



Full wwPDB EM Validation Report ⓘ

Apr 24, 2025 – 10:24 AM EDT

PDB ID : 9BMW / pdb_00009bmw
EMDB ID : EMD-44713
Title : State-7b-post2 of motor domain from full-length human dynein-1 in 5 mM ADP
Authors : Chai, P.; Zhang, K.
Deposited on : 2024-05-02
Resolution : 3.30 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.dev117
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

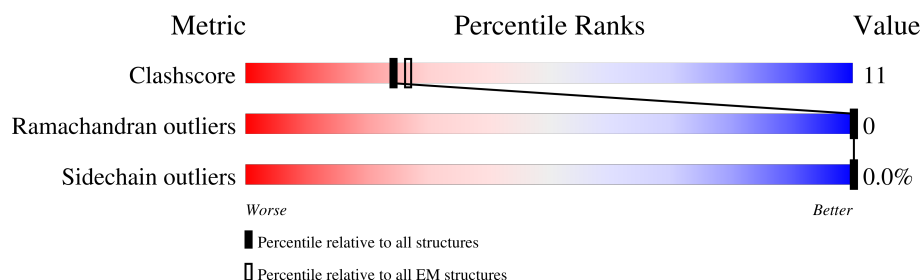
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	4646	<div> <div>10%</div> <div>49%</div> <div>17%</div> <div>35%</div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 24617 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	3043	24503	15606	4234	4541	122	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 31	C 10	N 5	O 13	P 3	0

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

Mol	Chain	Residues	Atoms		AltConf
4	A	2	Total 2	Mg 2	0





N4597	R4449	M4346	Y4180	A4074	A3918	M3791	L3731	L3634	D3546	VAL
T4598	T4452	Q4547	L4183	E4075	G3919	Q3792	L3732	V3635		GLU
E4599	L4452	M4348	A4184	G4076	R3923	E3793	K3733	Q3637		A3470
K4600	L4460	L4349	W4185	F4077	R3924	E3794	L3734	V3638		K3471
K4601	P4461	M4078	Q4079	Q4078	L3924	E3796	Q3735	E3639		V3472
		ASP	Q4079			T3796	G3736	S3640		N3473
		GLU						N3655		N3473
		GLU	I4189	I4084	E3933		E3737	R3561		R3474
		ASP	E4192	N4085	A3934	Y3801	F3738	D3557		A3556
		ASP	R4193	T4086	V3935	L3802	Q3739	E3558		S3475
		ALA	Y4205	A4087	V3936	P3803	L3740	R3559		R3476
		ALA	E4206	V4086	R3937			L3560		A3477
		GLU	K4089	K4089		S3809	R3741	R3556		L3478
						S3810	L3742	R3555		L3479
						I3811	L3743	W3562		L3479
						F3812	Q3743	Q3563		K3480
						T3813	Q3744	A3564		S3481
						M3815	L3745	L3567		L3482
						L3818	E3746	R3569		S3483
							K3747	V3660		A3484
						L3824	S3748	L3661		E3485
						S3828	L3749	T3663		R3486
						I3835	L3750	L3664		E3487
						Y3836	Q3751	G3665		K3581
						V3839	L3753	D3666		R3488
						L3846	N3754	Q3667		N3489
						R3855	E3755	D3668		E3490
						L3856	K3757	I3669		K3491
						I3859	V3756	D3670		S3492
						L3863	L3760	S3593		G3594
						F3864	L3761	Q3595		K3493
						Q3865	D3762	A3596		E3494
						N3869	D3763	T3597		T3495
						R3870	D3764	K3605		F3496
						R3873	T3765	D3606		M3601
						L3886	L3766	R3607		K3497
						K3891	L3767	S3612		N3498
						V3896	T3768	F3614		Q3499
						L3909	T3769	L3508		K3500
						R3910	L3770	S3510		S3501
						E3913	E3771	L3615		T3502
						I3914	N3772	D3616		G3505
						V3915	L3773	D3617		D3506
						L3916	K3774	A3618		C3507
						S3917	R3775	F3619		L3509
							E3776	R3620		S3510
							A3777	E3624		T3514
							A3778	F3629		A3515
							E3779	L3632		Y3516
							V3780	P3722		K3532
							T3781	D3723		S3533
							R3782	V3724		H3534
							K3783	D3725		H3535
							V3784	E3726		L3536
							E3785	K3727		Q3537
							E3786	R3728		N3540
							T3787	S3729		I3541
							D3788	D3730		Q3542
							V3789			F3543
										R3544
										T3545

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	41042	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	1.144	Depositor
Minimum map value	-0.610	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.15	Depositor
Map size (\AA)	329.984, 329.984, 329.984	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.0312, 1.0312, 1.0312	Depositor

5 Model quality

5.1 Standard geometry

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

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	0/25022	0.50	0/33900

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	24503	0	24573	518	0
2	A	81	0	36	2	0
3	A	31	0	12	2	0
4	A	2	0	0	0	0
All	All	24617	0	24621	518	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 11.

