0.42
1:A:3539:GLU:HA	1:A:3542:GLN:HG2	2.02	0.42
1:A:3597:LEU:HD23	1:A:3607:VAL:HG13	2.02	0.42
1:A:4547:ALA:HA	1:A:4550:VAL:HG22	2.02	0.42
1:A:689:GLU:HG2	1:A:770:TYR:CD1	2.55	0.42
1:A:1456:GLN:HA	1:A:1459:TRP:HD1	1.83	0.42
1:A:2315:LEU:HD23	1:A:2320:VAL:HG11	2.01	0.42
1:A:2827:ASP:HB2	1:A:2834:PRO:HB3	2.01	0.42
1:A:640:ARG:NH1	1:A:3674:TYR:OH	2.51	0.42
1:A:3726:SER:HB3	1:A:3729:GLU:HB3	2.02	0.42
1:A:5044:ILE:HD11	1:A:5132:ILE:HD13	2.02	0.42
1:A:642:ARG:HD2	1:A:4765:ARG:HH12	1.85	0.41
1:A:808:GLU:HG2	1:A:810:LEU:HD23	2.02	0.41
1:A:3958:VAL:HG21	1:A:3993:PHE:HB2	2.02	0.41
1:A:3814:MET:HE1	1:A:3865:GLU:HB2	2.02	0.41
1:A:3821:LYS:HG3	1:A:3869:LEU:HD11	2.02	0.41
1:A:4988:ASP:HA	1:A:5014:GLN:HG3	2.02	0.41
1:A:1054:GLU:O	1:A:1057:GLN:HG3	2.20	0.41
1:A:1395:HIS:NE2	1:A:1439:LEU:O	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1586:VAL:HG13	1:A:1646:LEU:HD23	2.01	0.41
1:A:1725:LYS:NZ	1:A:1729:GLN:OE1	2.50	0.41
1:A:2018:ILE:O	1:A:2059:VAL:HA	2.20	0.41
1:A:2755:GLU:OE1	1:A:2758:ARG:NH1	2.48	0.41
1:A:3058:MET:HG2	1:A:3106:ARG:HB2	2.02	0.41
1:A:3157:PHE:HE2	1:A:3242:LEU:HD13	1.85	0.41
1:A:4731:LEU:HD21	1:A:4827:VAL:HG11	2.03	0.41
1:A:662:ASP:OD1	1:A:662:ASP:N	2.54	0.41
1:A:1131:LYS:HA	1:A:1134:VAL:HG12	2.01	0.41
1:A:1710:CYS:SG	1:A:1711:GLU:N	2.93	0.41
1:A:2388:THR:HA	1:A:2391:ILE:HG12	2.03	0.41
1:A:4307:ARG:HG3	1:A:4308:SER:H	1.86	0.41
1:A:5033:ARG:HE	1:A:5038:LYS:HB2	1.86	0.41
1:A:5144:ASP:O	1:A:5148:ARG:HB3	2.21	0.41
1:A:2507:ARG:HE	1:A:2508:VAL:HG13	1.85	0.41
1:A:2694:LEU:HD22	1:A:2710:LYS:HG2	2.01	0.41
1:A:801:TYR:HD2	1:A:805:ILE:HD11	1.85	0.41
1:A:1018:VAL:HG23	1:A:1019:PHE:H	1.86	0.41
1:A:1324:GLN:HG3	1:A:1385:ALA:HB1	2.01	0.41
1:A:973:ILE:HG12	1:A:1004:ALA:HB2	2.02	0.41
1:A:1144:VAL:HG22	1:A:1147:LEU:HB2	2.03	0.41
1:A:3769:GLN:OE1	1:A:3772:ARG:NH2	2.53	0.41
1:A:4413:ASN:HB3	1:A:4421:MET:HE3	2.02	0.41
1:A:2428:ALA:HA	1:A:2431:THR:HG22	2.03	0.41
1:A:669:PRO:HG3	1:A:730:LEU:HD22	2.02	0.40
1:A:1806:ALA:HB2	1:A:1857:LEU:HD21	2.03	0.40
1:A:2805:ASP:HA	1:A:2845:ILE:HG23	2.01	0.40
1:A:4410:PRO:HB3	1:A:4611:LEU:HG	2.04	0.40
1:A:4895:ASP:OD1	1:A:4895:ASP:N	2.54	0.40
1:A:1365:LYS:HA	1:A:1365:LYS:HD3	1.84	0.40
1:A:2021:SER:OG	1:A:2022:THR:N	2.54	0.40
1:A:2722:LEU:HD23	1:A:2722:LEU:HA	1.86	0.40
1:A:3780:ARG:HH21	1:A:3842:PRO:HB3	1.85	0.40
1:A:2946:ARG:HG3	1:A:2978:LEU:HD22	2.03	0.40
1:A:3611:TRP:HD1	1:A:3656:PRO:HB3	1.87	0.40
1:A:1377:ARG:HD3	1:A:1462:LEU:HD22	2.03	0.40
1:A:1383:GLU:HB3	1:A:1472:LEU:HD23	2.04	0.40
1:A:1950:ILE:HG21	1:A:2085:LEU:HD12	2.03	0.40
1:A:2367:ILE:HG22	1:A:2371:PHE:HE1	1.86	0.40
1:A:4106:GLN:HA	1:A:4109:LYS:HG2	2.02	0.40
1:A:4232:LEU:HD22	1:A:4240:PHE:HE2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4409:LYS:HG2	1:A:4412:ARG:HH22	1.87	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	4394/5161 (85%)	3983 (91%)	404 (9%)	7 (0%)	43	74
2	B	151/166 (91%)	150 (99%)	1 (1%)	0	100	100
All	All	4545/5327 (85%)	4133 (91%)	405 (9%)	7 (0%)	44	74

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4600	GLN
1	A	1374	SER
1	A	4049	GLN
1	A	4166	PRO
1	A	5128	MET
1	A	2547	ASN
1	A	1373	ILE

5.3.2 Protein sidechains [i](#)

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

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	5201	4	32,33,33	0.32	0	48,52,52	0.29	0

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	5201	4	-	3/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

