



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 09:16 PM UTC

PDB ID : 9BM3 / pdb_00009bm3
EMDB ID : EMD-44686
Title : State-5a of motor domain from full-length human dynein-1 in 5 mM ATP
Authors : Chai, P.; Zhang, K.
Deposited on : 2024-05-02
Resolution : 3.49 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.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 EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

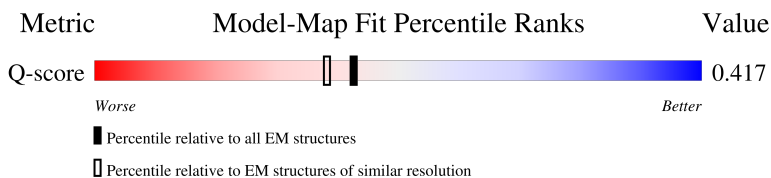
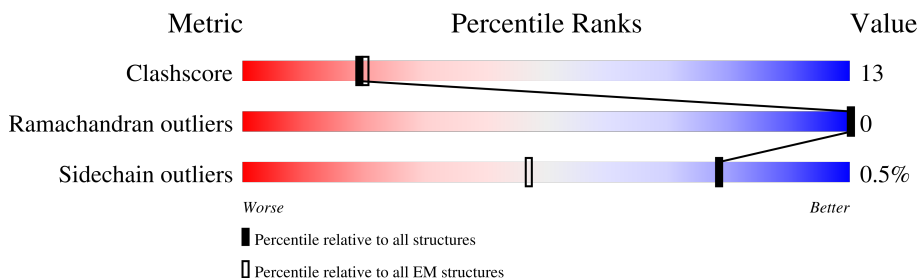
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

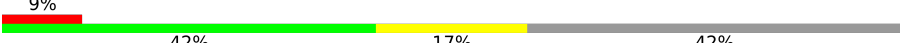
The reported resolution of this entry is 3.49 Å.

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	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13600 (2.99 - 3.99)

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	4646	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 21867 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2711	21755	13852	3757	4035	111	0	0

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



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

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

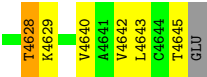


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	





C4510	M4377	M4296	K4171	M4043	R3937	I3835	N3754	L3679	D3591	A3484	LYS
L4511	L4380	P4297	S4172	M4043	F3944	Y3636	E3755	S3681	P3592	E3485	ASP
G4512	H4381	D4298	P4173	D4050	K3945	V3639	V3756	T3680	M3601	R3486	ASN
F4515	T4382	R4301	R4176	G4053	L3946	Y3641	K3757	F3688	I3600	E3487	GLN
Y4520	T4383	R4302	R4177	H4054	D3947	E3642	G3758	P3689	L3600	R3488	LYS
Y4520	W4387	E4303	R4178	H4055	L3948	N3643	R3759	D3690	L3600	R3489	ASN
Q4526	W4387	E4304	R4179	V4055	A3949	L3646	L3760	D3691	D3606	R3490	ALA
Y4527	L4390	F4305	F4186	L4058	V3951	L3846	L3761	L3692	R3607	E3491	GLU
Y4528	L4390	V4306	F4186	A4059	Q3952	L3851	D3762	L3693	K3608	T3492	VAL
S4535	Q4393	W4308	E4192	A4060	E3955	D3651	D3763	R3694	T3610	S3493	GLN
L4536	R4400	E4310	R4195	A4060	Q3956	Q3854	D3764	V3695	R3611	E3494	MET
E4537	F4412	L4212	R4195	H4063	F3957	L3856	T3765	T3697	S3613	T3495	ASN
E4538	F4412	L4212	Y4205	H4063	F3957	L3856	T3765	F3698	F3614	T3496	ASP
Y4543	F4413	P4318	Y4205	S4068	V3960	L3859	L3766	V3699	R3497	K3497	GLU
T4547	E4414	S4319	E4209	S4073	V3960	L3859	L3767	N3700	D3617	K3498	LEU
Q4548	R4415	E4320	E4210	S4073	P3966	L3863	T3768	F3701	D3617	N3498	ALA
Q4549	D4426	D4211	D4211	A4074	P3971	L3864	T3769	T3702	L3623	Q3499	ASN
G4550	W4434	R4213	R4213	E4075	L3972	F3867	E3771	V3703	L3623	K3500	ILE
A4551	V4435	D4220	D4220	A4080	K3974	A3867	L3770	T3704	S3501	S3501	ARG
T4552	C4438	L4224	L4224	A4087	S3976	R3873	E3771	S3707	T3502	T3502	ALA
D4554	E4439	D4227	A4227	A4087	E3977	D3882	E3777	A3719	D3506	D3506	TYR
S4557	Q4444	Q4347	Q4347	S4090	T3983	L3886	E3776	E3720	L3509	L3509	GLU
T4561	T4445	G4091	G4091	G4091	L3987	D3879	K3774	R3721	S3510	S3510	GLY
L4565	Y4447	L4233	L4233	R4092	L3982	T3882	E3778	V3635	Y3516	Y3516	MET
Q4566	L4448	S4234	S4234	R4092	L3982	T3882	E3778	Q3636	F3520	F3520	VAL
Q4567	R4449	K4237	K4237	M4095	F3996	L3886	E3779	V3638	F3529	F3529	LYS
L4577	Y4452	Y4252	Y4252	M4095	F3996	L3886	E3779	L3645	K3524	K3524	TRP
S4578	N4453	Q4253	Q4253	V4099	R4000	D3902	R3783	N3650	R3532	R3532	ALA
N4579	E4454	D4257	D4257	H4100	T4011	L3909	V3784	R3651	E3558	E3558	TYR
P4586	L4455	N4258	N4258	L4106	M4012	N3912	E3785	E3652	R3544	R3544	ALA
L4587	Y4457	E4259	E4259	M4107	L4013	E3913	E3786	V3653	T3545	T3545	ASP
T4588	W4457	F4260	F4260	P4118	G4014	L3914	T3787	V3654	D3546	D3546	LEU
Y4592	L4460	D4261	D4261	R4123	S4016	V3915	D3788	R3655	R3549	R3549	LYS
T4596	H4466	F4268	F4268	L4124	F4017	L3916	L3789	T3656	R3549	R3549	ARG
N4597	Y4467	S4277	S4277	M4128	L4020	S3917	V3790	G3657	L3553	L3553	VAL
T4598	Y4467	E4281	E4281	M4131	M4021	A3918	Q3792	G3658	E3558	E3558	GLU
E4599	M4473	F4282	F4282	M4131	E4022	G3919	E3793	R3659	R3570	R3570	ASN
K4600	T4474	K4283	K4283	V4134	Q4023	P3922	V3794	V3661	T3570	T3570	GLU
P4608	V4475	V4288	V4288	P4135	D4026	R3923	E3795	L3662	N3576	N3576	LEU
V4609	L4476	D4289	D4289	F4145	L4027	L3924	T3796	T3663	K3579	K3579	GLN
Y4610	W4478	G4290	G4290	V4146	L4027	L3924	L3742	L3664	L3477	L3477	LYS
L4611	W4478	H4291	H4291	F4147	L4030	Q3925	S3788	G3665	L3478	L3478	LEU
L4611	V4479	K4292	K4292	F4147	V4031	V3929	Q3799	D3666	L3479	L3479	GLU
L4618	G4500	D4293	D4293	T4160	P4037	V3933	Q3800	Q3667	K3481	K3481	ASP
L4619	A4501	W4375	W4375	V4166	P4040	E3933	Y3801	D3668	S3482	S3482	ALA
	K4505	V4376	V4376	S4167		V3935	C3808	L3671	L3482	L3482	
				R4168		V3936	T3811	S3674	S3483	S3483	
							E3816				
							S3817				
							K3819				
							Q3826				



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	65824	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.644	Depositor
Minimum map value	-0.354	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.12	Depositor
Map size ($\text{\AA}$)	332.80002, 332.80002, 332.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.832, 0.832, 0.832	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.18	0/22220	0.36	3/30121 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2812	PRO	CA-N-CD	-8.91	99.53	112.00
1	A	1848	PRO	CA-N-CD	-6.17	103.36	112.00
1	A	2020	PRO	CA-N-CD	-5.04	104.95	112.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	21755	0	21789	555	0
2	A	81	0	36	7	0
3	A	31	0	12	0	0
All	All	21867	0	21837	555	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 13.