All (518) 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:1698:ILE:HD13	1:A:1701:TRP:HE1	1.44	0.82
1:A:4099:VAL:HB	1:A:4106:LEU:HD21	1.65	0.77
1:A:2221:MET:HG2	1:A:2343:PHE:HB2	1.66	0.77
1:A:3601:MET:HE2	1:A:3634:LEU:HD23	1.66	0.76
1:A:4326:ASN:HD22	1:A:4581:ILE:HD13	1.49	0.74
1:A:2189:MET:HG3	1:A:2191:LEU:HD23	1.70	0.73
1:A:3756:VAL:HG23	1:A:3760:ILE:HG21	1.73	0.71
1:A:2943:LYS:NZ	2:A:4704:ADP:O1B	2.23	0.70
1:A:4096:LEU:HD13	1:A:4105:TRP:HH2	1.55	0.70
1:A:2386:PRO:HA	1:A:2416:GLN:HE22	1.56	0.69
1:A:2785:THR:HG22	1:A:2787:ASP:H	1.58	0.69
1:A:2943:LYS:HG2	1:A:3094:PHE:HE1	1.57	0.69
1:A:3069:ASN:HD21	1:A:3690:PRO:HB2	1.57	0.69
1:A:2413:LEU:HA	1:A:2416:GLN:HE21	1.57	0.68
1:A:1713:LEU:HD11	1:A:1872:TYR:HB2	1.75	0.68
1:A:4193:ARG:NH2	1:A:4637:GLU:O	2.21	0.68
1:A:3638:VAL:HG12	1:A:3681:THR:HB	1.75	0.68
1:A:1880:VAL:HG11	1:A:2049:ILE:HD13	1.74	0.68
1:A:2320:ASP:OD1	1:A:2358:ARG:NE	2.27	0.68
1:A:1332:VAL:HB	1:A:1377:LEU:HD22	1.76	0.67
1:A:3113:MET:O	1:A:3140:ARG:NH2	2.28	0.67
1:A:2131:LEU:HD12	1:A:2132:PRO:HD2	1.77	0.66
1:A:2956:LEU:HD13	1:A:2989:LYS:HB3	1.75	0.66
1:A:3593:SER:OG	1:A:3595:GLN:OE1	2.13	0.66
1:A:1511:PRO:HG2	1:A:3659:ARG:HE	1.60	0.66
1:A:4505:LYS:NZ	1:A:4554:ASP:O	2.27	0.66
1:A:2419:ALA:O	1:A:2423:MET:HG2	1.96	0.66
1:A:3742:LEU:HD11	1:A:3780:VAL:HG21	1.78	0.66
1:A:3886:LEU:HD11	1:A:4346:MET:HG3	1.79	0.65
1:A:2922:ILE:HD11	1:A:2935:LEU:HD21	1.78	0.64
1:A:1463:LEU:HA	1:A:1466:ILE:HD12	1.80	0.64
1:A:2923:ASP:OD2	1:A:2954:ASN:ND2	2.23	0.64
1:A:3553:LEU:O	1:A:3582:ARG:NH2	2.31	0.64
1:A:1857:LEU:HD22	1:A:1868:TYR:HB2	1.80	0.64
1:A:2901:TYR:OH	1:A:2909:LEU:N	2.27	0.63
1:A:2248:GLU:OE2	1:A:2248:GLU:N	2.31	0.63
1:A:2834:GLN:HG2	1:A:2843:ARG:HD3	1.81	0.62
1:A:4068:SER:HA	1:A:4095:MET:HB3	1.81	0.62
1:A:3955:GLU:N	1:A:3955:GLU:OE1	2.33	0.62
1:A:2987:ASN:OD1	1:A:3057:GLN:NE2	2.31	0.62
1:A:3151:HIS:ND1	1:A:3516:TYR:OH	2.21	0.62
1:A:3933:GLU:OE2	1:A:3937:ARG:NE	2.33	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4324:PRO:HB3	1:A:4638:ARG:NH1	2.14	0.62
1:A:1912:LYS:HG2	1:A:2041:MET:HG3	1.81	0.62