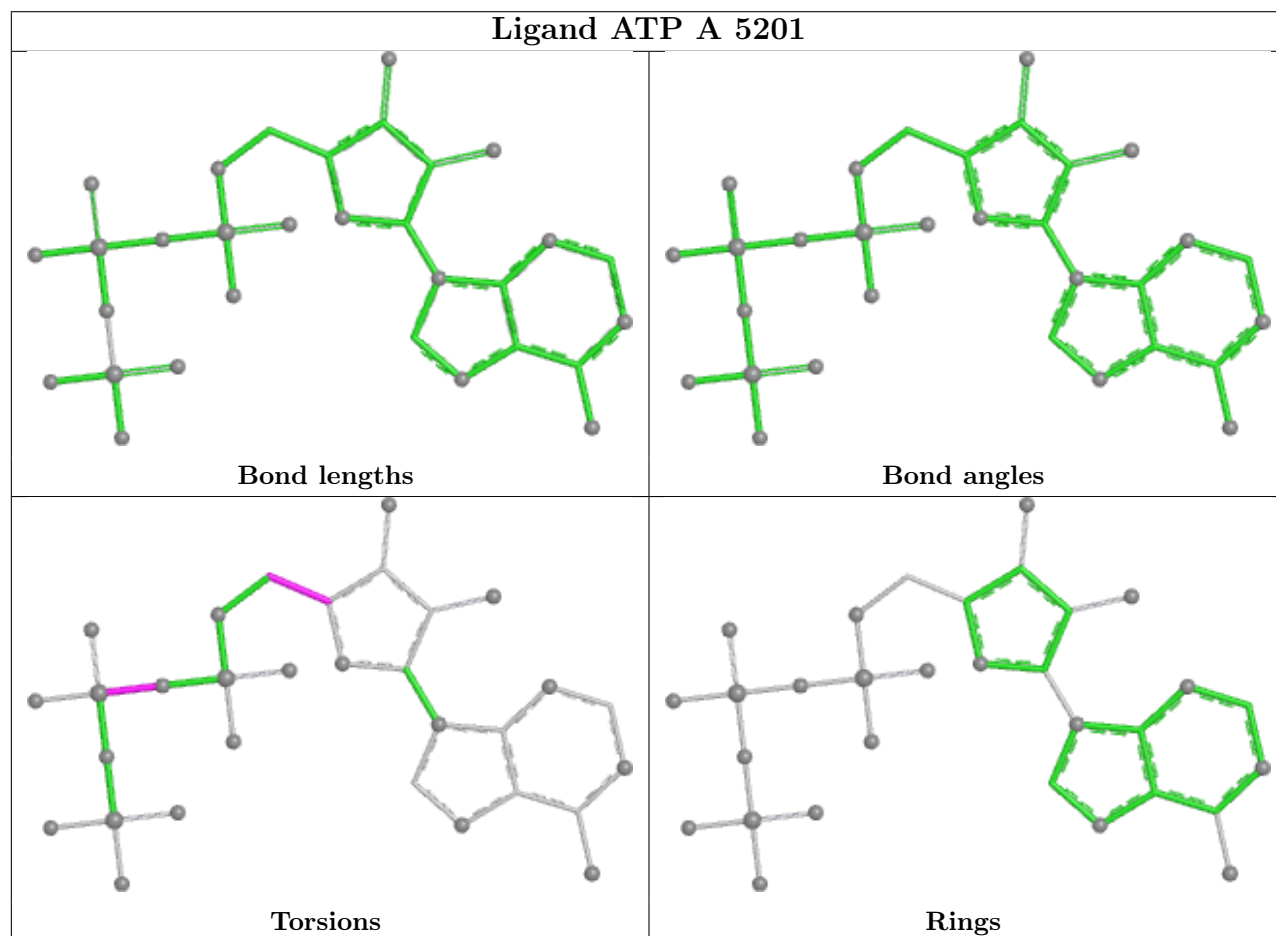
Mol	Chain	Res	Type	Atoms
3	A	5201	ATP	O4'-C4'-C5'-O5'
3	A	5201	ATP	C3'-C4'-C5'-O5'
3	A	5201	ATP	PA-O3A-PB-O2B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	5201	ATP	1	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.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

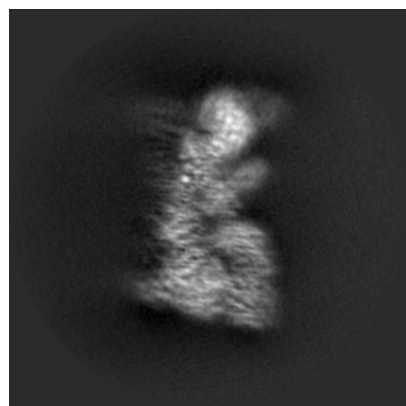
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12931. These allow visual inspection of the internal detail of the map and identification of artifacts.

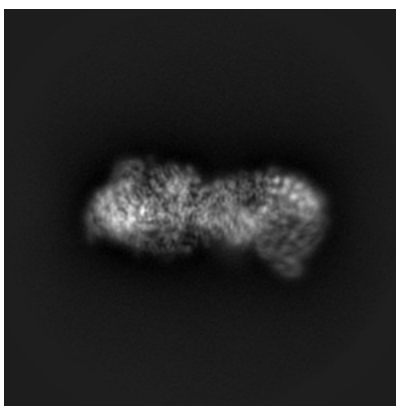
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