All (555) 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:3662:ILE:HD11	1:A:3671:LEU:HB2	1.54	0.87
1:A:3790:VAL:HG13	1:A:3794:VAL:HB	1.56	0.87
1:A:3661:LEU:HD11	1:A:3668:ASP:HB3	1.61	0.83
1:A:3731:LEU:HD12	1:A:3790:VAL:HG21	1.66	0.78
1:A:2053:MET:HE1	1:A:2094:LYS:HA	1.66	0.78
1:A:2925:ILE:HG21	1:A:2933:LEU:HG	1.67	0.77
1:A:4176:ARG:NH1	1:A:4220:ASP:OD1	2.18	0.76
1:A:3169:MET:HE1	1:A:3688:PHE:HB2	1.68	0.75
1:A:4040:PRO:HB3	1:A:4124:LEU:HD23	1.67	0.75
1:A:3992:LEU:O	1:A:3996:PHE:HB2	1.87	0.74
1:A:1950:GLN:HG2	1:A:2006:VAL:HG13	1.71	0.72
1:A:2494:LEU:O	1:A:2498:ILE:HD12	1.90	0.72
1:A:1635:GLU:HB3	1:A:2273:ARG:HB3	1.71	0.71
1:A:3733:LYS:O	1:A:3737:GLU:N	2.19	0.71
1:A:2910:VAL:HG11	1:A:3105:VAL:HG22	1.71	0.71
1:A:3198:GLN:HE22	1:A:3496:PHE:HD1	1.37	0.70
1:A:3983:ILE:HG13	1:A:4011:THR:HG22	1.74	0.70
1:A:2933:LEU:HB2	1:A:3065:VAL:HG23	1.74	0.70
1:A:2444:GLU:HG2	1:A:2510:MET:HE2	1.73	0.69
1:A:1925:ARG:HH12	1:A:2011:ASP:HB3	1.57	0.69
1:A:1960:PHE:HB3	1:A:2018:MET:HE3	1.75	0.69
1:A:2499:LEU:HD21	1:A:2518:ILE:HG21	1.75	0.69
1:A:4303:GLU:OE1	1:A:4303:GLU:N	2.26	0.68
1:A:3496:PHE:HA	1:A:3499:GLN:OE1	1.94	0.68
1:A:2287:ILE:HA	1:A:2294:GLU:HG3	1.78	0.66
1:A:1964:GLU:HG2	1:A:1967:MET:H	1.61	0.66
1:A:2446:ILE:HD11	1:A:2714:PRO:HB3	1.78	0.66
1:A:1679:ARG:HH21	1:A:2332:ARG:HH12	1.44	0.66
1:A:2671:MET:HE2	1:A:2675:GLY:HA2	1.77	0.66
1:A:3689:PRO:HG2	1:A:3692:LEU:HD23	1.78	0.66
1:A:1839:LEU:O	1:A:1843:ARG:NH1	2.28	0.66
1:A:1961:ASN:ND2	1:A:2019:ASN:O	2.29	0.65
1:A:3526:GLN:OE1	1:A:3549:ARG:NH2	2.29	0.65
1:A:3576:ASN:ND2	1:A:3700:ASN:O	2.29	0.65
1:A:3510:SER:HB3	1:A:3553:LEU:HD21	1.79	0.64
1:A:2615:MET:HG3	1:A:2658:TRP:HB2	1.80	0.64
1:A:3113:MET:HE1	1:A:3184:ALA:HA	1.79	0.64
1:A:3520:PHE:HB3	1:A:3524:MET:HB3	1.80	0.64
1:A:3691:ASP:O	1:A:3695:ARG:HG2	1.98	0.64
1:A:4505:LYS:NZ	1:A:4554:ASP:O	2.32	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2181:GLU:HG3	1:A:2244:LEU:HB2	1.80	0.63
1:A:2605:LEU:HD11	1:A:2709:VAL:HG11	1.80	0.63
1:A:1799:GLU:OE1	1:A:2109:GLN:NE2	2.32	0.63
1:A:1910:THR:HG22	1:A:2044:PRO:HD3	1.80	0.63
1:A:2453:ARG:NH1	1:A:2505:ASP:OD2	2.32	0.63
1:A:2221:MET:HG2	1:A:2343:PHE:HB2	1.81	0.62
1:A:2923:ASP:OD1	1:A:2954:ASN:ND2	2.31	0.62
1:A:1931:ASN:O	1:A:1931:ASN:ND2	2.32	0.62
1:A:3010:THR:HG22	1:A:3017:VAL:HG22	1.82	0.62
1:A:4305:PHE:O	1:A:4309:VAL:HG23	2.00	0.61
1:A:2226:SER:HB2	1:A:2726:ARG:HG2	1.81	0.61
1:A:3580:LEU:HD13	1:A:3600:ILE:HD11	1.82	0.61
1:A:1755:GLN:HG2	1:A:1814:GLU:OE1	2.00	0.61
1:A:3021:PHE:CE1	1:A:3029:LEU:HB2	2.36	0.61
1:A:4043:MET:HE1	1:A:4055:VAL:HB	1.83	0.61
1:A:2419:ALA:O	1:A:2423:MET:HG3	2.01	0.61
1:A:2107:ARG:NH2	1:A:2139:GLN:OE1	2.34	0.61
1:A:2893:VAL:HG13	1:A:2911:LEU:HD11	1.83	0.61
1:A:2220:LEU:HB2	1:A:2342:MET:HG2	1.83	0.60
1:A:2888:GLU:N	1:A:2888:GLU:OE1	2.33	0.60
1:A:4297:PRO:HG3	1:A:4308:TRP:CG	2.35	0.60
1:A:3650:ASN:OD1	1:A:3695:ARG:NH1	2.33	0.60
1:A:4027:LEU:HB3	1:A:4058:LEU:HD22	1.84	0.60
1:A:4043:MET:HG2	1:A:4147:PHE:HE2	1.65	0.60
1:A:2776:PHE:HA	1:A:2779:MET:HE3	1.82	0.60
1:A:3743:ARG:NH1	1:A:3743:ARG:O	2.35	0.60
1:A:3789:ILE:O	1:A:3793:GLU:N	2.32	0.60
1:A:3028:THR:HG22	1:A:3032:GLN:HE21	1.66	0.59
1:A:2483:ILE:O	1:A:2487:GLU:HG3	2.03	0.59
1:A:3882:THR:HG22	1:A:4339:MET:HG3	1.85	0.59
1:A:2047:GLN:NE2	1:A:2067:ASN:OD1	2.36	0.58
1:A:2995:ASP:OD1	1:A:2996:GLU:N	2.37	0.58
1:A:4318:PRO:HG2	1:A:4325:ASN:HA	1.86	0.58
1:A:2826:ALA:HA	1:A:2850:ILE:HD11	1.84	0.58
1:A:3909:LEU:HD21	1:A:4343:MET:HE2	1.85	0.58
1:A:3031:THR:O	1:A:3035:GLU:HG2	2.04	0.58
1:A:4037:PRO:HB2	1:A:4118:PRO:HG2	1.86	0.58
1:A:2179:ARG:NH1	1:A:2195:ASP:OD1	2.35	0.58
1:A:2694:ARG:O	1:A:2698:GLN:HA	2.04	0.58
1:A:1812:ILE:HG21	1:A:2056:SER:HA	1.86	0.58
1:A:4400:ARG:NH1	1:A:4414:GLU:OE2	2.37	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4178:ARG:HD2	1:A:4296:MET:HE1	1.85	0.58
1:A:3749:LEU:HD11	1:A:3770:LEU:HD23	1.85	0.58
1:A:3835:ILE:HD13	1:A:3867:ALA:HA	1.86	0.58
1:A:2606:PHE:O	1:A:2610:ARG:HG2	2.04	0.57
1:A:4543:VAL:HG13	1:A:4588:THR:HG23	1.86	0.57
1:A:3553:LEU:O	1:A:3582:ARG:NH1	2.37	0.57
1:A:1931:ASN:C	1:A:1931:ASN:HD22	2.12	0.57
1:A:3843:ASN:HB3	1:A:3846:LEU:HD12	1.87	0.57
1:A:3913:GLU:OE2	1:A:3913:GLU:N	2.38	0.57
1:A:3947:LEU:HA	1:A:3950:LYS:HD2	1.85	0.57
1:A:3654:ARG:HG3	1:A:3661:LEU:HB3	1.87	0.57
1:A:1961:ASN:HD21	1:A:2019:ASN:HB3	1.70	0.57
1:A:2461:MET:HG2	1:A:2583:THR:HG21	1.87	0.57
1:A:3107:LYS:HG3	1:A:3144:VAL:HG21	1.85	0.57
1:A:3733:LYS:HD3	1:A:3737:GLU:HG3	1.86	0.57
1:A:3946:ASP:HB2	1:A:3950:LYS:HE2	1.87	0.57
1:A:1907:PRO:HG2	1:A:1910:THR:HG21	1.87	0.56
1:A:1724:VAL:O	1:A:1728:GLY:N	2.38	0.56
1:A:3175:HIS:HB3	1:A:3516:TYR:HE1	1.69	0.56
1:A:3499:GLN:HA	1:A:3502:THR:HG22	1.86	0.56
1:A:3729:SER:O	1:A:3733:LYS:HG2	2.05	0.56
1:A:3746:GLU:HG2	1:A:3773:LEU:HD13	1.87	0.56
1:A:3791:MET:HE3	1:A:3791:MET:O	2.04	0.56
1:A:2073:PHE:HE2	1:A:2093:LEU:HA	1.70	0.56
1:A:1763:GLU:OE1	1:A:1845:TYR:OH	2.22	0.56
1:A:2623:SER:O	1:A:2626:THR:OG1	2.23	0.56
1:A:2816:LEU:HD23	1:A:2817:PRO:O	2.06	0.56
1:A:3654:ARG:HH11	1:A:3661:LEU:HG	1.71	0.56
1:A:3886:LEU:HD11	1:A:4346:MET:HG3	1.88	0.56
1:A:3488:ARG:O	1:A:3491:LYS:HG3	2.05	0.55
1:A:2612:LEU:HB3	1:A:2615:MET:CE	2.36	0.55
1:A:2936:ILE:HD11	1:A:3091:LEU:HD12	1.87	0.55
1:A:4460:LEU:HD21	1:A:4478:TRP:CD1	2.41	0.55
1:A:1888:CYS:HB2	1:A:2041:MET:HE1	1.88	0.55
1:A:3071:SER:O	1:A:3075:LEU:N	2.38	0.55
1:A:1860:GLN:HG2	1:A:1865:LYS:HG2	1.88	0.55
1:A:2797:ARG:NH1	1:A:3087:ASN:OD1	2.37	0.55
1:A:3661:LEU:HD12	1:A:3662:ILE:H	1.72	0.55
1:A:2840:ASP:OD1	1:A:2843:ARG:NH2	2.39	0.55
1:A:1687:LYS:HG2	1:A:1712:THR:HG22	1.89	0.55
1:A:1939:GLN:H	1:A:1939:GLN:CD	2.15	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2085:HIS:HB2	1:A:2361:MET:HG2	1.88	0.55
1:A:3189:GLU:OE2	1:A:3582:ARG:NH2	2.39	0.55
1:A:3898:GLU:OE1	1:A:3983:ILE:HD13	2.06	0.55
1:A:2569:VAL:HG11	1:A:2747:ILE:HA	1.88	0.55
1:A:3601:MET:HE1	1:A:3611:ARG:HB2	1.88	0.55
1:A:3951:VAL:HG22	1:A:3957:PHE:HE2	1.69	0.55
1:A:2321:ASP:OD2	1:A:2321:ASP:N	2.34	0.55
1:A:2065:LEU:HD13	1:A:2137:LEU:HD22	1.88	0.54
1:A:1979:GLN:O	1:A:1983:ARG:HG3	2.07	0.54
1:A:2784:PHE:HB2	1:A:2794:TYR:HE2	1.72	0.54
1:A:3113:MET:HG3	1:A:3115:LEU:HD11	1.88	0.54
1:A:1631:PHE:HE2	1:A:1656:LYS:HB3	1.73	0.54
1:A:2068:LYS:NZ	1:A:4535:SER:OG	2.40	0.54
1:A:2665:GLU:HB3	1:A:2668:LEU:HB2	1.90	0.54
1:A:3030:MET:HG3	1:A:3047:HIS:CD2	2.43	0.54
1:A:4512:GLY:HA3	1:A:4645:THR:HG23	1.89	0.54
1:A:1647:VAL:HG11	1:A:1692:ILE:HD13	1.89	0.54
1:A:2110:LYS:HA	1:A:2113:ARG:NH1	2.23	0.54
1:A:2445:HIS:CD2	1:A:2449:LEU:HD22	2.43	0.54
1:A:2737:ASP:OD2	1:A:2738:TYR:N	2.40	0.54
1:A:4186:PHE:HE1	1:A:4268:PHE:HB3	1.73	0.54
1:A:1814:GLU:OE1	1:A:1818:GLN:NE2	2.39	0.54
1:A:3017:VAL:HB	1:A:3020:LEU:HD23	1.90	0.54
1:A:4021:MET:HE3	1:A:4021:MET:HA	1.90	0.54
1:A:4209:GLU:OE1	1:A:4213:ARG:NH2	2.40	0.54
1:A:1816:VAL:HG11	1:A:2052:VAL:HG22	1.90	0.53
1:A:1900:LEU:HD21	1:A:2037:ARG:HH21	1.73	0.53
1:A:2901:TYR:OH	1:A:2909:LEU:N	2.36	0.53
1:A:3614:PHE:HZ	1:A:3645:LEU:HD11	1.72	0.53
1:A:2759:ILE:HD12	1:A:2762:LEU:HD23	1.88	0.53
1:A:3929:VAL:O	1:A:3933:GLU:HG3	2.08	0.53
1:A:4475:VAL:O	1:A:4479:VAL:HG23	2.08	0.53
1:A:1713:LEU:HD22	1:A:1749:LEU:HD21	1.91	0.53
1:A:1788:THR:O	1:A:1791:VAL:HG12	2.08	0.53
1:A:3655:ARG:NE	1:A:3660:VAL:HG22	2.22	0.53
1:A:3759:ARG:HG3	1:A:3760:ILE:HG12	1.89	0.53
1:A:2757:ARG:HA	1:A:2763:ARG:HH21	1.74	0.53
1:A:3021:PHE:CD1	1:A:3025:GLU:HG3	2.42	0.53
1:A:4160:THR:HG23	1:A:4212:LEU:HD21	1.91	0.53
1:A:4260:PHE:HE2	1:A:4618:LEU:HD11	1.73	0.53
1:A:1685:MET:HE2	1:A:1685:MET:HA	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3721:ARG:HB3	1:A:3724:VAL:HB	1.90	0.53
1:A:4192:GLU:OE1	1:A:4195:ARG:NH1	2.41	0.53
1:A:1769:MET:HE1	1:A:1777:PRO:HD2	1.91	0.53
1:A:1945:PHE:HE1	1:A:1975:VAL:HG12	1.74	0.53
1:A:3722:PRO:HA	1:A:3725:ASP:HB3	1.91	0.53
1:A:3506:ASP:OD2	1:A:3544:ARG:HD2	2.09	0.53
1:A:1972:SER:HB2	1:A:2031:ASN:HD21	1.74	0.52
1:A:2066:ALA:HA	1:A:2069:ILE:HG22	1.91	0.52
1:A:1971:VAL:O	1:A:1975:VAL:HG13	2.10	0.52
1:A:2622:PHE:HZ	1:A:2631:LEU:HD21	1.75	0.52
1:A:1967:MET:HA	1:A:1967:MET:HE2	1.92	0.52
1:A:2469:VAL:HG22	1:A:2481:MET:HE1	1.91	0.52
1:A:2569:VAL:HB	1:A:2747:ILE:HG13	1.91	0.52
1:A:1628:ARG:HA	1:A:1951:VAL:HG22	1.91	0.52
1:A:3044:LEU:HB3	1:A:3049:GLU:HG3	1.92	0.52
1:A:3588:LEU:HD23	1:A:3698:PHE:HE1	1.74	0.52
1:A:2441:PHE:HA	1:A:2449:LEU:HD23	1.91	0.52
1:A:2811:ARG:HB3	1:A:2812:PRO:HD2	1.91	0.52
1:A:3971:PRO:HG2	1:A:3973:LEU:HD11	1.91	0.52
1:A:2449:LEU:HA	1:A:2453:ARG:HH21	1.75	0.52
1:A:3495:THR:O	1:A:3498:ASN:HB3	2.10	0.51
1:A:4526:GLN:HA	1:A:4536:LEU:HD21	1.91	0.51
1:A:4444:GLN:O	1:A:4449:ARG:NH1	2.43	0.51
1:A:4567:GLY:HA3	1:A:4640:VAL:HG22	1.92	0.51
1:A:4311:LEU:O	1:A:4311:LEU:HD23	2.11	0.51
1:A:4554:ASP:N	1:A:4557:SER:OG	2.43	0.51
1:A:1784:ASN:O	1:A:1787:VAL:HG12	2.11	0.51
1:A:3839:VAL:HG21	1:A:3863:LEU:HA	1.92	0.51
1:A:3944:PHE:CE1	1:A:3974:TRP:HB3	2.45	0.51
1:A:2992:PHE:HB3	1:A:3064:VAL:HA	1.92	0.51
1:A:1630:TYR:HD1	1:A:1947:GLY:HA2	1.75	0.51
1:A:1686:PHE:HA	1:A:1712:THR:HG21	1.93	0.51
1:A:2481:MET:HG3	1:A:2485:GLN:NE2	2.26	0.51
1:A:3734:LEU:HD22	1:A:3783:LYS:HB3	1.91	0.51
1:A:3796:THR:HA	1:A:3799:GLN:HG3	1.93	0.51
1:A:2300:TRP:CD2	1:A:2342:MET:HE1	2.45	0.51
1:A:4068:SER:HA	1:A:4095:MET:HB3	1.93	0.51
1:A:2568:VAL:HG23	1:A:2603:MET:HE1	1.93	0.51
1:A:3151:HIS:ND1	1:A:3516:TYR:OH	2.41	0.51
1:A:3114:ASP:OD2	1:A:3114:ASP:N	2.44	0.50
1:A:2297:LYS:HB2	1:A:2299:GLN:HE22	1.77	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4205:TYR:OH	1:A:4261:ASP:OD2	2.25	0.50
1:A:3791:MET:O	1:A:3795:GLU:HG2	2.12	0.50
1:A:3721:ARG:O	1:A:3725:ASP:N	2.34	0.50
1:A:1653:HIS:HA	1:A:1656:LYS:HD2	1.93	0.50
1:A:3030:MET:HA	1:A:3030:MET:HE3	1.93	0.50
1:A:3783:LYS:O	1:A:3787:THR:HG23	2.11	0.50
1:A:2612:LEU:HB3	1:A:2615:MET:HE3	1.93	0.50
1:A:3690:PRO:HA	1:A:3693:CYS:SG	2.51	0.50
1:A:2094:LYS:HD2	2:A:4701:ADP:H1'	1.93	0.50
1:A:2771:ALA:O	1:A:2775:GLU:N	2.38	0.50
1:A:4387:TRP:HZ3	1:A:4455:LEU:HD21	1.75	0.50
1:A:4326:ASN:ND2	1:A:4579:ASN:O	2.44	0.50
1:A:4387:TRP:HZ2	1:A:4476:ILE:HG13	1.77	0.50
1:A:1844:PHE:HZ	1:A:1922:GLN:HE21	1.60	0.49
1:A:2461:MET:CE	1:A:2497:ALA:HA	2.42	0.49
1:A:3101:ALA:O	1:A:3105:VAL:HG23	2.12	0.49
1:A:4171:LYS:HG3	1:A:4172:SER:H	1.76	0.49
1:A:2872:LEU:HD12	1:A:2920:LEU:HD12	1.93	0.49
1:A:3043:MET:HE3	1:A:3043:MET:HA	1.94	0.49
1:A:3488:ARG:HH21	1:A:3489:TRP:CG	2.30	0.49
1:A:3609:ILE:HD11	1:A:3634:LEU:HB2	1.94	0.49
1:A:1722:THR:O	1:A:1726:ILE:HG12	2.13	0.49
1:A:2694:ARG:O	1:A:2698:GLN:CA	2.60	0.49
1:A:4277:SER:HA	1:A:4282:PHE:CG	2.47	0.49
1:A:4566:GLN:O	1:A:4640:VAL:HA	2.12	0.49
1:A:2446:ILE:HG22	1:A:2505:ASP:O	2.11	0.49
1:A:4100:HIS:HB2	1:A:4131:ASN:HD21	1.76	0.49
1:A:3161:LEU:HB3	1:A:3168:THR:HG22	1.95	0.49
1:A:3661:LEU:HD12	1:A:3662:ILE:N	2.27	0.49
1:A:4336:GLY:O	1:A:4340:ILE:HG12	2.12	0.49
1:A:2562:VAL:O	1:A:2804:ARG:NH1	2.46	0.49
1:A:3974:TRP:NE1	1:A:3976:GLU:OE2	2.46	0.49
1:A:3916:LEU:HD21	1:A:3937:ARG:HG2	1.95	0.49
1:A:1853:VAL:HA	1:A:1856:GLN:HG3	1.94	0.49
1:A:2228:SER:HB3	1:A:2364:PHE:HB3	1.94	0.49
1:A:3785:GLU:O	1:A:3789:ILE:HG13	2.12	0.49
1:A:4609:VAL:HG22	1:A:4642:VAL:HB	1.95	0.49
1:A:2682:PHE:O	1:A:2686:MET:HE2	2.13	0.49
1:A:4381:HIS:NE2	1:A:4439:GLU:OE2	2.45	0.48
1:A:4610:TYR:HB2	1:A:4643:LEU:HD22	1.95	0.48
1:A:2123:ASP:O	1:A:2127:ILE:HG13	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3021:PHE:CE1	1:A:3025:GLU:HG3	2.48	0.48
1:A:2191:LEU:HD11	1:A:2232:MET:HE2	1.94	0.48
1:A:2437:LEU:HD21	1:A:2451:ARG:HG3	1.95	0.48
1:A:2518:ILE:HA	1:A:2521:ILE:HG12	1.94	0.48
1:A:2961:ILE:HD11	1:A:2994:MET:HE1	1.96	0.48
1:A:4179:LEU:HD12	1:A:4223:LEU:HD11	1.94	0.48
1:A:4306:VAL:O	1:A:4310:GLU:HG2	2.13	0.48
1:A:2448:ASP:O	1:A:2453:ARG:NH2	2.47	0.48
1:A:2865:LYS:O	1:A:2865:LYS:NZ	2.40	0.48
1:A:2601:LYS:HG2	1:A:2736:VAL:HB	1.94	0.48
1:A:2694:ARG:O	1:A:2698:GLN:N	2.47	0.48
1:A:3040:GLU:OE1	1:A:3053:TRP:NE1	2.46	0.48
1:A:3206:ARG:O	1:A:3210:GLU:HG2	2.13	0.48
1:A:2511:ARG:HB3	1:A:2535:ILE:CD1	2.43	0.48
1:A:2519:ARG:HG2	1:A:2526:LEU:HD13	1.96	0.48
1:A:2977:ARG:HG3	1:A:3020:LEU:HB3	1.95	0.48
1:A:3154:LEU:HD21	1:A:3532:TRP:HZ2	1.77	0.48
1:A:4528:VAL:HG11	1:A:4592:TRP:HB2	1.95	0.48
1:A:2511:ARG:HB3	1:A:2535:ILE:HD13	1.96	0.48
1:A:3951:VAL:HG22	1:A:3957:PHE:CE2	2.48	0.48
1:A:1632:VAL:HB	1:A:1636:ASP:HB2	1.96	0.48
1:A:4013:LEU:HD23	1:A:4017:PHE:CZ	2.48	0.48
1:A:2050:ALA:O	1:A:2051:GLN:C	2.57	0.47
1:A:2312:VAL:HG21	1:A:2355:THR:HG21	1.95	0.47
1:A:3115:LEU:HD22	1:A:3143:ILE:HG13	1.96	0.47
1:A:1739:ILE:HG23	1:A:1804:ARG:HD3	1.96	0.47
1:A:3771:GLU:O	1:A:3775:ARG:HG2	2.13	0.47
1:A:3499:GLN:HA	1:A:3502:THR:CG2	2.45	0.47
1:A:4013:LEU:HD23	1:A:4017:PHE:CE2	2.49	0.47
1:A:4168:ARG:NH1	1:A:4220:ASP:OD2	2.43	0.47
1:A:4387:TRP:CZ3	1:A:4455:LEU:HD21	2.50	0.47
1:A:1631:PHE:HA	1:A:1947:GLY:HA3	1.96	0.47
1:A:1976:GLN:HG2	1:A:1980:GLU:OE2	2.15	0.47
1:A:2465:ALA:HB2	1:A:2493:TYR:CD1	2.49	0.47
1:A:2956:LEU:HG	1:A:2989:LYS:HB2	1.96	0.47
1:A:2989:LYS:NZ	1:A:3061:ASN:OD1	2.47	0.47
1:A:4288:VAL:O	1:A:4319:SER:OG	2.23	0.47
1:A:2337:PRO:O	1:A:2340:ARG:NH1	2.48	0.47
1:A:2797:ARG:NH2	2:A:4703:ADP:O3A	2.48	0.47
1:A:2963:VAL:HG21	1:A:2998:ASN:HB3	1.95	0.47
1:A:4031:VAL:HG21	1:A:4058:LEU:HD21	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4176:ARG:NH2	1:A:4224:ASP:OD1	2.44	0.47
1:A:4381:HIS:HD2	1:A:4438:CYS:HB3	1.78	0.47
1:A:2087:ASP:HB2	1:A:2356:VAL:HG12	1.97	0.47
1:A:2615:MET:H	1:A:2615:MET:HE2	1.80	0.47
1:A:2623:SER:HA	1:A:2668:LEU:HD23	1.95	0.47
1:A:3158:ASN:ND2	1:A:3169:MET:O	2.36	0.47
1:A:2227:GLY:HA2	1:A:2452:LEU:HD12	1.97	0.47
1:A:2819:GLU:HA	1:A:2861:ILE:HD11	1.95	0.47
1:A:3629:PHE:CD1	1:A:3629:PHE:N	2.82	0.47
1:A:4178:ARG:NH1	1:A:4296:MET:HE1	2.30	0.47
1:A:2048:LEU:O	1:A:2049:ILE:C	2.58	0.47
1:A:2644:THR:OG1	1:A:2647:GLY:O	2.24	0.47
1:A:2890:ARG:NH1	1:A:2911:LEU:O	2.48	0.47
1:A:3197:GLN:OE1	1:A:3496:PHE:HE1	1.97	0.47
1:A:3793:GLU:O	1:A:3797:VAL:HG23	2.15	0.47
1:A:2527:PRO:HD2	1:A:2534:ILE:HG22	1.97	0.46
1:A:3638:VAL:HG11	1:A:3679:LEU:HB3	1.97	0.46
1:A:2029:PRO:HG2	1:A:2032:LEU:HD12	1.96	0.46
1:A:4346:MET:HE3	1:A:4346:MET:HA	1.96	0.46
1:A:1724:VAL:HA	1:A:1727:PHE:HD1	1.80	0.46
1:A:2498:ILE:HG23	1:A:2502:LEU:HD22	1.97	0.46
1:A:4257:ASP:OD2	1:A:4258:ASN:N	2.49	0.46
1:A:2231:SER:OG	1:A:2344:GLU:OE2	2.31	0.46
1:A:4565:LEU:HD13	1:A:4642:VAL:HG22	1.97	0.46
1:A:2354:ALA:HB1	1:A:2358:ARG:HE	1.80	0.46
1:A:2939:SER:O	1:A:3172:THR:HB	2.15	0.46
1:A:3158:ASN:HD22	1:A:3171:ILE:HG13	1.80	0.46
1:A:4020:ILE:HA	1:A:4023:GLN:NE2	2.31	0.46
1:A:4166:VAL:HG12	1:A:4302:ARG:HH12	1.79	0.46
1:A:2564:ALA:HB3	1:A:2567:VAL:HG22	1.96	0.46
1:A:2278:GLY:O	1:A:2282:HIS:N	2.40	0.46
1:A:2743:SER:O	1:A:2747:ILE:HG22	2.15	0.46
1:A:3002:SER:O	1:A:3006:GLU:HG2	2.16	0.46
1:A:3836:TYR:HE1	1:A:3840:LEU:HD11	1.81	0.46
1:A:3851:ASP:HB3	1:A:3854:GLN:HG2	1.98	0.46
1:A:4128:MET:SD	1:A:4134:VAL:HG21	2.56	0.46
1:A:3113:MET:HG3	1:A:3115:LEU:CD1	2.46	0.46
1:A:4099:VAL:HB	1:A:4106:LEU:HD21	1.97	0.46
1:A:4446:ASN:OD1	1:A:4447:TYR:N	2.46	0.46
1:A:3099:THR:HG23	1:A:3148:VAL:HG11	1.97	0.46
1:A:2431:GLY:O	1:A:2435:LYS:HE2	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3492:THR:O	1:A:3496:PHE:HB2	2.16	0.46
1:A:3641:TYR:HD2	1:A:3692:LEU:HD21	1.81	0.45
1:A:1888:CYS:O	1:A:1892:MET:HG2	2.16	0.45
1:A:1909:GLY:HA2	2:A:4701:ADP:H5'2	1.99	0.45
1:A:2461:MET:CG	1:A:2583:THR:HG21	2.46	0.45
1:A:4510:CYS:HG	1:A:4561:THR:HG1	1.59	0.45
1:A:2739:PRO:HD2	1:A:2796:PRO:HG2	1.99	0.45
1:A:3126:MET:HE2	1:A:3126:MET:HA	1.99	0.45
1:A:3485:GLU:O	1:A:3489:TRP:HD1	1.99	0.45
1:A:1911:GLY:O	1:A:1912:LYS:C	2.60	0.45
1:A:3641:TYR:CD2	1:A:3692:LEU:HD21	2.52	0.45
1:A:4473:MET:HG3	1:A:4477:GLN:HB2	1.99	0.45
1:A:4535:SER:O	1:A:4538:GLU:HG2	2.17	0.45
1:A:4547:THR:HA	1:A:4586:PRO:HB2	1.98	0.45
1:A:2049:ILE:HD13	1:A:2090:LEU:HD21	1.98	0.45
1:A:2512:ALA:O	1:A:2516:GLU:HG2	2.16	0.45
1:A:2964:HIS:HA	1:A:3643:PRO:HD2	1.97	0.45
1:A:3817:SER:HB2	1:A:4346:MET:HE1	1.98	0.45
1:A:1985:HIS:NE2	1:A:2010:PRO:HB3	2.32	0.45
1:A:2206:LYS:HD3	1:A:2206:LYS:HA	1.82	0.45
1:A:2596:PRO:O	1:A:2601:LYS:NZ	2.45	0.45
1:A:3579:MET:HE3	1:A:3579:MET:HB2	1.84	0.45
1:A:4289:ASP:N	1:A:4289:ASP:OD1	2.50	0.45
1:A:2107:ARG:HH12	1:A:2135:GLU:CD	2.24	0.45
1:A:2307:VAL:HG23	1:A:2311:TRP:CZ2	2.52	0.45
1:A:2802:TRP:CZ2	1:A:2829:ALA:HB2	2.51	0.45
1:A:3960:TRP:CZ3	1:A:3996:PHE:HD2	2.35	0.45
1:A:2107:ARG:NH1	1:A:2135:GLU:OE1	2.48	0.45
1:A:2926:PHE:HA	1:A:3063:HIS:CD2	2.52	0.45
1:A:1779:HIS:CE1	1:A:1826:ILE:HD12	2.52	0.44
1:A:1946:VAL:HG12	1:A:2001:LEU:HD13	1.98	0.44
1:A:2079:GLN:O	1:A:4415:ARG:NH2	2.50	0.44
1:A:2257:LYS:HA	1:A:2257:LYS:HD2	1.74	0.44
1:A:3191:ARG:NE	1:A:3195:GLU:OE1	2.50	0.44
1:A:3218:LEU:HD21	1:A:3760:ILE:O	2.17	0.44
1:A:3721:ARG:HH21	1:A:3724:VAL:HG11	1.82	0.44
1:A:3787:THR:O	1:A:3790:VAL:HB	2.16	0.44
1:A:3983:ILE:HG12	1:A:4012:ASN:OD1	2.18	0.44
1:A:4186:PHE:HE2	1:A:4252:TYR:CD1	2.36	0.44
1:A:2648:VAL:HG13	1:A:2701:VAL:HG22	1.99	0.44
1:A:3113:MET:HE2	1:A:3113:MET:HB3	1.80	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3873:ARG:HD3	1:A:4021:MET:HE1	1.98	0.44
1:A:2495:VAL:HG11	1:A:2526:LEU:HD21	1.99	0.44
1:A:2762:LEU:HD11	1:A:2821:LEU:HD22	1.99	0.44
1:A:2790:PRO:HB3	1:A:3076:LYS:HG3	1.99	0.44
1:A:3488:ARG:HE	1:A:3489:TRP:CD1	2.36	0.44
1:A:3789:ILE:HG22	1:A:3793:GLU:HG2	1.98	0.44
1:A:2571:THR:H	1:A:2574:THR:HB	1.82	0.44
1:A:4211:ASP:HB3	1:A:4252:TYR:CE2	2.53	0.44
1:A:2220:LEU:O	1:A:2342:MET:HA	2.17	0.44
1:A:2231:SER:HA	1:A:2234:TRP:CD1	2.53	0.44
1:A:2913:ASN:OD1	1:A:2913:ASN:N	2.50	0.44
1:A:3194:LEU:O	1:A:3198:GLN:HG2	2.17	0.44
1:A:1658:PHE:CG	1:A:1661:VAL:HB	2.53	0.44
1:A:2973:ASP:O	1:A:2977:ARG:HD3	2.17	0.44
1:A:2979:VAL:HG21	1:A:2992:PHE:CE2	2.53	0.44
1:A:2594:CYS:O	1:A:2735:TYR:HA	2.18	0.44
1:A:2943:LYS:HE2	1:A:2943:LYS:HB2	1.84	0.44
1:A:2964:HIS:H	1:A:2967:TYR:HB2	1.83	0.44
1:A:3808:CYS:HG	1:A:3836:TYR:HE2	1.62	0.44
1:A:2181:GLU:OE1	1:A:2243:ARG:NH1	2.51	0.44
1:A:2503:SER:HB3	1:A:2514:LEU:HD22	1.99	0.44
1:A:2694:ARG:NE	1:A:2697:ASP:OD1	2.50	0.44
1:A:2943:LYS:HG3	1:A:3094:PHE:CD2	2.53	0.44
1:A:3030:MET:HA	1:A:3033:CYS:SG	2.57	0.44
1:A:3117:LYS:HE3	1:A:3119:ASN:ND2	2.32	0.44
1:A:4178:ARG:HH11	1:A:4296:MET:HE1	1.83	0.44
1:A:2325:LEU:O	1:A:2332:ARG:HA	2.17	0.43
1:A:2762:LEU:HD21	1:A:2821:LEU:HB2	1.99	0.43
1:A:3056:SER:O	1:A:3059:ILE:HG22	2.18	0.43
1:A:3638:VAL:HG22	1:A:3681:THR:HG22	2.00	0.43
1:A:3780:VAL:O	1:A:3784:VAL:HG23	2.18	0.43
1:A:1623:ARG:HB3	1:A:1630:TYR:HD2	1.83	0.43
1:A:1912:LYS:HB2	1:A:1912:LYS:HE2	1.80	0.43
1:A:2497:ALA:O	1:A:2501:SER:HB2	2.17	0.43
1:A:3529:PHE:CE2	1:A:3549:ARG:HD3	2.53	0.43
1:A:2748:TYR:HH	1:A:2800:THR:HG1	1.65	0.43
1:A:2831:ARG:HB3	1:A:2924:ARG:NH2	2.33	0.43
1:A:2937:GLY:C	1:A:3070:PRO:HD3	2.43	0.43
1:A:3704:THR:H	1:A:3707:SER:HB3	1.83	0.43
1:A:3966:PRO:HD2	1:A:4000:ARG:HG3	2.00	0.43
1:A:4031:VAL:O	1:A:4123:ARG:NH2	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1945:PHE:CE1	1:A:1975:VAL:HG12	2.54	0.43
1:A:2445:HIS:ND1	1:A:2505:ASP:OD1	2.45	0.43
1:A:2449:LEU:HD11	1:A:2454:CYS:SG	2.58	0.43
1:A:2762:LEU:HD12	1:A:2765:TYR:HB2	2.00	0.43
1:A:3606:ASP:N	1:A:3606:ASP:OD1	2.50	0.43
1:A:3681:THR:HG21	1:A:3688:PHE:HZ	1.83	0.43
1:A:4260:PHE:CE2	1:A:4608:PRO:HB3	2.53	0.43
1:A:1751:VAL:O	1:A:1755:GLN:HG3	2.19	0.43
1:A:1850:GLN:HB3	1:A:1856:GLN:HG2	1.99	0.43
1:A:3103:TYR:CE2	1:A:3107:LYS:HD2	2.53	0.43
1:A:3743:ARG:HA	1:A:3743:ARG:HD2	1.90	0.43
1:A:1925:ARG:HH22	1:A:2011:ASP:CG	2.27	0.43
1:A:2896:ARG:HD2	1:A:2896:ARG:HA	1.75	0.43
1:A:3767:ILE:HA	1:A:3770:LEU:HD12	1.99	0.43
1:A:3846:LEU:HD21	1:A:3859:ILE:HG13	2.00	0.43
1:A:1779:HIS:ND1	1:A:1826:ILE:HD12	2.34	0.43
1:A:2596:PRO:HB2	1:A:2738:TYR:CE1	2.54	0.43
1:A:2873:TYR:CE2	1:A:2883:PRO:HD3	2.54	0.43
1:A:3558:GLU:OE1	1:A:3581:LYS:NZ	2.52	0.43
1:A:4288:VAL:HG23	1:A:4289:ASP:OD1	2.19	0.43
1:A:2202:MET:HE2	1:A:2202:MET:HB3	1.73	0.43
1:A:2873:TYR:CZ	1:A:2883:PRO:HD3	2.53	0.43
1:A:4106:LEU:HD23	1:A:4106:LEU:HA	1.81	0.43
1:A:1926:PHE:O	1:A:1953:ALA:HB1	2.19	0.43
1:A:1944:ILE:HD12	1:A:1944:ILE:HA	1.93	0.43
1:A:2092:ALA:O	1:A:2093:LEU:C	2.61	0.43
1:A:2492:ARG:HG2	1:A:2545:TRP:NE1	2.34	0.43
1:A:2602:THR:HG23	1:A:2662:PHE:HE2	1.83	0.43
1:A:2652:PRO:HD2	1:A:2705:ARG:CZ	2.49	0.43
1:A:3601:MET:HE3	1:A:3611:ARG:HE	1.84	0.43
1:A:3655:ARG:HH21	1:A:3660:VAL:HG13	1.84	0.43
1:A:3692:LEU:O	1:A:3696:VAL:HG22	2.18	0.43
1:A:4283:LYS:NZ	1:A:4293:ASP:OD2	2.36	0.43
1:A:1950:GLN:NE2	1:A:2007:LYS:H	2.17	0.43
1:A:2265:TYR:O	1:A:2281:THR:OG1	2.29	0.43
1:A:2615:MET:SD	1:A:2615:MET:N	2.92	0.43
1:A:4227:ALA:HB2	1:A:4233:ILE:HD12	2.00	0.43
1:A:3591:ASP:OD1	1:A:3591:ASP:N	2.49	0.42
1:A:4628:THR:O	1:A:4629:LYS:HG2	2.19	0.42
1:A:1843:ARG:NH2	1:A:1860:GLN:HB3	2.34	0.42
1:A:1929:VAL:HG22	1:A:1956:CYS:HB3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1985:HIS:CD2	1:A:2010:PRO:HB3	2.54	0.42
1:A:2315:LEU:HD23	1:A:2315:LEU:HA	1.87	0.42
1:A:1664:ILE:HD12	1:A:1666:LEU:HD11	2.01	0.42
1:A:2209:GLN:O	1:A:2213:ILE:HG12	2.20	0.42
1:A:2299:GLN:N	1:A:2299:GLN:OE1	2.53	0.42
1:A:2483:ILE:HD12	1:A:2483:ILE:HA	1.85	0.42
1:A:4179:LEU:HD23	1:A:4179:LEU:HA	1.86	0.42
1:A:4234:SER:HB3	1:A:4237:LYS:HG2	2.01	0.42
1:A:4288:VAL:HG22	1:A:4293:ASP:HA	2.02	0.42
1:A:2286:LYS:NZ	1:A:2291:VAL:HB	2.35	0.42
1:A:3719:ALA:HB3	1:A:3840:LEU:HD13	2.01	0.42
1:A:1882:THR:O	1:A:1883:PRO:C	2.62	0.42
1:A:2799:MET:HE3	1:A:2799:MET:HB3	1.79	0.42
1:A:4467:TYR:HB3	1:A:4515:PHE:HD2	1.85	0.42
1:A:1628:ARG:HG3	1:A:1706:GLU:OE1	2.19	0.42
1:A:2779:MET:HA	1:A:2782:GLU:HB3	2.00	0.42
1:A:2779:MET:O	1:A:2783:ARG:N	2.53	0.42
1:A:3787:THR:HA	1:A:3790:VAL:HB	2.00	0.42
1:A:1789:LEU:HD13	1:A:1815:LEU:HB3	2.02	0.42
1:A:2783:ARG:HH21	1:A:2845:TRP:CD1	2.37	0.42
1:A:4435:VAL:O	1:A:4439:GLU:HG2	2.20	0.42
1:A:2744:LEU:HA	1:A:2747:ILE:HG22	2.02	0.42
1:A:4380:LEU:HA	1:A:4383:THR:HG22	2.00	0.42
1:A:1635:GLU:HG2	1:A:1636:ASP:H	1.85	0.42
1:A:1769:MET:CE	1:A:1777:PRO:HD2	2.50	0.42
1:A:2012:MET:SD	1:A:2013:ALA:N	2.93	0.42
1:A:2590:PRO:O	1:A:2732:PRO:HD2	2.19	0.42
1:A:3879:ASP:O	1:A:3882:THR:OG1	2.30	0.42
1:A:2239:LYS:HD2	1:A:2239:LYS:HA	1.76	0.42
1:A:2995:ASP:OD1	1:A:2995:ASP:C	2.62	0.42
1:A:3488:ARG:HD2	1:A:3746:GLU:OE1	2.20	0.42
1:A:2277:ASP:OD1	1:A:2277:ASP:N	2.53	0.41
1:A:3169:MET:SD	1:A:3693:CYS:HB3	2.59	0.41
1:A:3612:THR:O	1:A:3635:VAL:HA	2.20	0.41
1:A:3935:VAL:HG13	1:A:3947:LEU:HD23	2.01	0.41
1:A:3178:ASP:OD2	1:A:3585:ARG:NE	2.44	0.41
1:A:3495:THR:HG23	1:A:3496:PHE:HD2	1.86	0.41
1:A:3747:LYS:O	1:A:3751:GLN:HG2	2.20	0.41
1:A:4173:PRO:HG2	1:A:4176:ARG:HB2	2.02	0.41
1:A:1659:ALA:O	1:A:1679:ARG:NH2	2.51	0.41
1:A:1724:VAL:HA	1:A:1727:PHE:CD1	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2620:LEU:HD11	1:A:2634:THR:HG21	2.02	0.41
1:A:2979:VAL:HG21	1:A:2992:PHE:HE2	1.85	0.41
1:A:3924:ILE:HG23	1:A:3952:GLN:NE2	2.35	0.41
1:A:2704:GLU:HG3	1:A:2705:ARG:HG3	2.03	0.41
1:A:3004:PHE:N	1:A:3004:PHE:CD1	2.88	0.41
1:A:3110:THR:O	1:A:3140:ARG:NH1	2.53	0.41
1:A:3154:LEU:HD12	1:A:3171:ILE:HD13	2.02	0.41
1:A:2527:PRO:HG3	1:A:2545:TRP:CG	2.55	0.41
1:A:3181:ASN:ND2	1:A:3584:ASN:OD1	2.53	0.41
1:A:2603:MET:HE3	2:A:4703:ADP:C4	2.54	0.41
1:A:2911:LEU:HA	1:A:2911:LEU:HD23	1.76	0.41
1:A:3801:TYR:CD1	1:A:3856:LEU:HD13	2.54	0.41
1:A:3811:ILE:HD11	1:A:3864:PHE:CE1	2.55	0.41
1:A:4611:LEU:HB2	1:A:4619:ILE:HD11	2.01	0.41
1:A:1789:LEU:HD12	1:A:1789:LEU:HA	1.89	0.41
1:A:1887:ARG:NH2	1:A:4253:GLY:O	2.53	0.41
1:A:3115:LEU:HD22	1:A:3143:ILE:HG21	2.01	0.41
1:A:4412:PHE:CZ	1:A:4520:TYR:HB2	2.55	0.41
1:A:2600:GLY:H	2:A:4703:ADP:H5'2	1.86	0.41
1:A:2612:LEU:HB3	1:A:2615:MET:HE2	2.03	0.41
1:A:2747:ILE:HD12	2:A:4703:ADP:C6	2.56	0.41
1:A:3592:PRO:HG3	1:A:3702:THR:HG22	2.02	0.41
1:A:1623:ARG:HE	1:A:1637:LEU:HD22	1.86	0.41
1:A:1780:SER:O	1:A:1784:ASN:N	2.43	0.41
1:A:2300:TRP:CE3	1:A:2342:MET:HE1	2.56	0.41
1:A:2311:TRP:CD1	1:A:2311:TRP:H	2.37	0.41
1:A:2449:LEU:HA	1:A:2449:LEU:HD12	1.77	0.41
1:A:2570:PRO:O	1:A:2746:GLN:NE2	2.54	0.41
1:A:2755:MET:HE2	1:A:2755:MET:HB3	1.77	0.41
1:A:2992:PHE:HE1	1:A:2994:MET:SD	2.43	0.41
1:A:3607:ARG:O	1:A:3608:LYS:HG2	2.20	0.41
1:A:3766:ILE:HD12	1:A:3766:ILE:HA	1.92	0.41
1:A:3801:TYR:HD1	1:A:3856:LEU:HD13	1.85	0.41
1:A:3841:TYR:O	1:A:3842:GLU:HG2	2.21	0.41
1:A:4297:PRO:HG3	1:A:4308:TRP:CD2	2.56	0.41
1:A:4577:LEU:HD23	1:A:4577:LEU:HA	1.79	0.41
1:A:2747:ILE:HD11	2:A:4703:ADP:C2	2.56	0.41
1:A:2749:GLY:N	1:A:2770:THR:HG21	2.36	0.41
1:A:3509:LEU:HD23	1:A:3509:LEU:HA	1.88	0.41
1:A:3614:PHE:HE2	1:A:3641:TYR:HD1	1.69	0.41
1:A:4374:PRO:HG2	1:A:4377:MET:HB2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2286:LYS:HE2	1:A:2292:ARG:NH1	2.35	0.40
1:A:2855:LEU:HD13	1:A:2855:LEU:HA	1.87	0.40
1:A:3788:ASP:O	1:A:3791:MET:HB3	2.21	0.40
1:A:3808:CYS:SG	1:A:3836:TYR:HE2	2.43	0.40
1:A:2668:LEU:O	1:A:2721:LYS:NZ	2.48	0.40
1:A:2822:ILE:HD11	1:A:2858:PHE:CD2	2.56	0.40
1:A:3194:LEU:HD23	1:A:3500:MET:HE2	2.03	0.40
1:A:3544:ARG:O	1:A:3544:ARG:HG2	2.21	0.40
1:A:3983:ILE:O	1:A:3987:ILE:HG22	2.20	0.40
1:A:4107:MET:HG2	1:A:4135:PRO:HB3	2.02	0.40
1:A:1675:GLY:HA3	1:A:1685:MET:HE2	2.04	0.40
1:A:1698:ILE:HD12	1:A:1701:TRP:NE1	2.36	0.40
1:A:3039:LYS:HA	1:A:3039:LYS:HD3	1.86	0.40
1:A:3783:LYS:HA	1:A:3783:LYS:HD3	1.76	0.40
1:A:3819:LYS:HB2	1:A:3826:GLN:OE1	2.21	0.40
1:A:4030:ILE:HG21	1:A:4145:PHE:CZ	2.56	0.40
1:A:2183:LYS:HB2	1:A:2183:LYS:HE2	1.86	0.40
1:A:3614:PHE:CD1	1:A:3635:VAL:HG11	2.56	0.40
1:A:3642:ASP:OD2	1:A:3642:ASP:C	2.65	0.40
1:A:4448:LEU:O	1:A:4452:ILE:HG12	2.21	0.40
1:A:1882:THR:HB	1:A:2045:ASP:HB2	2.04	0.40
1:A:1941:MET:O	1:A:1944:ILE:HG22	2.22	0.40
1:A:2763:ARG:HH11	1:A:2763:ARG:HG2	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	2699/4646 (58%)	2635 (98%)	64 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	2407/4125 (58%)	2395 (100%)	12 (0%)	81 80