1:A:2816:LEU:HD11	1:A:2820:GLY:HA3	1.82	0.62
1:A:1661:VAL:HG22	1:A:1676:ILE:HG21	1.82	0.61
1:A:2291:VAL:HG23	1:A:2292:ARG:HG2	1.81	0.61
1:A:1529:ARG:HH21	1:A:1592:LEU:HG	1.64	0.61
1:A:1713:LEU:HD22	1:A:1749:LEU:HD21	1.81	0.61
1:A:3909:LEU:HB3	1:A:4344:LEU:HD13	1.82	0.61
1:A:4071:ILE:HG23	1:A:4077:PHE:HE1	1.65	0.61
1:A:4574:LYS:NZ	1:A:4625:GLU:OE1	2.29	0.61
1:A:3828:SER:HB3	1:A:4140:ARG:HG2	1.83	0.60
1:A:4069:ILE:HD13	1:A:4079:GLN:HG2	1.83	0.60
1:A:4511:LEU:HD23	1:A:4560:VAL:HG13	1.83	0.60
1:A:3078:ARG:HA	1:A:3081:THR:HG22	1.83	0.60
1:A:4629:LYS:HE3	1:A:4629:LYS:HA	1.83	0.60
1:A:4482:PHE:O	1:A:4486:ILE:HG12	2.01	0.60
1:A:1717:LEU:HB2	1:A:1749:LEU:HD12	1.83	0.59
1:A:2448:ASP:OD2	1:A:2725:HIS:NE2	2.35	0.59
1:A:2930:GLN:HB2	1:A:3059:ILE:HG23	1.83	0.59
1:A:1800:GLN:OE1	1:A:1804:ARG:NH1	2.34	0.59
1:A:1721:VAL:HA	1:A:1724:VAL:HG12	1.83	0.59
1:A:2609:LEU:HD21	1:A:2615:MET:HB2	1.84	0.59
1:A:2775:GLU:OE1	1:A:2857:HIS:NE2	2.35	0.59
1:A:1864:ALA:HB2	1:A:1897:GLU:HB2	1.84	0.59
1:A:1816:VAL:HG11	1:A:2052:VAL:HG22	1.83	0.59
1:A:4631:ASP:O	1:A:4634:SER:OG	2.16	0.59
1:A:2112:LYS:HG3	1:A:2122:VAL:HG11	1.84	0.59
1:A:2413:LEU:HD21	1:A:2417:ARG:HH21	1.67	0.59
1:A:2983:SER:HB3	1:A:2990:ILE:HD12	1.84	0.59
1:A:2054:LEU:HG	1:A:2097:LEU:HD22	1.84	0.58
1:A:1490:TRP:CH2	1:A:1537:TRP:HD1	2.21	0.58
1:A:3772:ASN:HA	1:A:3775:ARG:HH11	1.67	0.58
1:A:1928:LEU:HD12	1:A:1948:LEU:HD21	1.86	0.58
1:A:4574:LYS:HG2	1:A:4627:ALA:HB2	1.84	0.58
1:A:1720:SER:HB2	1:A:1745:TYR:CD1	2.38	0.58
1:A:2610:ARG:HG2	1:A:2610:ARG:HH11	1.68	0.57
1:A:2925:ILE:HD12	1:A:3090:VAL:HG11	1.86	0.57
1:A:2970:GLU:N	1:A:2970:GLU:OE1	2.36	0.57
1:A:3910:ARG:NH2	1:A:4348:MET:SD	2.77	0.57
1:A:3914:ILE:H	1:A:3937:ARG:HH12	1.52	0.57
1:A:2346:GLN:HB2	1:A:2726:ARG:HD2	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4153:VAL:HG22	1:A:4192:GLU:HG3	1.87	0.57
1:A:2191:LEU:HD12	3:A:4702:ATP:C6	2.40	0.57
1:A:3839:VAL:HG21	1:A:3863:LEU:HA	1.87	0.57
1:A:2571:THR:H	1:A:2574:THR:HB	1.70	0.57
1:A:2994:MET:HB2	1:A:2998:ASN:HD21	1.70	0.57
1:A:1750:VAL:HG12	1:A:1811:LEU:HD21	1.85	0.57