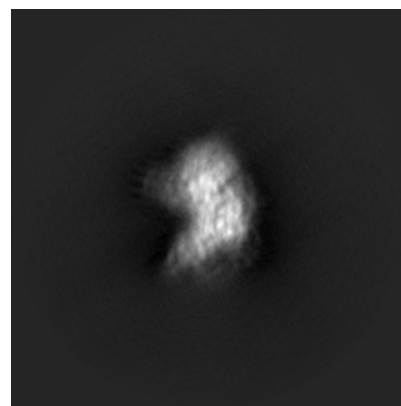
6.1.1 Primary map



X

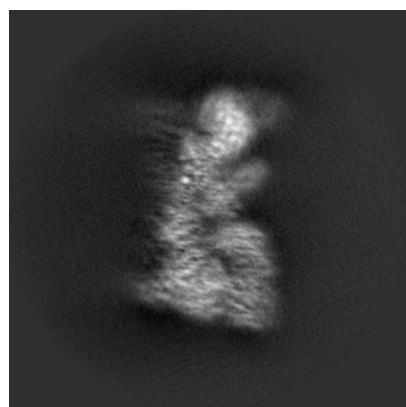


Y

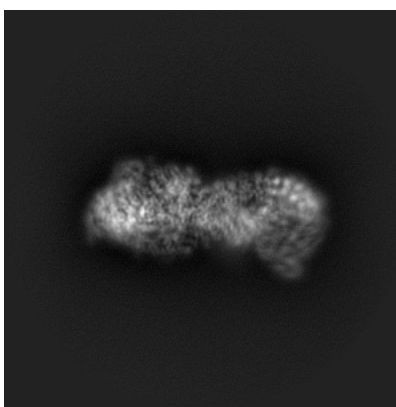


Z

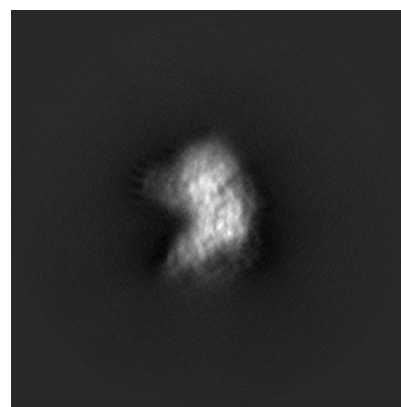
6.1.2 Raw map



X



Y

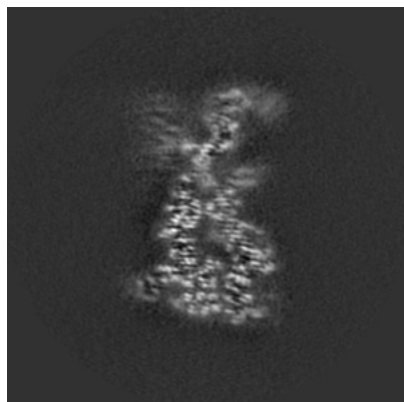


Z

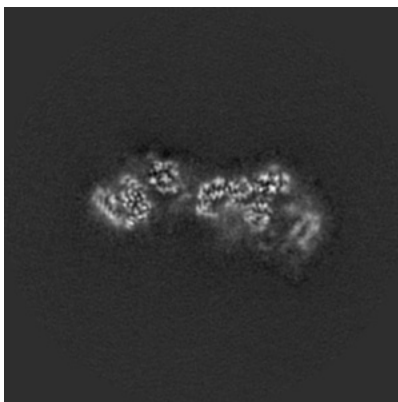
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

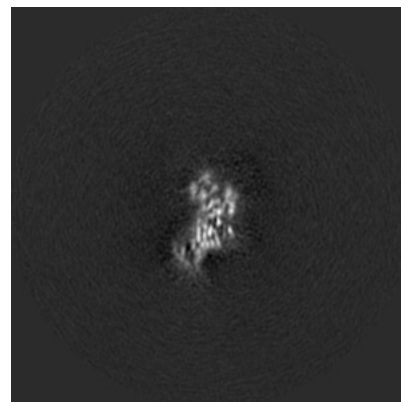
6.2.1 Primary map



X Index: 176

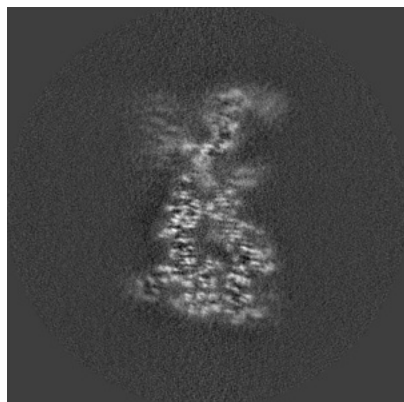


Y Index: 176

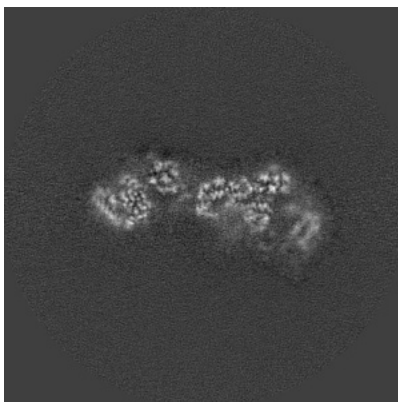


Z Index: 176

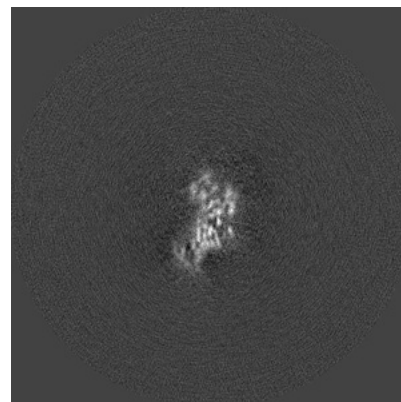
6.2.2 Raw map



X Index: 176



Y Index: 176

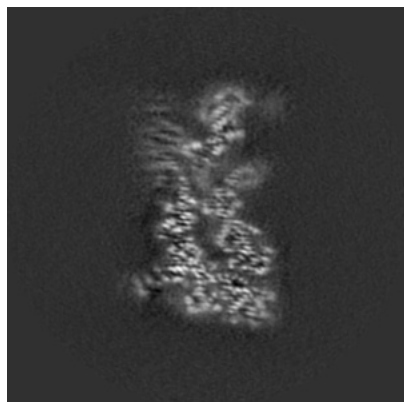


Z Index: 176

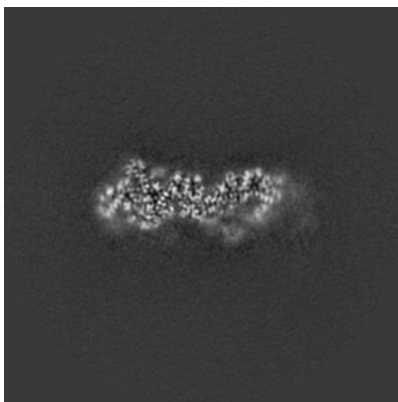
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