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1878	LYS
1	A	1879	LEU
1	A	1880	VAL
1	A	1884	LEU
1	A	1885	THR
1	A	1914	GLU
1	A	1931	ASN
1	A	1964	GLU
1	A	2043	LYS
1	A	2090	LEU
1	A	3795	GLU
1	A	4628	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1817	HIS
1	A	1850	GLN
1	A	1922	GLN
1	A	1973	GLN
1	A	2005	GLN
1	A	2109	GLN
1	A	2130	ASN
1	A	2169	GLN
1	A	2171	HIS
1	A	2314	ASN
1	A	2464	GLN
1	A	2482	GLN
1	A	2549	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2834	GLN
1	A	3032	GLN
1	A	3047	HIS
1	A	3181	ASN
1	A	3214	GLN
1	A	3535	HIS
1	A	3563	GLN
1	A	3744	GLN
1	A	3772	ASN
1	A	3800	GLN
1	A	3845	ASN
1	A	3854	GLN
1	A	4023	GLN
1	A	4114	HIS
1	A	4325	ASN
1	A	4397	HIS
1	A	4466	HIS
1	A	4490	GLN
1	A	4566	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](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ADP	A	4701	-	28,29,29	0.44	0	43,45,45	0.45	0
2	ADP	A	4704	-	28,29,29	1.38	4 (14%)	43,45,45	1.79	8 (18%)
2	ADP	A	4703	-	28,29,29	1.40	4 (14%)	43,45,45	1.90	8 (18%)
3	ATP	A	4702	-	32,33,33	0.51	0	48,52,52	0.56	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
2	ADP	A	4701	-	-	2/16/32/32	0/3/3/3
2	ADP	A	4704	-	-	4/16/32/32	0/3/3/3
2	ADP	A	4703	-	-	4/16/32/32	0/3/3/3
3	ATP	A	4702	-	-	1/22/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4703	ADP	C5-C4	4.70	1.47	1.39
2	A	4704	ADP	C5-C4	4.51	1.47	1.39
2	A	4703	ADP	C5-C6	2.66	1.48	1.41
2	A	4704	ADP	C5-C6	2.56	1.48	1.41
2	A	4704	ADP	C5-N7	-2.41	1.34	1.39
2	A	4703	ADP	C5-N7	-2.35	1.34	1.39
2	A	4704	ADP	C8-N7	2.27	1.36	1.31
2	A	4703	ADP	C8-N7	2.23	1.36	1.31