1:A:1463:LEU:HD13	1:A:1466:ILE:HD12	1.87	0.57
1:A:3074:GLY:O	1:A:3078:ARG:NE	2.35	0.57
1:A:3691:ASP:OD1	1:A:3692:LEU:N	2.37	0.57
1:A:3913:GLU:HG3	1:A:4476:ILE:HD13	1.87	0.57
1:A:1487:ILE:HD13	1:A:1537:TRP:HE1	1.70	0.56
1:A:1721:VAL:O	1:A:1725:GLU:HG2	2.05	0.56
1:A:1626:PHE:CE1	1:A:1628:ARG:HB2	2.39	0.56
1:A:3055:THR:O	1:A:3059:ILE:HD12	2.06	0.56
1:A:3739:GLN:HA	1:A:3742:LEU:HD12	1.87	0.56
1:A:1539:ASP:OD2	1:A:1543:ARG:NH1	2.35	0.56
1:A:3731:LEU:HD11	1:A:3790:VAL:HG12	1.86	0.56
1:A:2516:GLU:O	1:A:2520:ARG:HG3	2.06	0.56
1:A:2755:MET:SD	1:A:2807:PHE:HB2	2.45	0.56
1:A:2726:ARG:NH1	3:A:4702:ATP:O3G	2.39	0.56
1:A:4075:GLU:N	1:A:4075:GLU:OE1	2.39	0.56
1:A:1398:MET:SD	1:A:1399:LEU:HD22	2.47	0.55
1:A:2816:LEU:HD12	1:A:2817:PRO:HD2	1.88	0.55
1:A:3208:ILE:HG23	1:A:3482:LEU:HD12	1.87	0.55
1:A:2413:LEU:HA	1:A:2416:GLN:NE2	2.22	0.55
1:A:4414:GLU:O	1:A:4418:LYS:HG3	2.07	0.55
1:A:2590:PRO:HB2	1:A:2731:VAL:HG12	1.87	0.55
1:A:2976:LEU:HA	1:A:2979:VAL:HG12	1.89	0.55
1:A:3935:VAL:HG22	1:A:3996:PHE:HE1	1.72	0.55
1:A:2616:GLU:N	1:A:2616:GLU:OE1	2.40	0.55
1:A:1961:ASN:HD21	1:A:2019:ASN:HB3	1.71	0.55
1:A:2102:ASN:OD1	1:A:2105:ARG:NH2	2.35	0.55
1:A:3154:LEU:HD13	1:A:3516:TYR:CD1	2.42	0.55
1:A:3811:ILE:O	1:A:3815:MET:HG3	2.07	0.55
1:A:2449:LEU:HD11	1:A:2454:CYS:SG	2.46	0.54
1:A:3967:GLU:HG2	1:A:4007:MET:HE1	1.89	0.54
1:A:1561:LEU:HB3	1:A:1564:GLU:HB2	1.89	0.54
1:A:2146:VAL:HA	1:A:2149:LEU:HD12	1.89	0.54
1:A:3846:LEU:HD21	1:A:3859:ILE:HG13	1.88	0.54
1:A:1623:ARG:NH2	1:A:1634:ASP:OD1	2.41	0.54
1:A:3551:GLU:OE2	1:A:3559:ARG:NH1	2.38	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2065:LEU:HD11	1:A:2133:GLU:HB3	1.90	0.54
1:A:1571:ILE:HG23	1:A:1604:LEU:HD22	1.89	0.54
1:A:2265:TYR:OH	1:A:2311:TRP:O	2.18	0.54
1:A:3763:ASP:OD2	1:A:3765:THR:OG1	2.25	0.54
1:A:4180:TYR:OH	1:A:4220:ASP:OD2	2.25	0.54
1:A:2290:SER:HB3	1:A:2295:LEU:HG	1.90	0.53
1:A:4547:THR:HG22	1:A:4586:PRO:HG2	1.89	0.53
1:A:2919:VAL:HG13	1:A:2950:VAL:HG22	1.90	0.53
1:A:3486:ARG:O	1:A:3490:GLU:HG2	2.07	0.53
1:A:1843:ARG:NH1	1:A:1845:TYR:OH	2.42	0.53
1:A:1927:VAL:HG22	1:A:1954:TRP:HB2	1.91	0.53