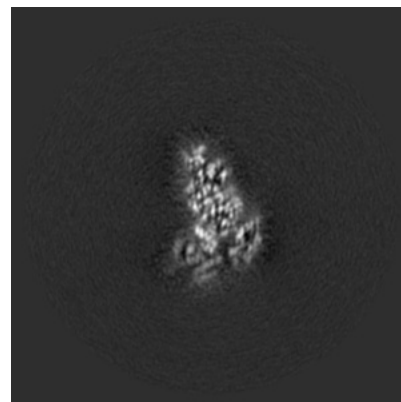
6.3.1 Primary map



X Index: 172

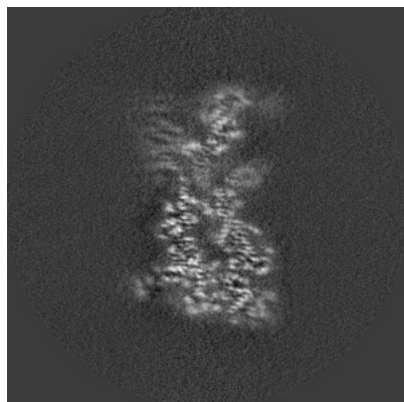


Y Index: 159

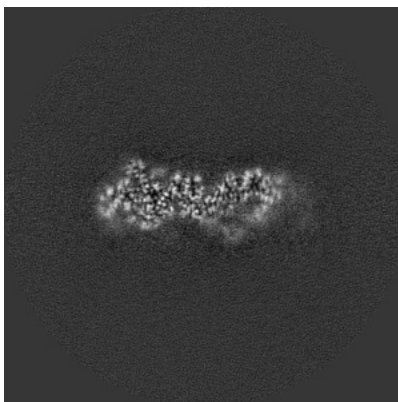


Z Index: 111

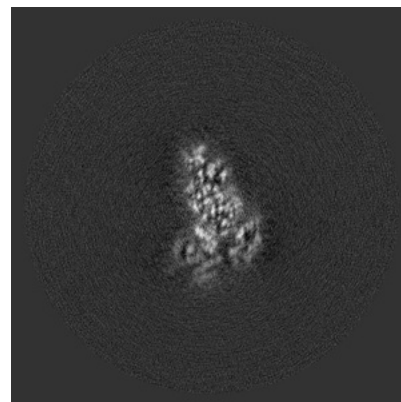
6.3.2 Raw map



X Index: 173



Y Index: 159

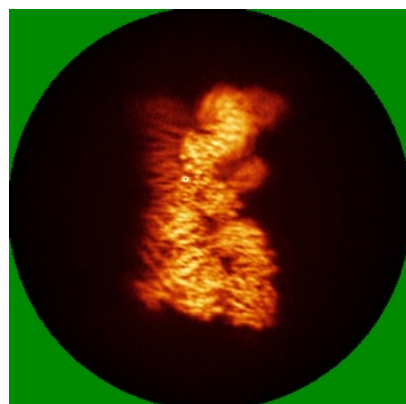


Z Index: 111

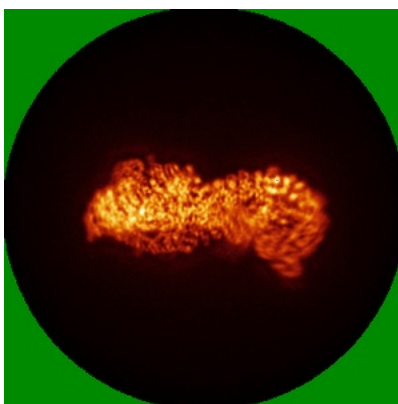
The images above show the largest variance slices of the map in three orthogonal directions.

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

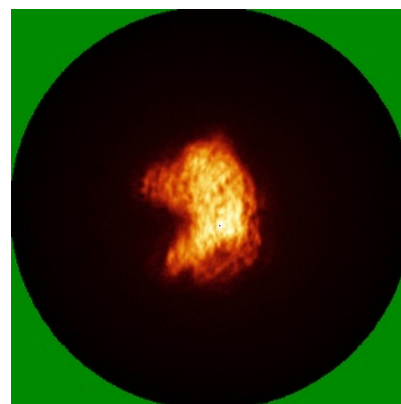
6.4.1 Primary map



X

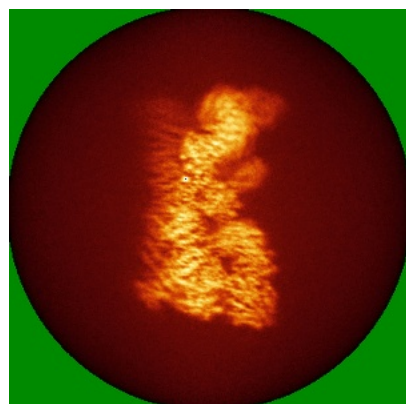


Y

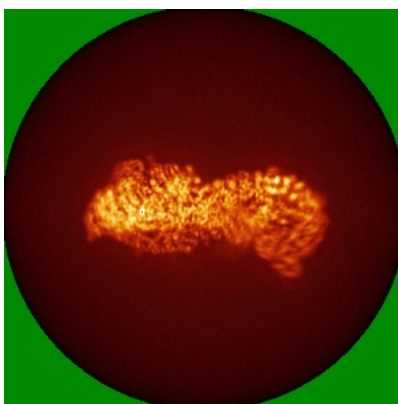


Z

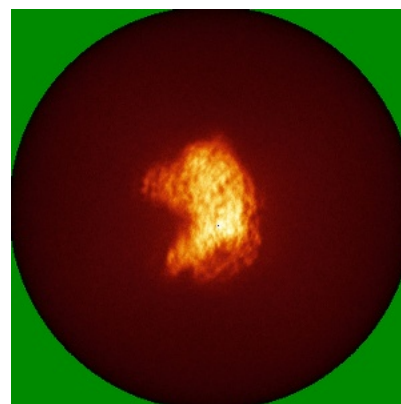
6.4.2 Raw map



X



Y



Z

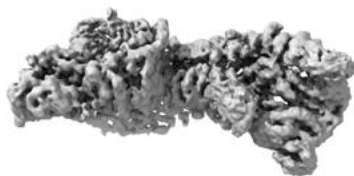
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

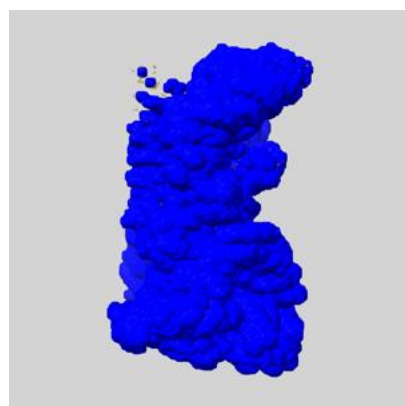
6.6 Mask visualisation [i](#)

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

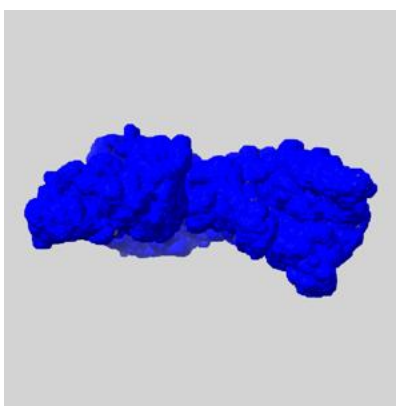
A mask typically either:

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

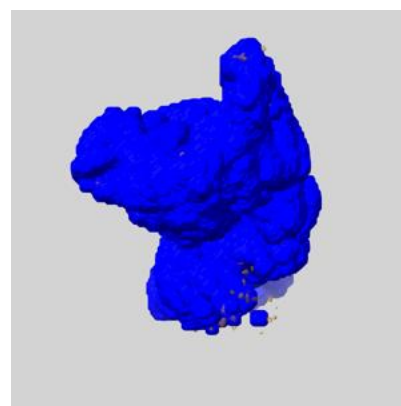
6.6.1 emd_12931_msk_1.map [i](#)



X



Y

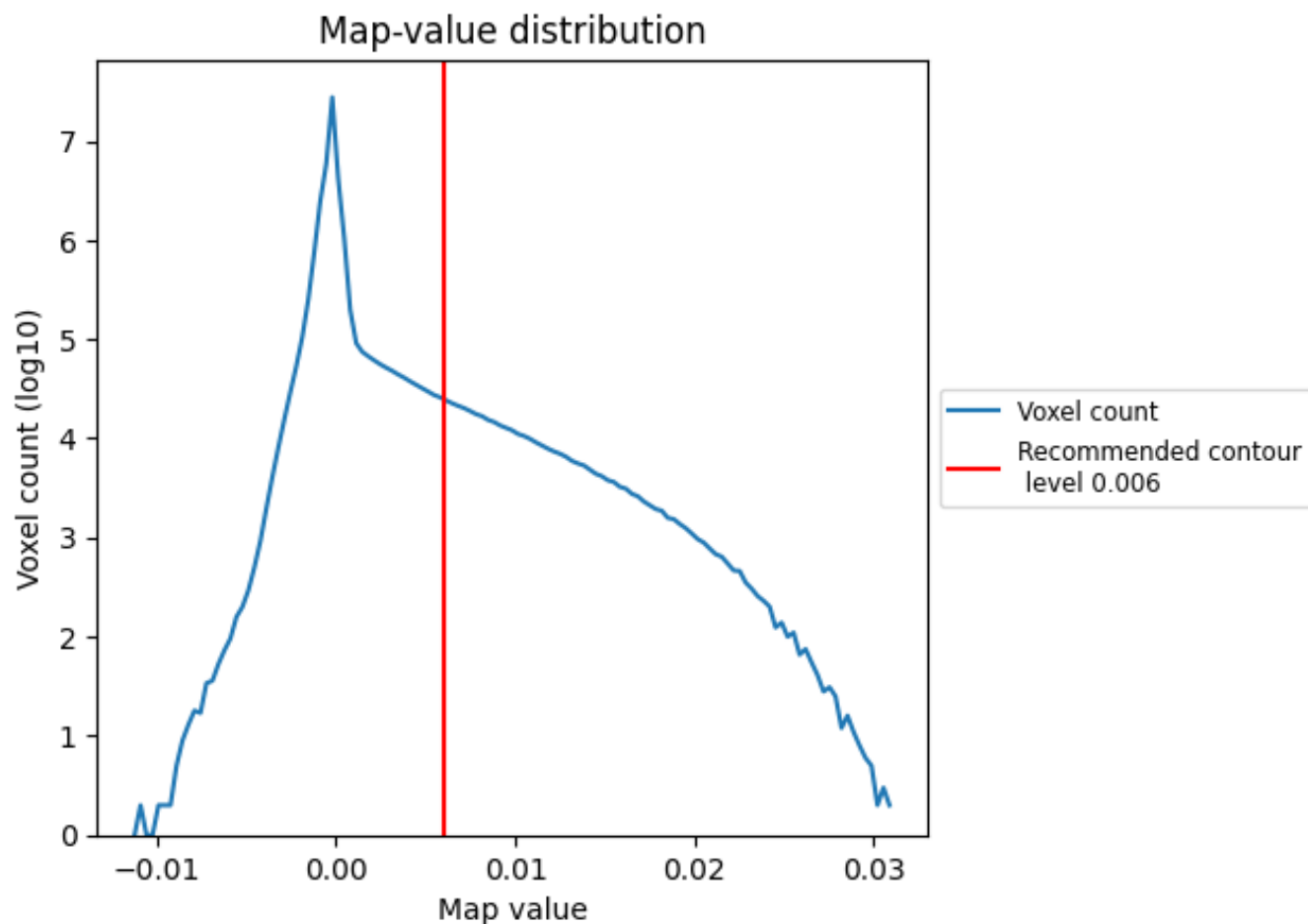


Z

7 Map analysis [i](#)

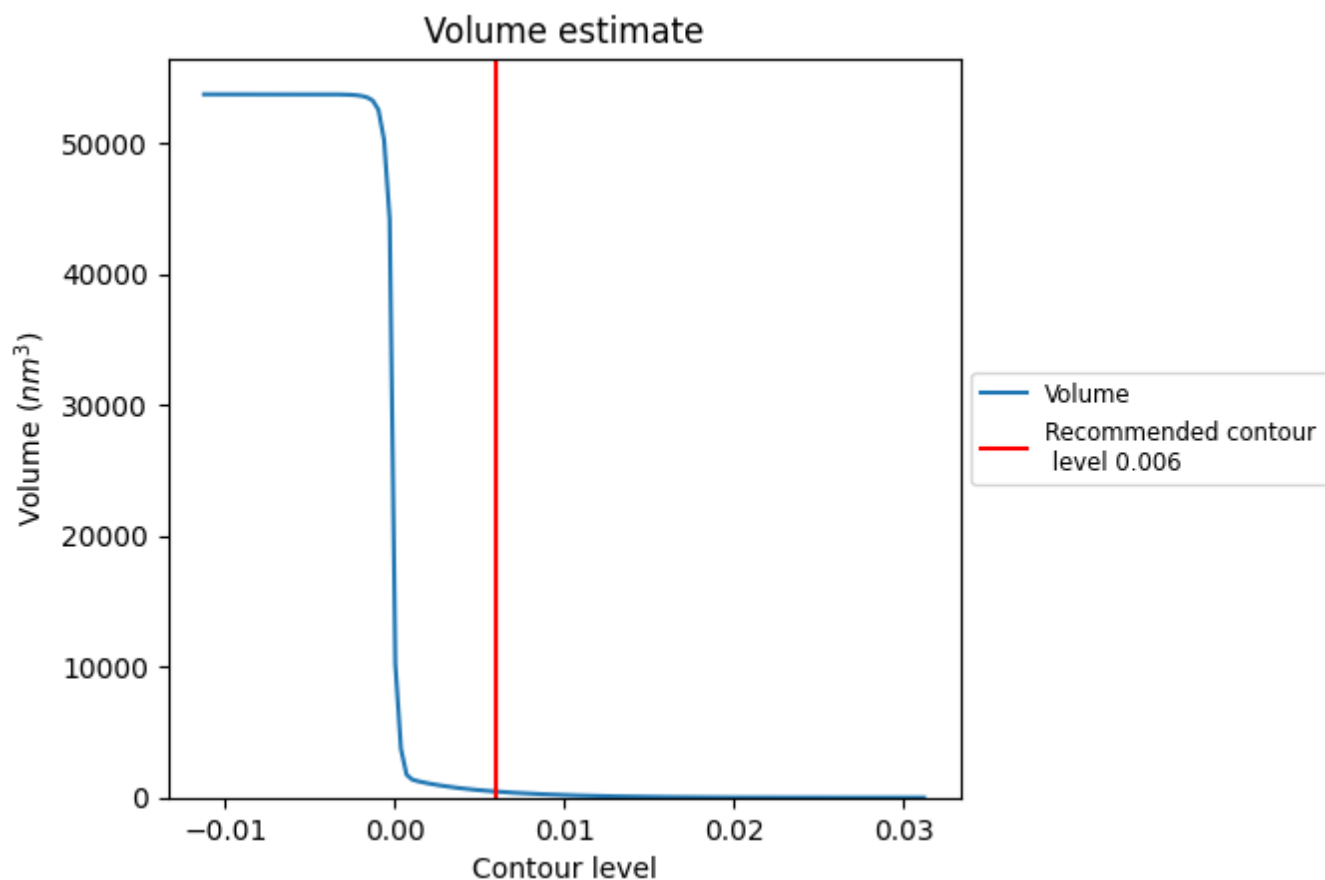
This section contains the results of statistical analysis of the map.