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4703	ADP	C5-C4-N3	-6.11	118.30	126.72
2	A	4704	ADP	C5-C4-N3	-5.64	118.95	126.72
2	A	4703	ADP	N3-C4-N9	4.98	135.64	127.17
2	A	4704	ADP	N3-C4-N9	4.43	134.71	127.17
2	A	4703	ADP	C2-N3-C4	3.89	121.33	111.83
2	A	4704	ADP	C2-N3-C4	3.59	120.60	111.83
2	A	4703	ADP	N3-C2-N1	-3.52	123.26	128.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4704	ADP	C4-C5-N7	-3.36	106.74	110.58
2	A	4704	ADP	N3-C2-N1	-3.20	123.75	128.58
2	A	4703	ADP	C4-C5-N7	-3.18	106.95	110.58
2	A	4703	ADP	C3'-C2'-C1'	2.83	106.81	101.46
2	A	4704	ADP	C4-N9-C8	2.56	108.42	105.74
2	A	4703	ADP	C4-N9-C8	2.46	108.32	105.74
2	A	4704	ADP	C5-N7-C8	2.40	107.22	103.45
2	A	4703	ADP	C5-N7-C8	2.35	107.15	103.45
2	A	4704	ADP	C3'-C2'-C1'	2.28	105.78	101.46