1:A:4619:ILE:HG22	1:A:4620:PHE:HD1	1.73	0.53
1:A:3667:GLN:N	1:A:3667:GLN:OE1	2.41	0.53
1:A:3103:TYR:OH	1:A:3141:GLU:OE1	2.18	0.53
1:A:4448:LEU:O	1:A:4452:ILE:HG12	2.08	0.53
1:A:2936:ILE:HG22	1:A:3070:PRO:HG3	1.90	0.52
1:A:3505:GLY:HA3	1:A:3543:PHE:HB3	1.91	0.52
1:A:2066:ALA:HA	1:A:2069:ILE:HG22	1.91	0.52
1:A:4564:LYS:HG3	1:A:4646:GLU:HB2	1.90	0.52
1:A:2873:TYR:HE1	1:A:2883:PRO:HD3	1.73	0.52
1:A:3580:LEU:HD21	1:A:3589:ILE:HD11	1.91	0.52
1:A:3755:GLU:OE2	1:A:3759:ARG:NH1	2.42	0.52
1:A:2750:THR:HG22	1:A:2753:ARG:HH22	1.74	0.52
1:A:1571:ILE:HD11	1:A:1607:LEU:HB3	1.91	0.52
1:A:1831:ASP:OD1	1:A:1832:ASN:N	2.41	0.52
1:A:4104:GLY:O	1:A:4108:GLN:HG2	2.09	0.52
1:A:4264:LEU:O	1:A:4267:THR:OG1	2.25	0.52
1:A:2910:VAL:HG22	1:A:3108:GLU:HG2	1.92	0.52
1:A:2393:GLU:HB3	1:A:2397:ARG:HH12	1.75	0.52
1:A:1411:ARG:NH2	1:A:1456:GLU:OE1	2.39	0.51
1:A:4460:LEU:HA	1:A:4475:VAL:HG22	1.91	0.51
1:A:4560:VAL:HB	1:A:4588:THR:HB	1.91	0.51
1:A:2231:SER:HA	1:A:2234:TRP:CD1	2.45	0.51
1:A:3723:ASP:O	1:A:3727:LYS:HG3	2.11	0.51
1:A:1336:LEU:HD11	1:A:1386:VAL:HG21	1.93	0.51
1:A:2258:ALA:HB1	1:A:2682:PHE:HD1	1.75	0.51
1:A:2045:ASP:O	1:A:2049:ILE:HG12	2.11	0.51
1:A:2223:VAL:HG12	1:A:2223:VAL:O	2.11	0.51
1:A:2519:ARG:HG3	1:A:2526:LEU:HD12	1.92	0.51
1:A:2838:VAL:HA	1:A:3093:TRP:CD1	2.46	0.51
1:A:4485:ARG:NH1	1:A:4513:GLY:O	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2666:ILE:HG22	1:A:2723:LEU:HD21	1.92	0.51
1:A:1546:TYR:O	1:A:1550:ILE:HG12	2.10	0.51
1:A:1476:ASP:HB3	1:A:1488:ARG:NH1	2.26	0.51
1:A:2577:HIS:O	1:A:2581:LEU:HD23	2.11	0.51
1:A:3690:PRO:HA	1:A:3693:CYS:HB2	1.93	0.51
1:A:3947:LEU:O	1:A:3951:VAL:HG23	2.11	0.51
1:A:2651:ALA:HB1	1:A:2705:ARG:HH21	1.76	0.51
1:A:2965:ARG:NH2	1:A:2966:LYS:HD3	2.26	0.51
1:A:2192:THR:HB	1:A:2373:MET:HB3	1.94	0.50
1:A:1466:ILE:HG12	1:A:1500:HIS:CE1	2.45	0.50
1:A:1638:LEU:HD23	1:A:1641:ILE:HD11	1.93	0.50
1:A:2306:ASP:N	1:A:2306:ASP:OD1	2.43	0.50
1:A:2993:ILE:HG12	1:A:3065:VAL:HB	1.93	0.50
1:A:3611:ARG:NH1	1:A:3636:GLN:OE1	2.44	0.50
1:A:2591:LEU:HD12	1:A:2592:VAL:H	1.76	0.50
1:A:1698:ILE:HA	1:A:1701:TRP:NE1	2.27	0.50