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.

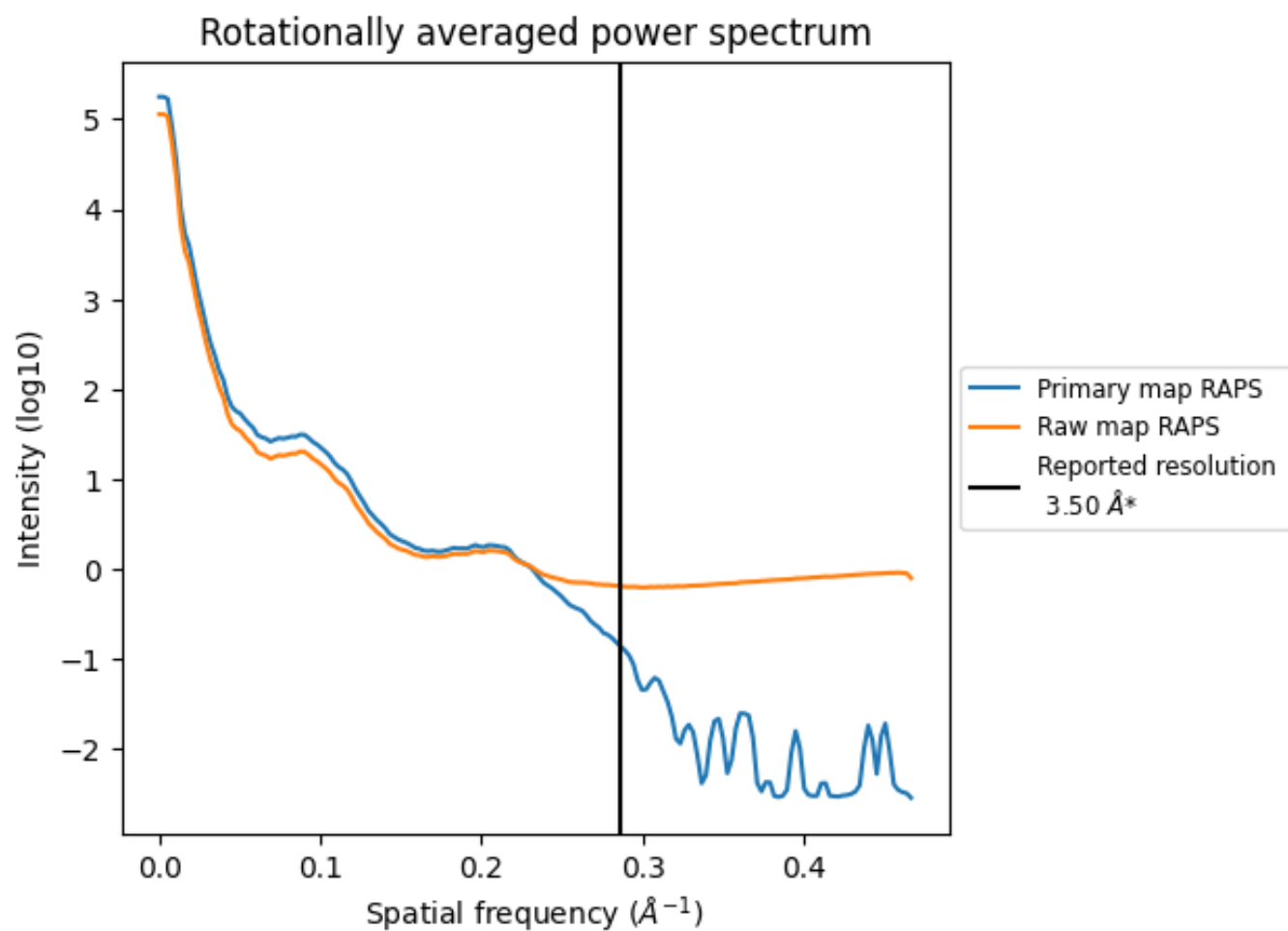
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 457 nm^3 ; this corresponds to an approximate mass of 412 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 ⓘ