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	4703	ADP	C5'-O5'-PA-O1A
2	A	4703	ADP	C5'-O5'-PA-O2A
2	A	4703	ADP	C5'-O5'-PA-O3A
2	A	4704	ADP	PA-O3A-PB-O2B
2	A	4704	ADP	PA-O3A-PB-O3B
2	A	4704	ADP	C5'-O5'-PA-O1A
2	A	4701	ADP	O4'-C4'-C5'-O5'
3	A	4702	ATP	O4'-C4'-C5'-O5'
2	A	4701	ADP	C3'-C4'-C5'-O5'
2	A	4704	ADP	C3'-C4'-C5'-O5'
2	A	4703	ADP	O4'-C4'-C5'-O5'

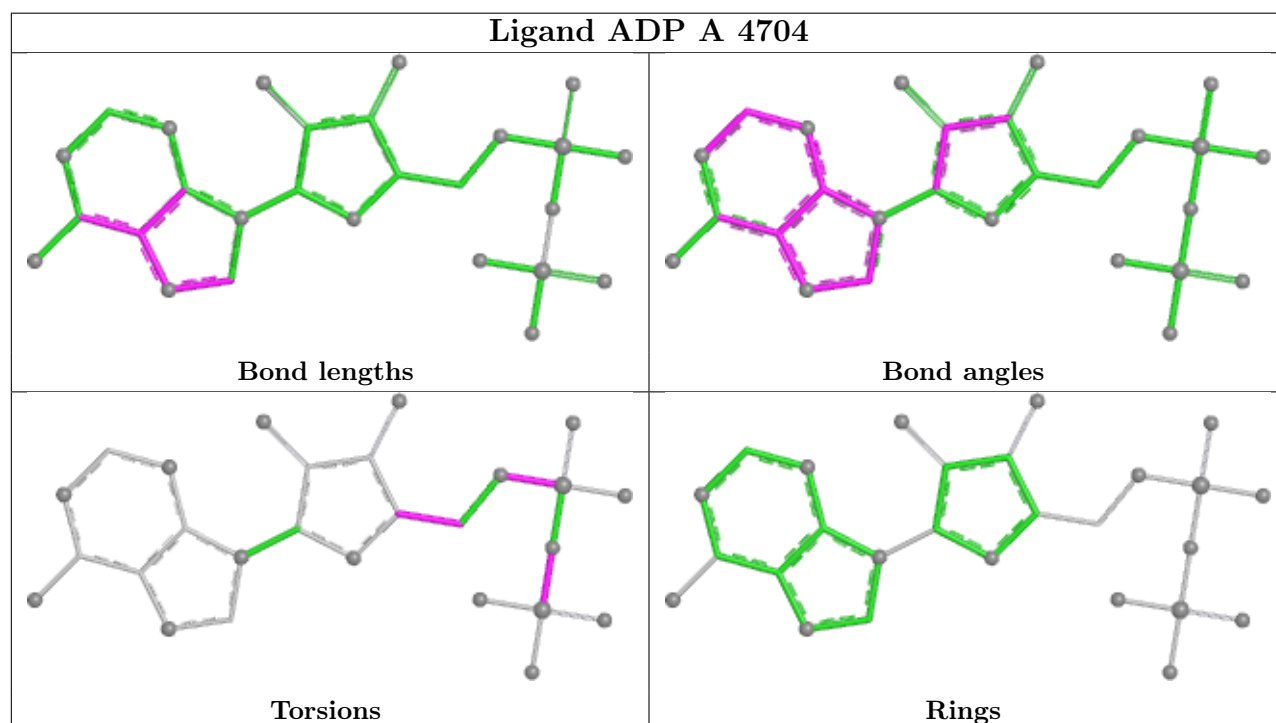
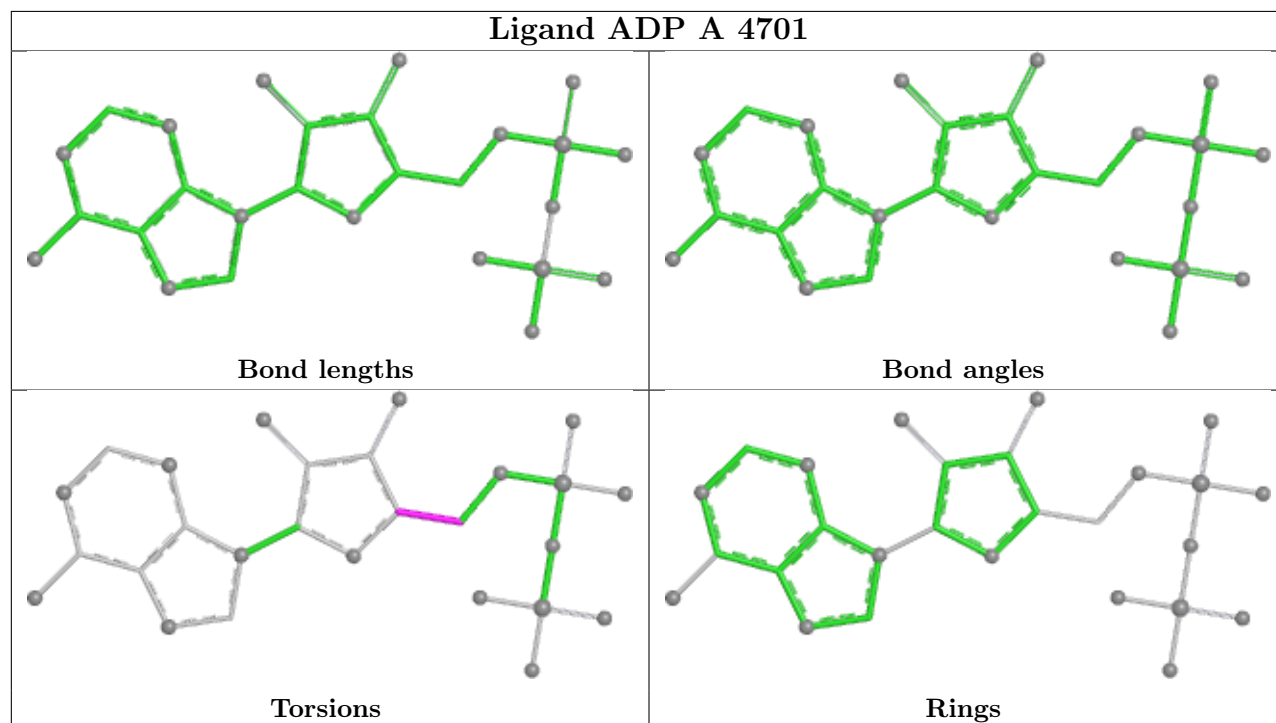
There are no ring outliers.

2 monomers are involved in 7 short contacts:

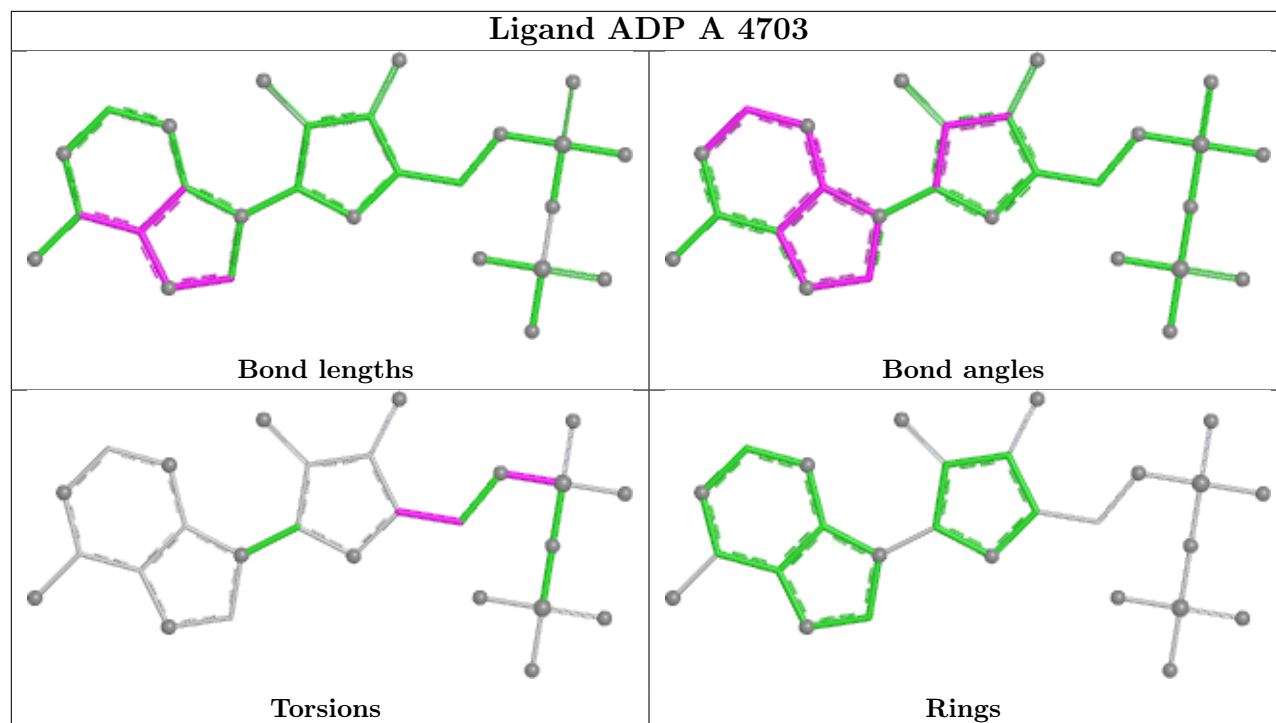
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4701	ADP	2	0
2	A	4703	ADP	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

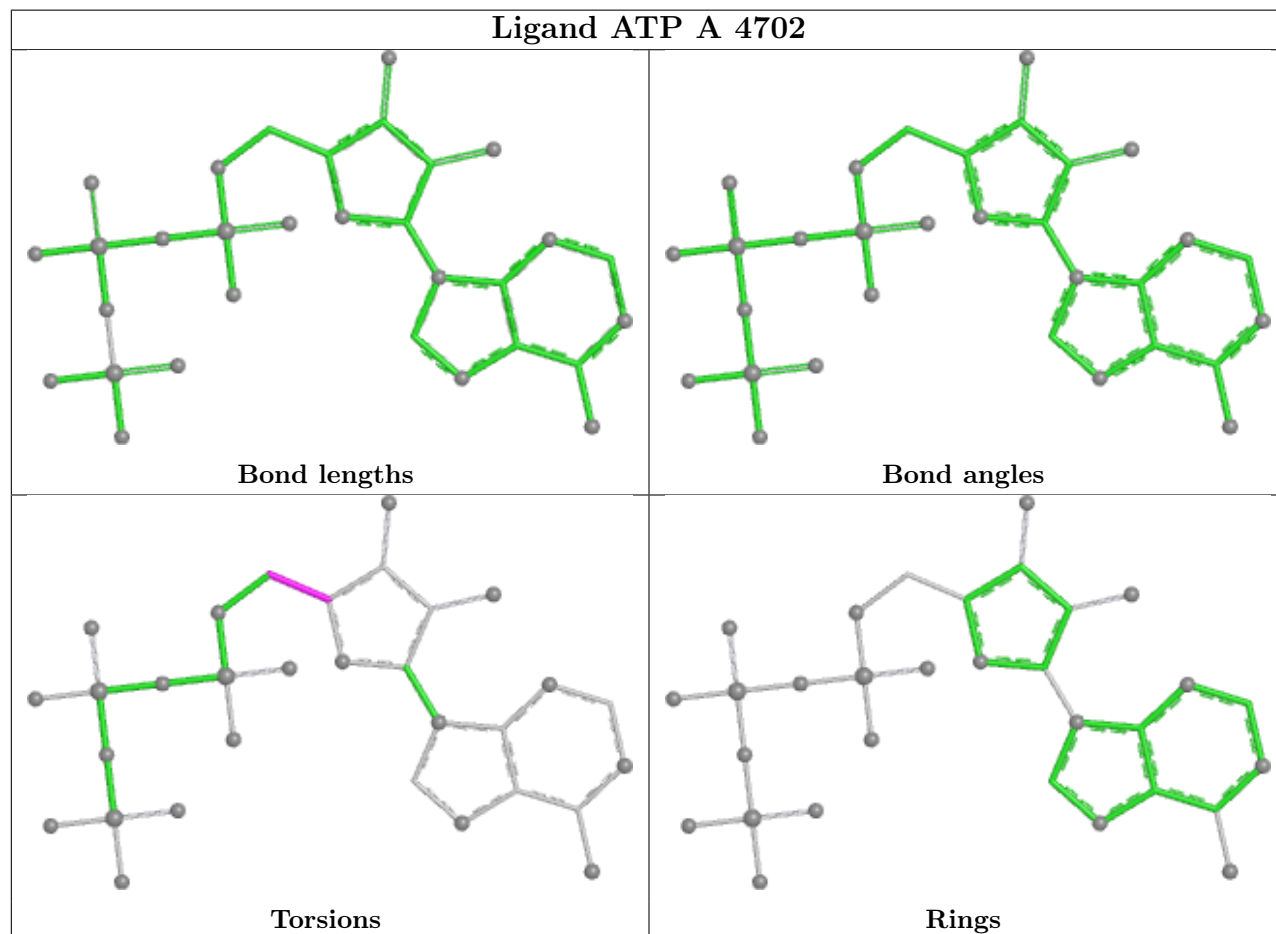
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



Ligand ADP A 4703



Ligand ATP A 4702



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

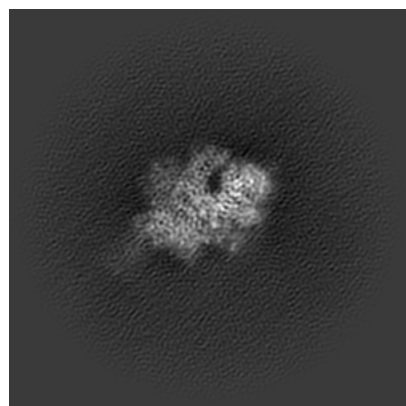
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44686. These allow visual inspection of the internal detail of the map and identification of artifacts.