1:A:3873:ARG:HH11	1:A:4025:LEU:HD12	1.77	0.50
1:A:4176:ARG:NH2	1:A:4224:ASP:OD1	2.42	0.50
1:A:1632:VAL:HG22	1:A:1636:ASP:HB2	1.94	0.50
1:A:2327:LEU:HD12	1:A:2331:GLU:HB3	1.94	0.50
1:A:2395:GLN:HB3	1:A:2398:ARG:HH22	1.77	0.50
1:A:3891:LYS:HD2	1:A:4013:LEU:HD23	1.92	0.50
1:A:2778:THR:O	1:A:2782:GLU:HG2	2.12	0.50
1:A:2973:ASP:OD1	1:A:3007:ARG:NE	2.45	0.50
1:A:3801:TYR:CE1	1:A:3856:LEU:HD12	2.47	0.49
1:A:2304:ASP:OD2	1:A:2684:ARG:NH2	2.45	0.49
1:A:2905:LEU:HD11	1:A:2948:ARG:HH21	1.77	0.49
1:A:4445:THR:O	1:A:4449:ARG:HG2	2.11	0.49
1:A:1741:TRP:CH2	1:A:1750:VAL:HG13	2.47	0.49
1:A:2755:MET:HE3	1:A:2803:VAL:HG13	1.95	0.49
1:A:2943:LYS:HE2	1:A:3067:THR:HB	1.94	0.49
1:A:3600:ILE:HD11	1:A:3634:LEU:HD22	1.93	0.49
1:A:2329:ASN:OD1	1:A:2330:GLY:N	2.46	0.49
1:A:2589:LYS:HE3	1:A:2732:PRO:HD3	1.95	0.49
1:A:4391:ILE:O	1:A:4428:ARG:NH2	2.45	0.49
1:A:1438:ASP:HB3	1:A:1441:LYS:HB3	1.94	0.49
1:A:1470:TRP:HE1	1:A:1500:HIS:CD2	2.30	0.49
1:A:1547:LEU:HD12	1:A:1551:PHE:HE2	1.76	0.49
1:A:2619:GLY:HA2	1:A:2662:PHE:HB3	1.94	0.49
1:A:3151:HIS:CD2	1:A:3155:HIS:HE2	2.30	0.49
1:A:3612:THR:HG22	1:A:3619:PHE:HD1	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2149:LEU:HD11	1:A:2157:LEU:HD22	1.95	0.49
1:A:4185:TRP:O	1:A:4189:ILE:HG12	2.12	0.49
1:A:4303:GLU:HG2	1:A:4304:GLU:N	2.28	0.49
1:A:1907:PRO:O	1:A:1912:LYS:NZ	2.45	0.49
1:A:1420:LEU:HD13	1:A:1437:VAL:HG11	1.95	0.49
1:A:1462:PHE:O	1:A:1466:ILE:HG13	2.13	0.49
1:A:1744:LYS:C	1:A:1745:TYR:HD2	2.16	0.49
1:A:2743:SER:O	1:A:2747:ILE:HG22	2.13	0.49
1:A:4445:THR:HG22	1:A:4448:LEU:HB2	1.94	0.49
1:A:3614:PHE:CE1	1:A:3635:VAL:HG11	2.47	0.49
1:A:1537:TRP:CZ2	1:A:1579:MET:HE2	2.47	0.48
1:A:3028:THR:O	1:A:3031:THR:OG1	2.18	0.48
1:A:3551:GLU:OE1	1:A:3733:LYS:HA	2.12	0.48
1:A:4097:LYS:HA	1:A:4127:THR:HG22	1.95	0.48
1:A:2191:LEU:HD11	1:A:2232:MET:HG2	1.95	0.48
1:A:2684:ARG:HH12	1:A:2726:ARG:NE	2.11	0.48
1:A:2835:ASP:OD1	1:A:2921:ARG:NH1	2.46	0.48
1:A:3708:LEU:HD22	1:A:3809:SER:HA	1.95	0.48
1:A:3824:LEU:HD11	1:A:4144:ILE:HG21	1.94	0.48
1:A:4128:MET:CE	1:A:4134:VAL:HG11	2.43	0.48
1:A:1363:LEU:HD11	1:A:1435:TRP:HH2	1.77	0.48