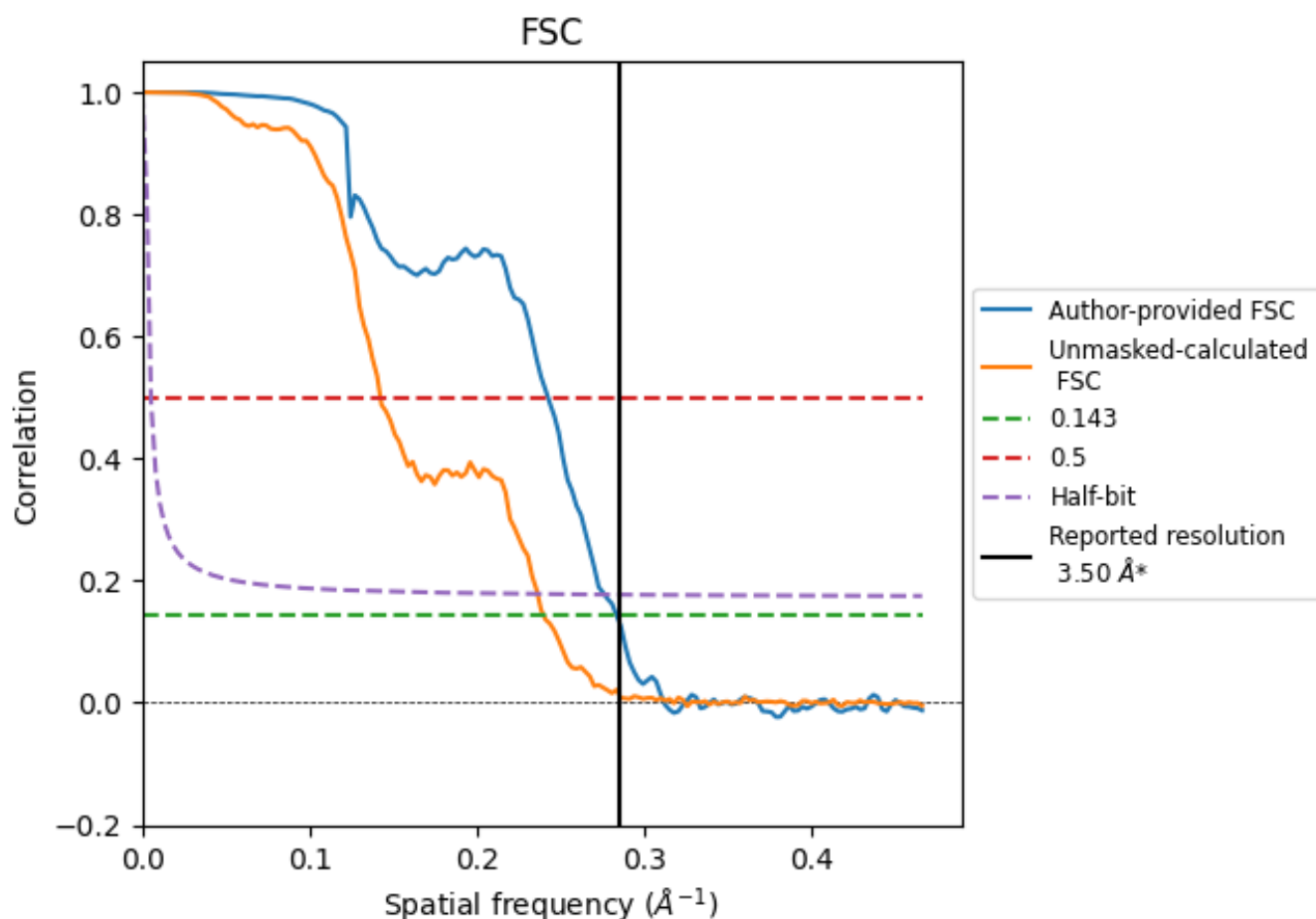


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.286 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

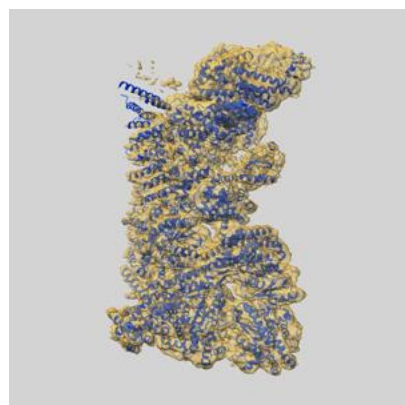
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.52	4.12	3.62
Unmasked-calculated*	4.16	7.02	4.23

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.16 differs from the reported value 3.5 by more than 10 %

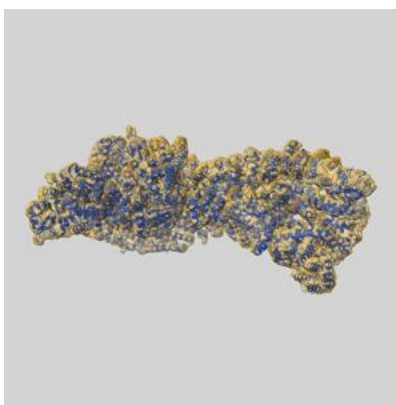
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12931 and PDB model 7OIK. Per-residue inclusion information can be found in section [3](#) on page [6](#).

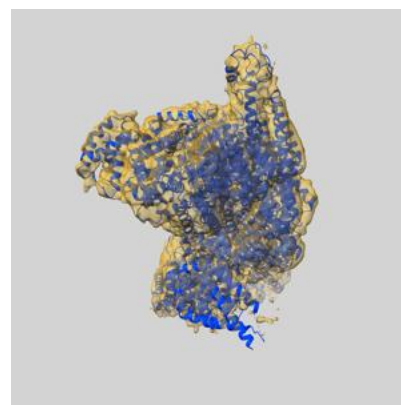
9.1 Map-model overlay [i](#)