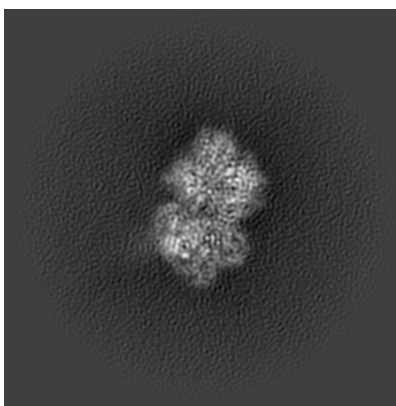
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

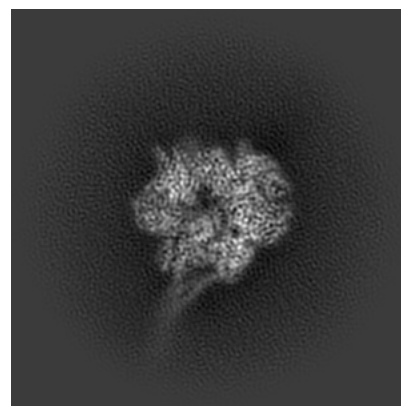
6.1.1 Primary map



X

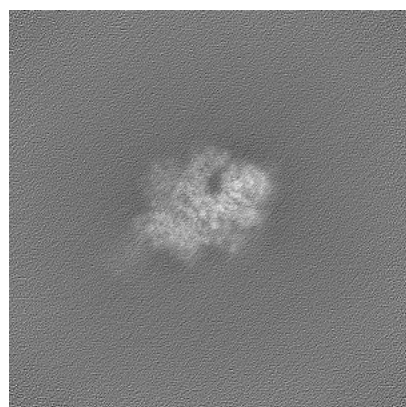


Y

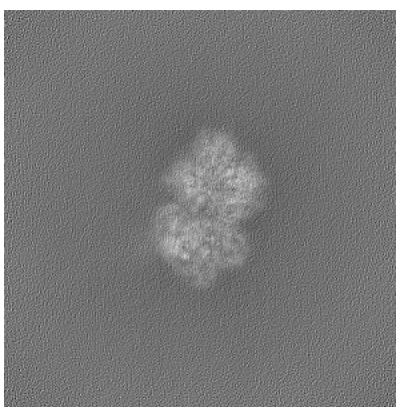


Z

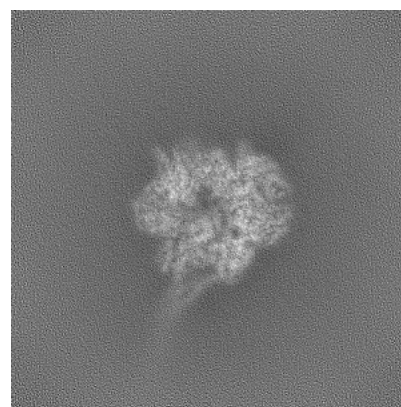
6.1.2 Raw map



X



Y

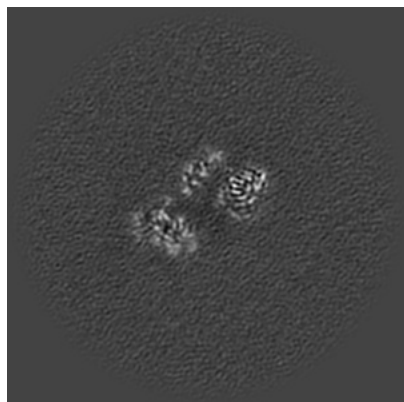


Z

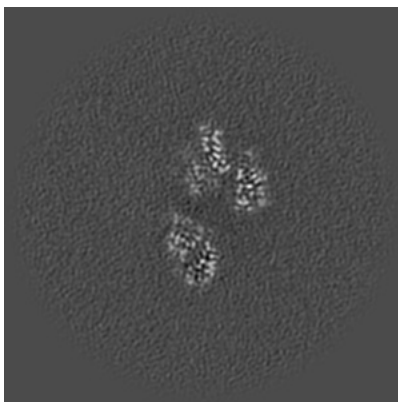
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

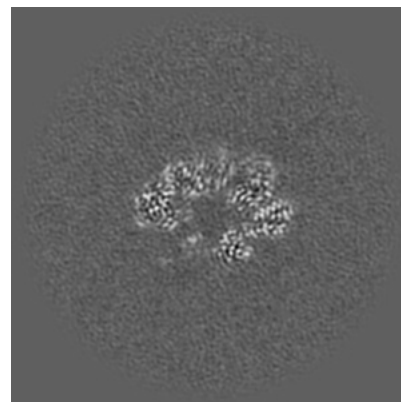
6.2.1 Primary map



X Index: 200

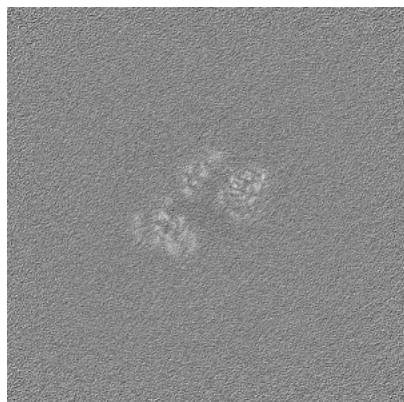


Y Index: 200

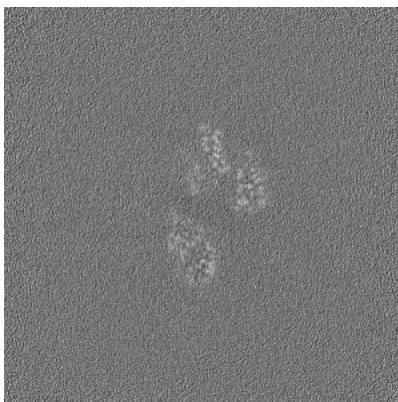


Z Index: 200

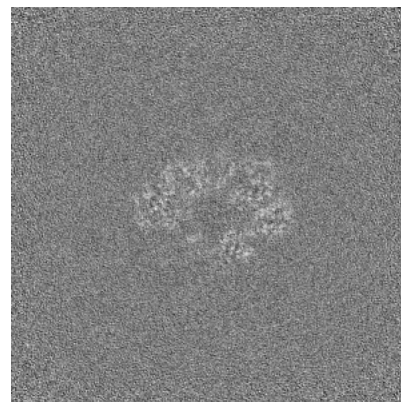
6.2.2 Raw map



X Index: 200



Y Index: 200

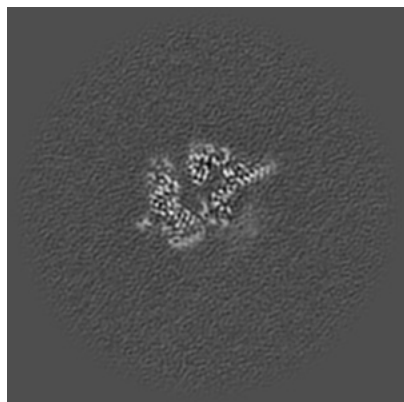


Z Index: 200

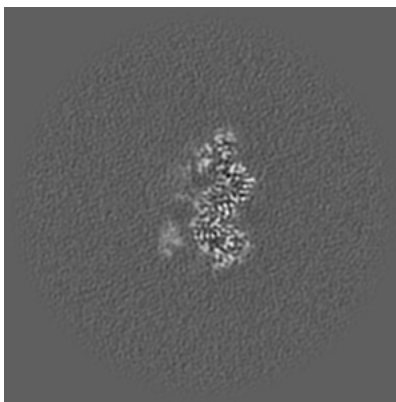
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

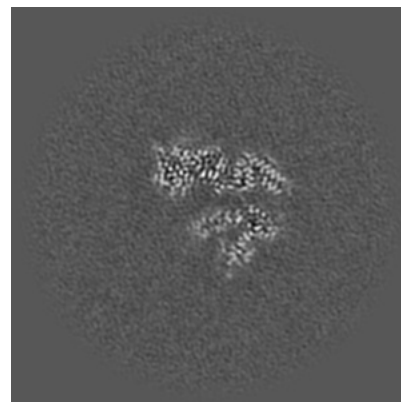
6.3.1 Primary map



X Index: 229

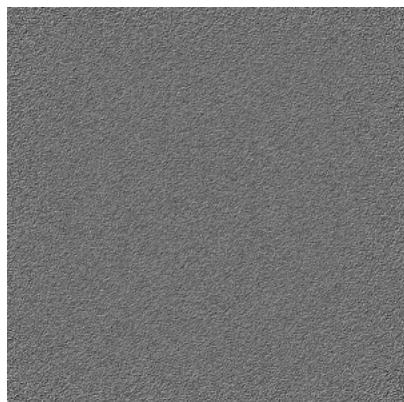


Y Index: 226

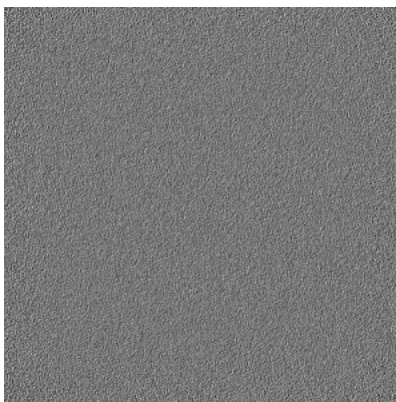


Z Index: 225

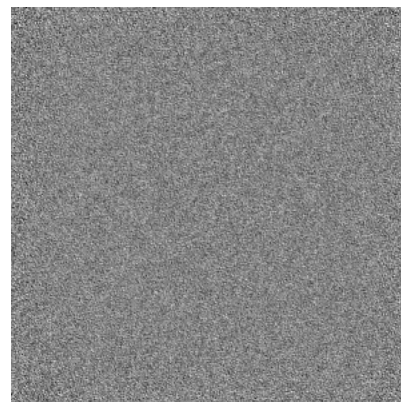
6.3.2 Raw map



X Index: 0



Y Index: 0

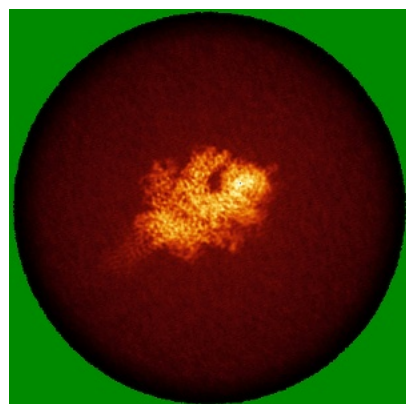


Z Index: 0

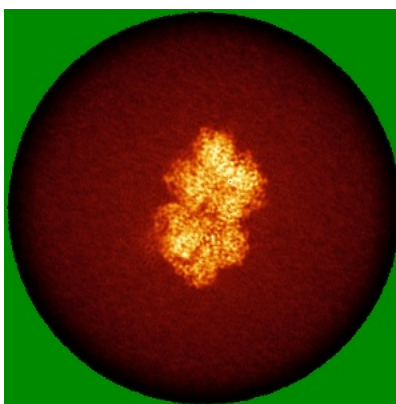
The images above show the largest variance slices of the map in three orthogonal directions.