1:A:2747:ILE:O	1:A:2750:THR:OG1	2.21	0.48
1:A:1717:LEU:HB2	1:A:1749:LEU:CD1	2.44	0.48
1:A:2325:LEU:HB3	1:A:2333:LEU:HB2	1.96	0.48
1:A:3601:MET:O	1:A:3605:LYS:HG2	2.13	0.48
1:A:2265:TYR:OH	1:A:2315:LEU:HG	2.14	0.48
1:A:4154:LYS:O	1:A:4158:LEU:HD23	2.13	0.48
1:A:1490:TRP:HZ3	1:A:1534:PHE:CD2	2.32	0.48
1:A:2767:GLU:HG2	1:A:2768:PRO:HD3	1.95	0.47
1:A:4168:ARG:NH2	1:A:4217:ASP:OD1	2.47	0.47
1:A:2437:LEU:HD21	1:A:2451:ARG:HG3	1.96	0.47
1:A:4119:HIS:CD2	1:A:4120:ALA:H	2.32	0.47
1:A:3967:GLU:N	1:A:3967:GLU:OE1	2.48	0.47
1:A:1486:LEU:HB3	1:A:1541:GLN:NE2	2.29	0.47
1:A:2995:ASP:OD1	1:A:2996:GLU:N	2.37	0.47
1:A:3534:HIS:HA	1:A:3537:GLN:HG2	1.97	0.47
1:A:3731:LEU:HD13	1:A:3791:MET:HG2	1.96	0.47
1:A:4609:VAL:HG22	1:A:4642:VAL:HB	1.96	0.47
1:A:2605:LEU:HD13	1:A:2662:PHE:CE2	2.50	0.47
1:A:1490:TRP:CH2	1:A:1537:TRP:CD1	3.01	0.47
1:A:1582:VAL:HG23	1:A:1591:VAL:HG22	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2755:MET:CE	1:A:2803:VAL:HG13	2.45	0.47
1:A:2972:PHE:CE1	1:A:2976:LEU:HD11	2.50	0.47
1:A:4226:THR:HG21	1:A:4239:PRO:HD3	1.97	0.47
1:A:2728:LEU:HA	1:A:2731:VAL:HG22	1.96	0.47
1:A:3027:ALA:O	1:A:3031:THR:HG23	2.14	0.47
1:A:4508:HIS:HE1	1:A:4553:LEU:HD21	1.79	0.47
1:A:4528:VAL:HG11	1:A:4592:TRP:HB2	1.96	0.47
1:A:2107:ARG:NH2	1:A:2139:GLN:OE1	2.47	0.47
1:A:2773:MET:HG3	1:A:2825:TRP:HE1	1.80	0.47
1:A:4324:PRO:HB2	1:A:4326:ASN:OD1	2.13	0.47
1:A:4445:THR:HG23	1:A:4448:LEU:H	1.80	0.47
1:A:2260:SER:OG	1:A:2263:HIS:ND1	2.48	0.47
1:A:2413:LEU:HG	1:A:2417:ARG:HE	1.80	0.47
1:A:2982:ARG:HG2	1:A:2990:ILE:HD11	1.97	0.47
1:A:3192:SER:O	1:A:3196:GLU:OE1	2.33	0.47
1:A:3716:VAL:HG23	1:A:3836:TYR:OH	2.15	0.47
1:A:2422:ILE:HD13	1:A:2487:GLU:HA	1.97	0.46
1:A:2517:TYR:O	1:A:2521:ILE:HG12	2.15	0.46
1:A:2623:SER:HB3	1:A:3006:GLU:OE1	2.15	0.46
1:A:1892:MET:SD	1:A:1902:GLY:HA3	2.55	0.46
1:A:2882:ILE:HG13	1:A:2883:PRO:HD2	1.97	0.46
1:A:3870:ARG:NH2	1:A:4034:GLU:OE1	2.46	0.46
1:A:4434:VAL:HA	1:A:4437:VAL:HG12	1.97	0.46
1:A:2305:GLY:O	1:A:2345:VAL:HG12	2.15	0.46
1:A:2464:GLN:NE2	1:A:2468:ASN:OD1	2.48	0.46
1:A:2593:LEU:HD13	1:A:2605:LEU:HD12	1.97	0.46