X



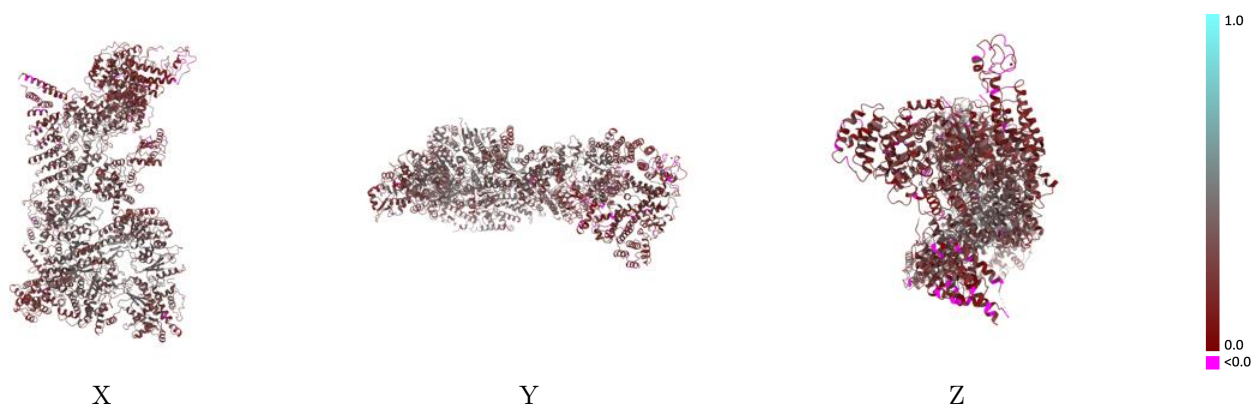
Y



Z

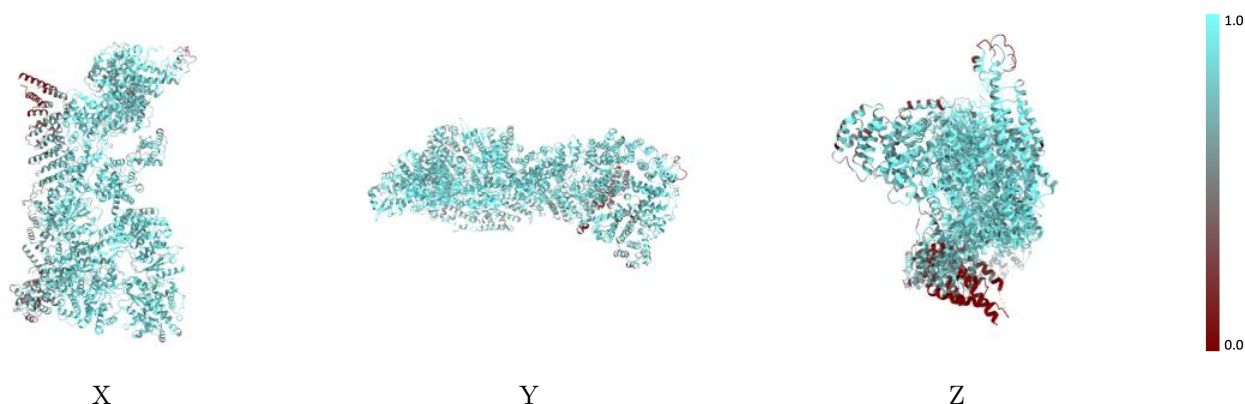
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



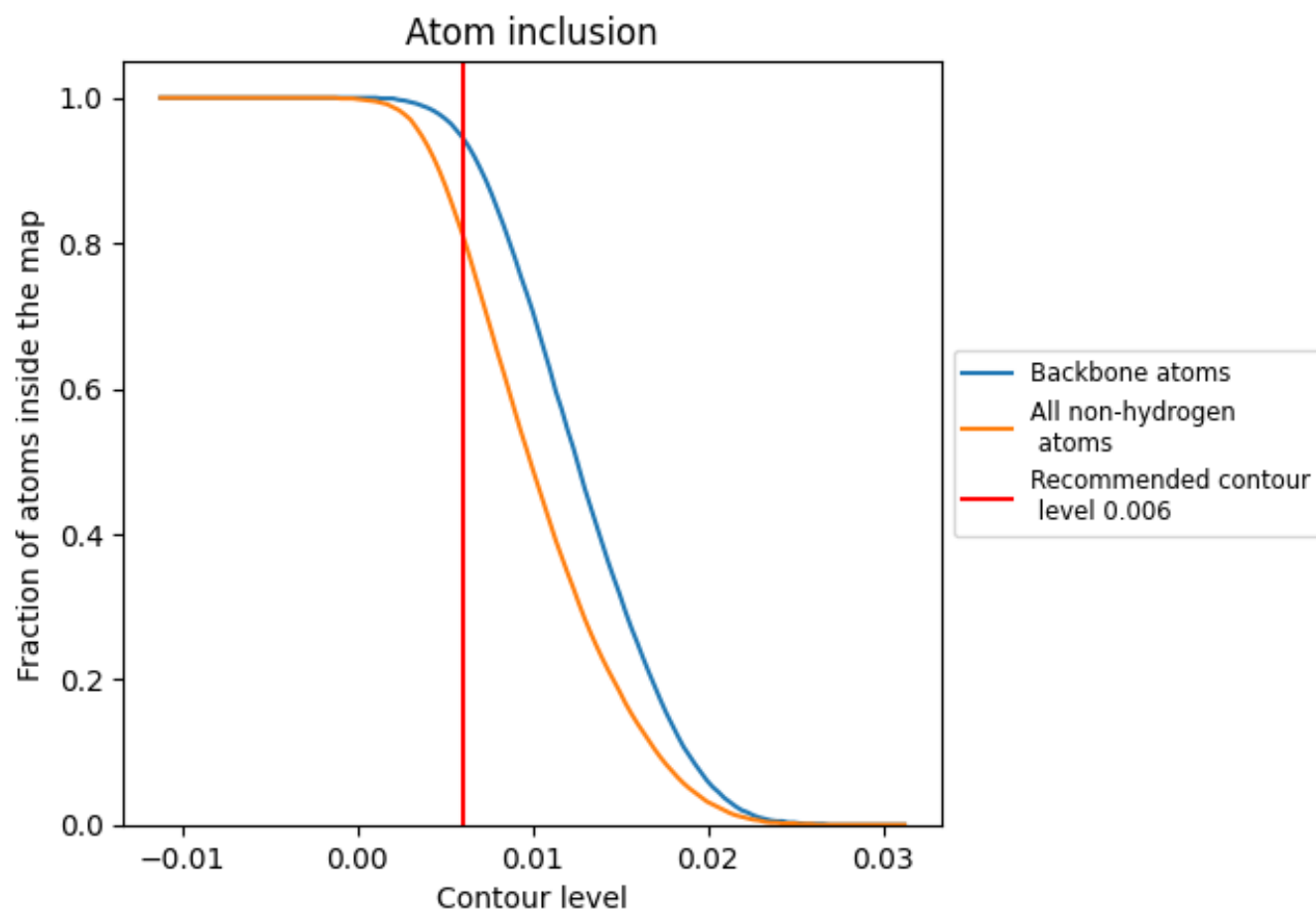
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.006).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 81% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8110	0.2940
A	0.8130	0.2970
B	0.7660	0.1960