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

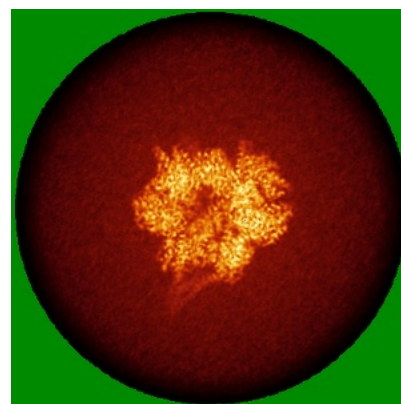
6.4.1 Primary map



X

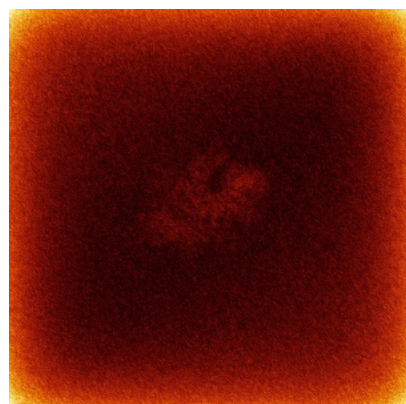


Y

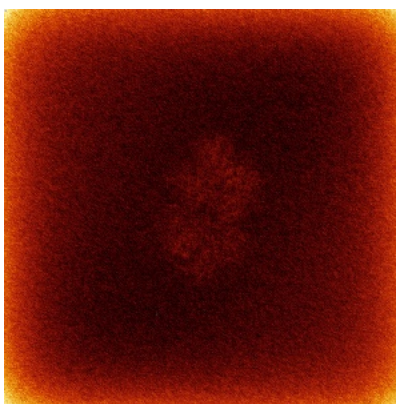


Z

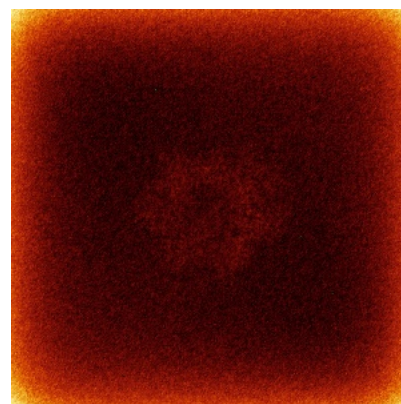
6.4.2 Raw map



X



Y



Z

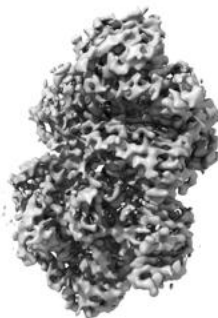
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

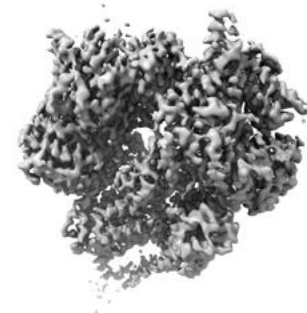
6.5.1 Primary map



X



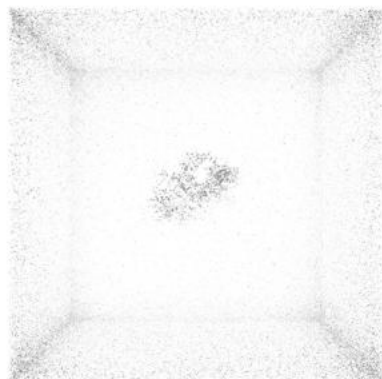
Y



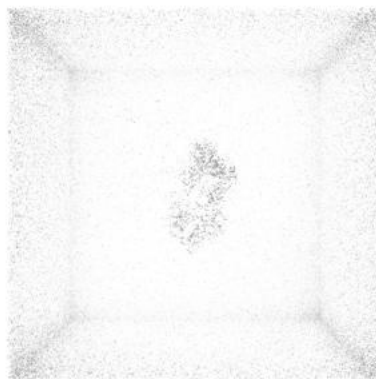
Z

The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

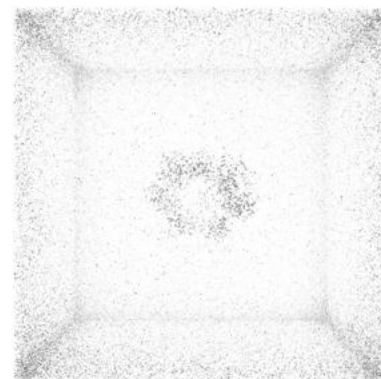
6.5.2 Raw map



X



Y



Z

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.

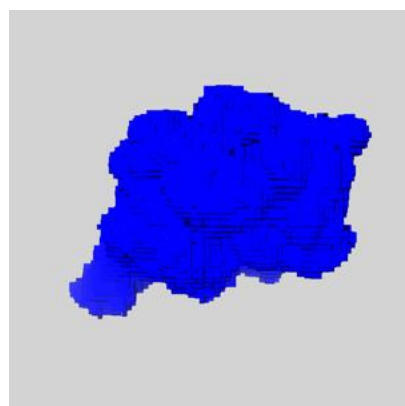
6.6 Mask visualisation [i](#)

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

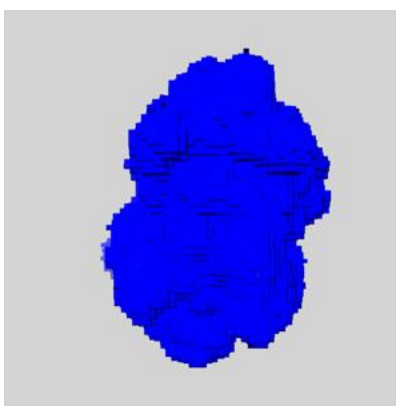
A mask typically either:

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

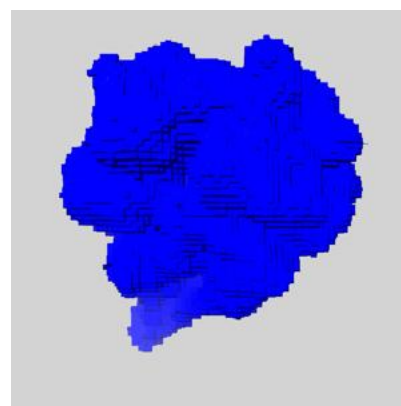
6.6.1 emd_44686_msk_1.map [i](#)



X



Y

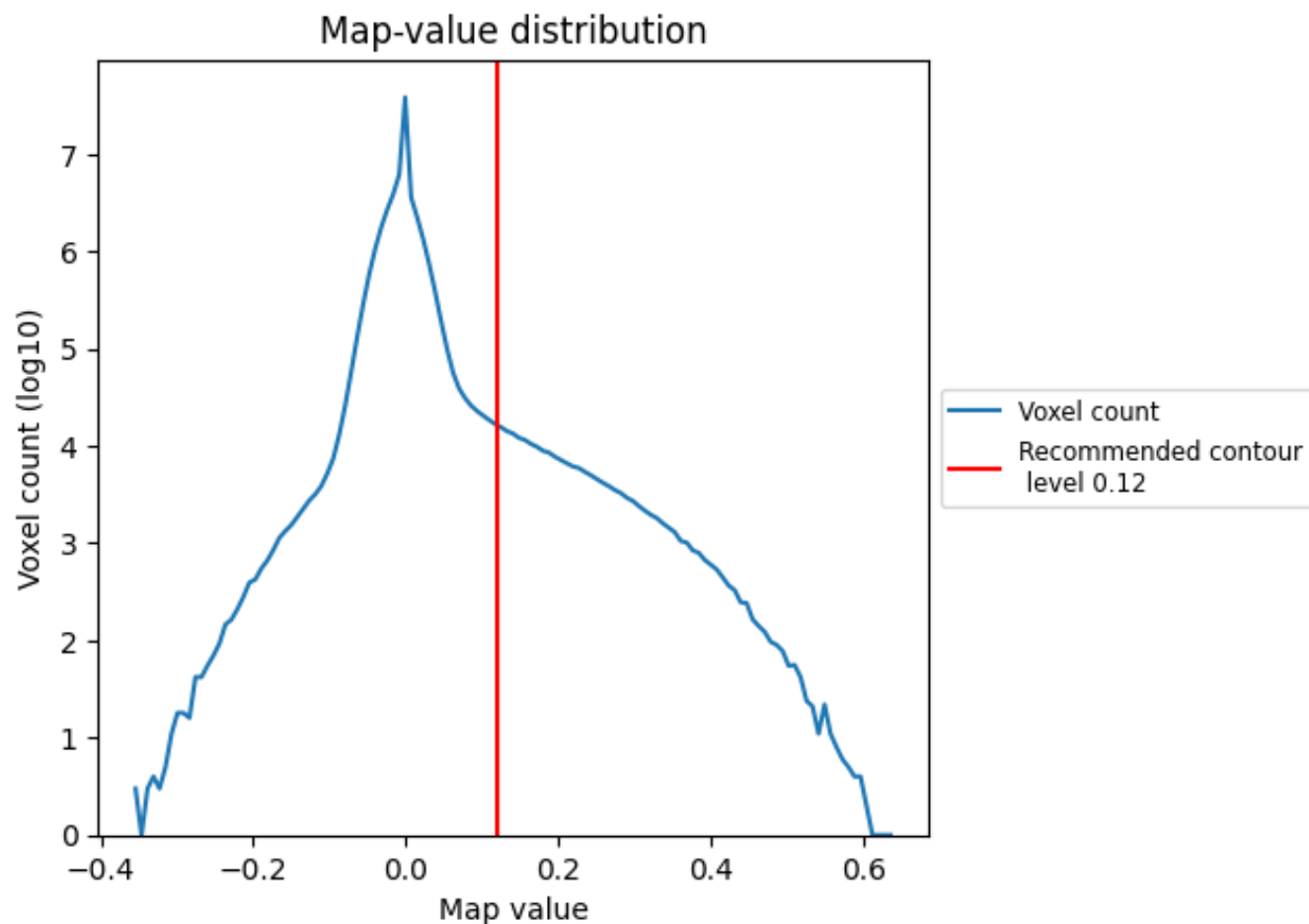


Z

7 Map analysis [i](#)

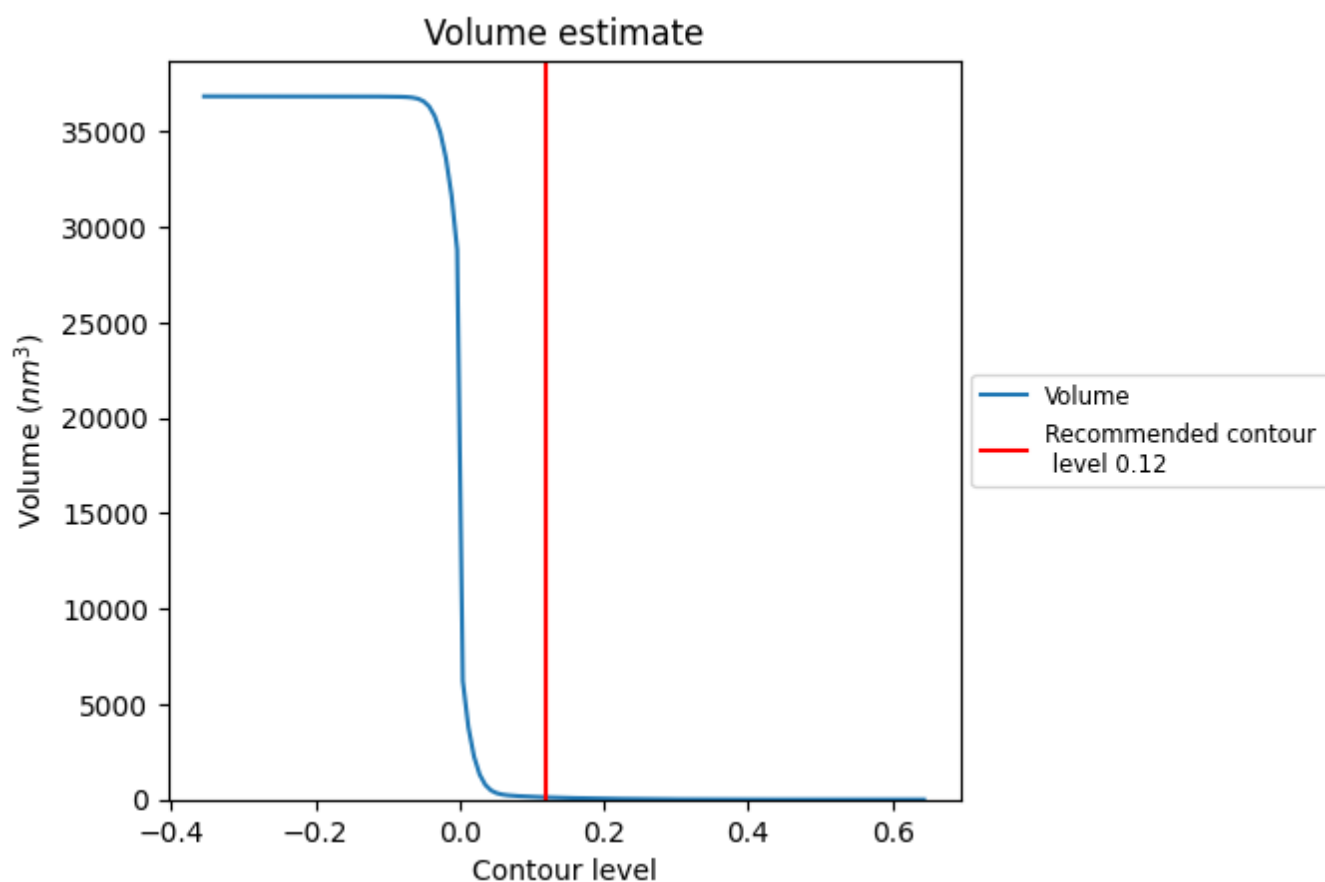
This section contains the results of statistical analysis of the map.

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.

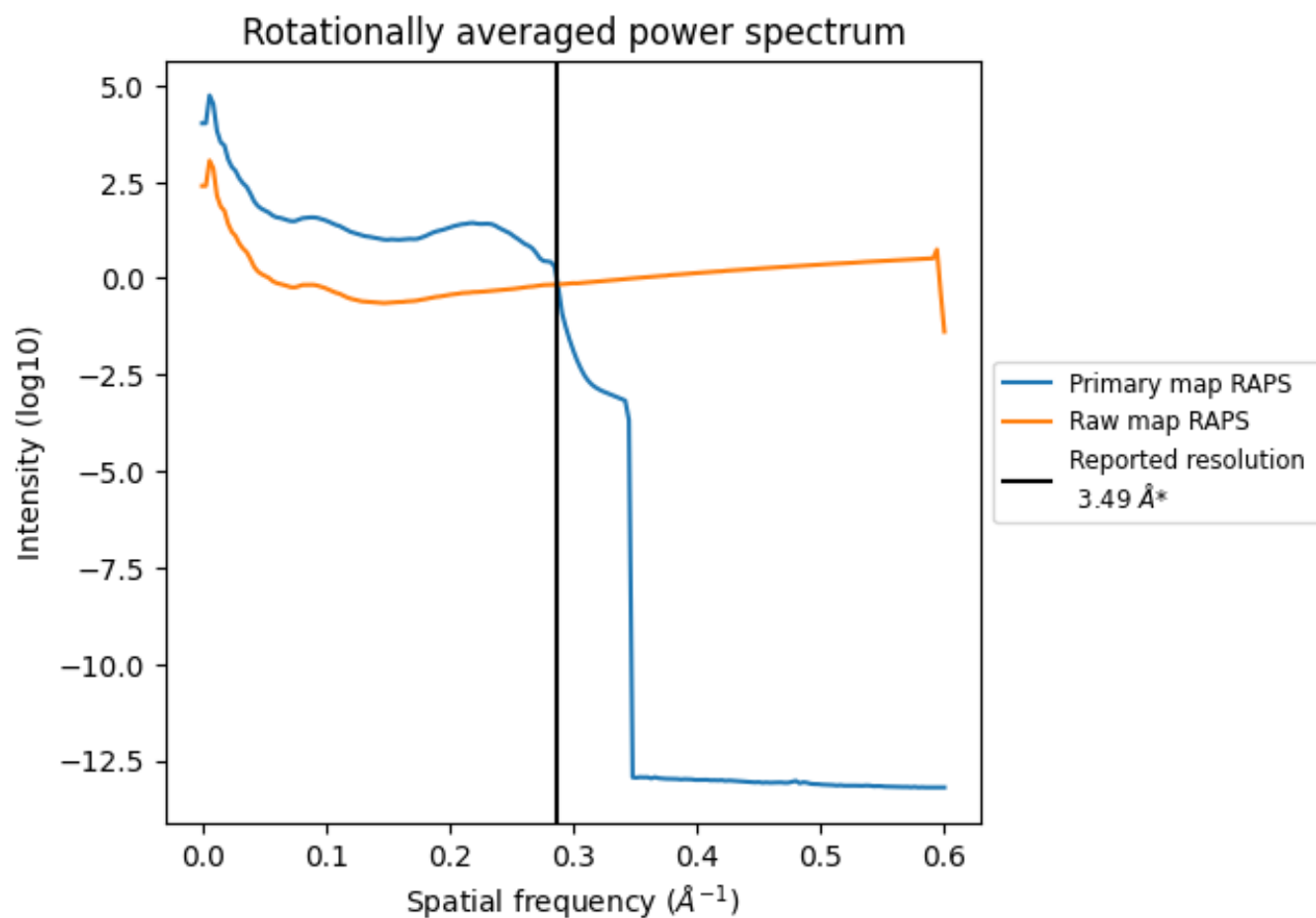
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 118 nm^3 ; this corresponds to an approximate mass of 107 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 ⓘ

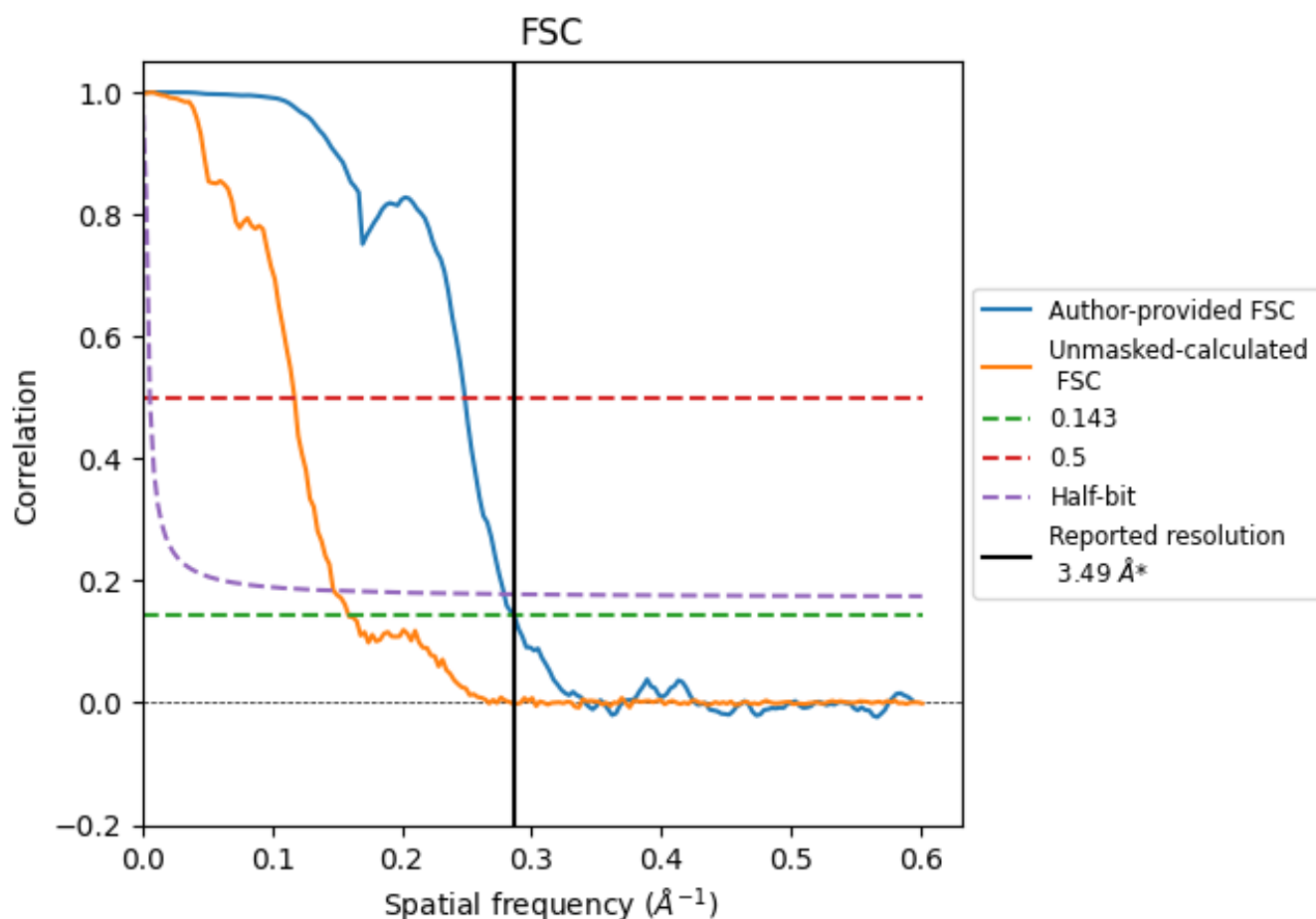


*Reported resolution corresponds to spatial frequency of 0.287 $\text{\AA}^{-1}$

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 0.287 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

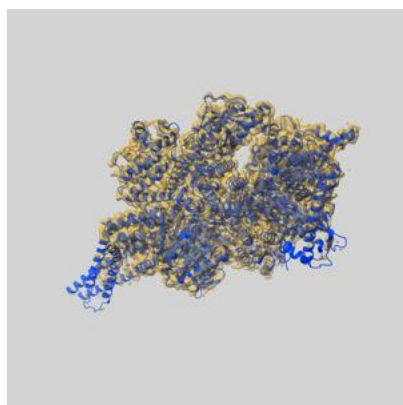
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.49	-	-
Author-provided FSC curve	3.49	4.02	3.59
Unmasked-calculated*	6.29	8.53	6.78

*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 6.29 differs from the reported value 3.49 by more than 10 %

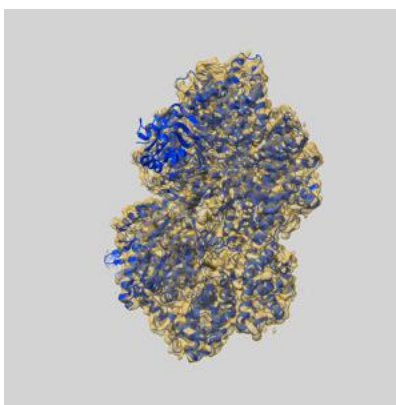
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44686 and PDB model 9BM3. Per-residue inclusion information can be found in section 3 on page 5.

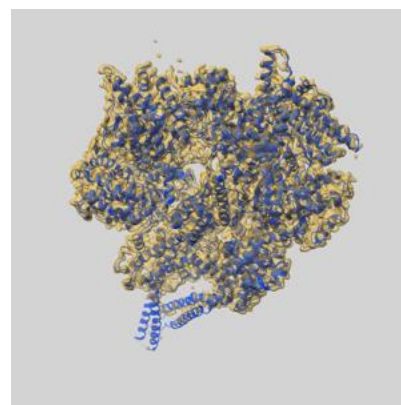
9.1 Map-model overlay [i](#)



X



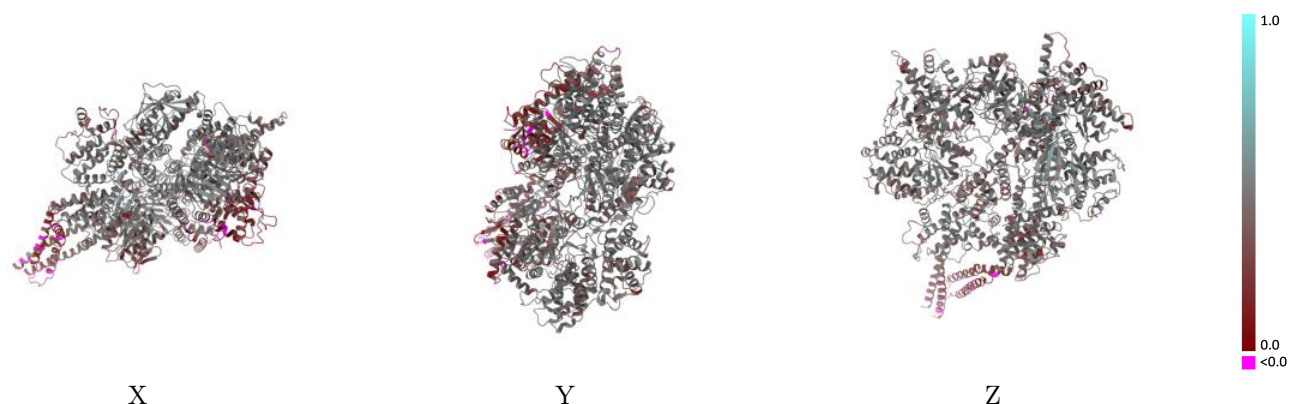
Y



Z

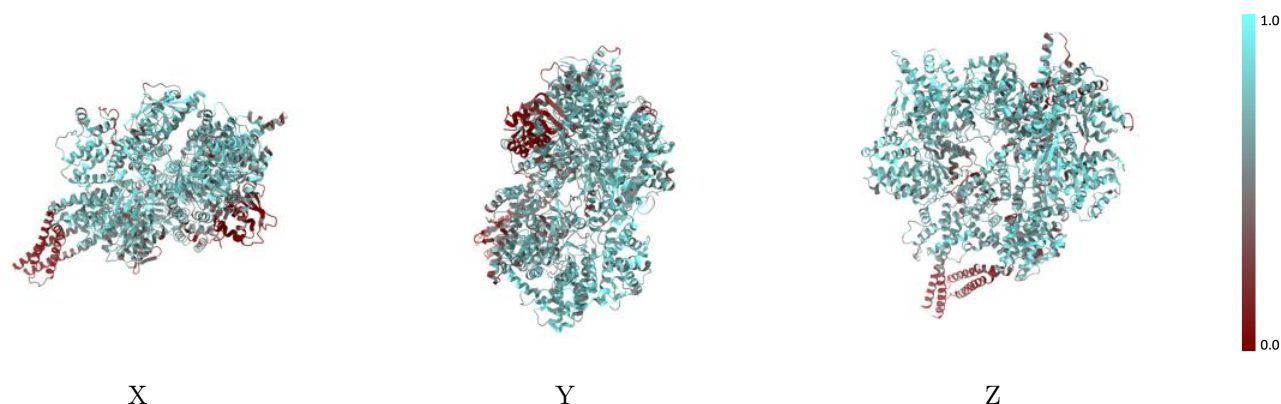
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



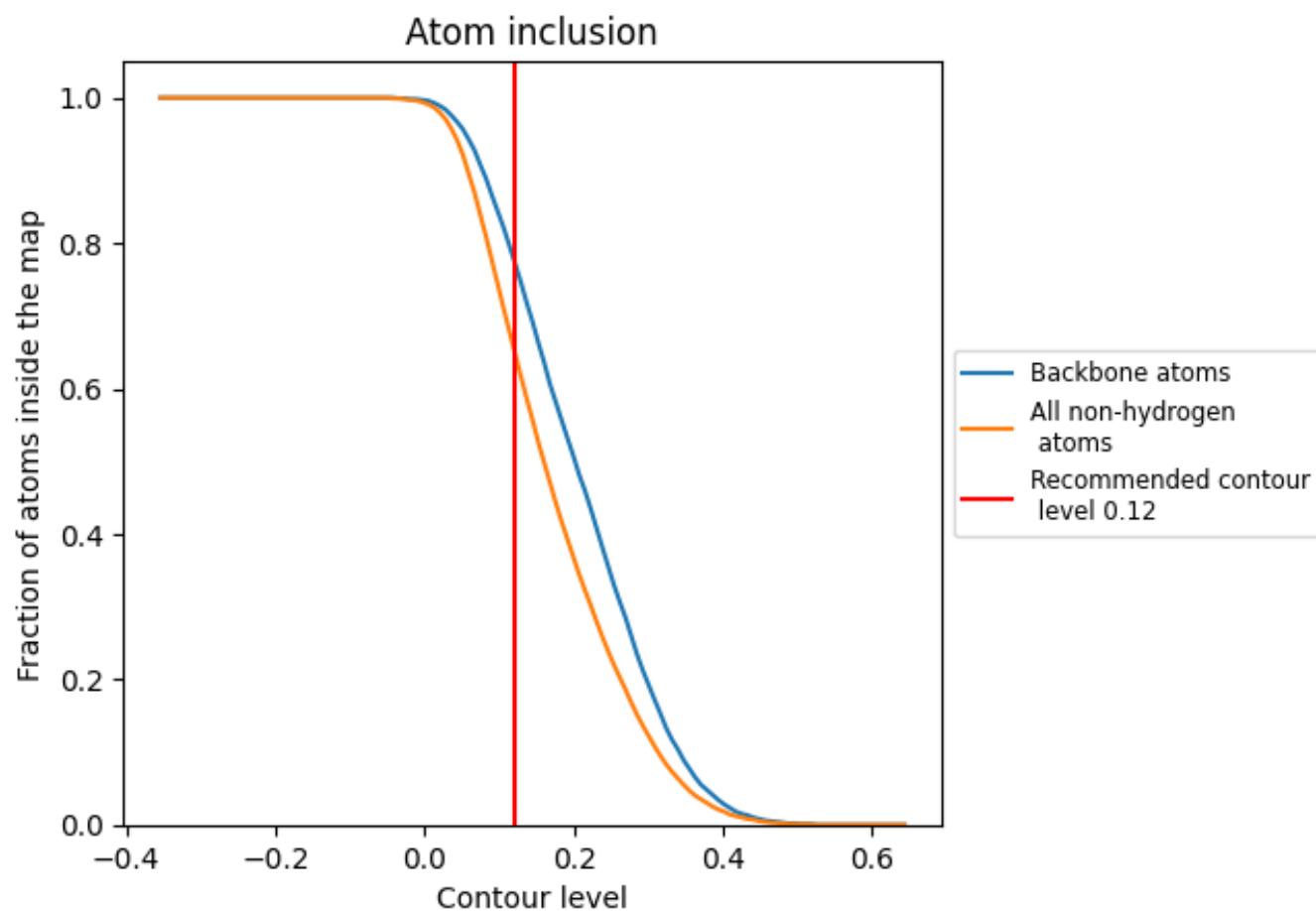
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 65% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6530	0.4170
A	0.6530	0.4170