1:A:2935:LEU:HD22	1:A:3094:PHE:CZ	2.50	0.46
1:A:4306:VAL:HA	1:A:4309:VAL:HG12	1.96	0.46
1:A:2072:PHE:HE2	1:A:2141:VAL:HG11	1.81	0.46
1:A:2211:TYR:HB2	1:A:2237:LEU:HD11	1.97	0.46
1:A:3536:LEU:HD23	1:A:3541:ILE:HG21	1.97	0.46
1:A:3756:VAL:HG13	1:A:3756:VAL:O	2.15	0.46
1:A:1363:LEU:HD11	1:A:1435:TRP:CH2	2.50	0.46
1:A:4271:ARG:HH11	1:A:4271:ARG:HG2	1.81	0.46
1:A:2033:LYS:NZ	1:A:4206:GLU:OE2	2.35	0.46
1:A:3474:ARG:HE	1:A:3764:ASP:HB3	1.80	0.46
1:A:3614:PHE:CE2	1:A:3641:TYR:HA	2.51	0.46
1:A:4112:LYS:O	1:A:4116:LEU:HG	2.15	0.46
1:A:1526:LYS:O	1:A:1530:ILE:HG22	2.15	0.46
1:A:1658:PHE:HB2	1:A:1661:VAL:HB	1.97	0.46
1:A:1937:ASP:OD2	1:A:1940:ALA:HB3	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2741:PRO:O	1:A:2745:THR:HG23	2.16	0.46
1:A:3562:TRP:HZ2	1:A:3581:LYS:HD3	1.80	0.46
1:A:3999:ASP:OD1	1:A:4000:ARG:N	2.48	0.46
1:A:1355:GLN:HG3	1:A:1358:LYS:H	1.80	0.46
1:A:1793:ALA:HA	1:A:1796:VAL:HG12	1.98	0.46
1:A:3482:LEU:O	1:A:3485:GLU:HG3	2.16	0.46
1:A:1724:VAL:HA	1:A:1727:PHE:HB2	1.98	0.46
1:A:2096:VAL:HG11	1:A:2141:VAL:HG22	1.98	0.46
1:A:3967:GLU:HG2	1:A:4007:MET:CE	2.45	0.46
1:A:2936:ILE:HG21	1:A:3093:TRP:CZ3	2.50	0.45
1:A:4381:HIS:HB2	1:A:4438:CYS:HB3	1.97	0.45
1:A:1920:GLY:HA3	1:A:1927:VAL:HG21	1.97	0.45
1:A:2797:ARG:HH12	1:A:3088:ARG:HH12	1.63	0.45
1:A:3215:VAL:HG11	1:A:3478:LEU:HD23	1.99	0.45
1:A:2591:LEU:HD13	1:A:2732:PRO:HG2	1.99	0.45
1:A:3689:PRO:HB2	1:A:3691:ASP:OD1	2.17	0.45
1:A:1409:LYS:HB3	1:A:1410:ASP:H	1.58	0.45
1:A:2189:MET:HG3	1:A:2191:LEU:CD2	2.43	0.45
1:A:2224:GLY:H	1:A:2230:LYS:HD3	1.80	0.45
1:A:4084:ILE:O	1:A:4088:VAL:HG23	2.17	0.45
1:A:1720:SER:HB2	1:A:1745:TYR:CE1	2.50	0.45
1:A:1720:SER:HB2	1:A:1745:TYR:HD1	1.81	0.45
1:A:2826:ALA:O	1:A:2830:LEU:HD23	2.17	0.45
1:A:3108:GLU:HG3	1:A:3109:PHE:HD1	1.82	0.45
1:A:1374:PRO:HD2	1:A:1377:LEU:HD12	1.98	0.45
1:A:2382:LEU:HD23	1:A:2420:ALA:HB2	1.99	0.45
1:A:2790:PRO:HG2	1:A:3075:LEU:HD23	1.98	0.45
1:A:4482:PHE:CE2	1:A:4486:ILE:HD11	2.50	0.45
1:A:1356:PRO:HB3	1:A:1401:ILE:HG12	1.98	0.45
1:A:2684:ARG:NH1	1:A:2726:ARG:HB3	2.31	0.45
1:A:4442:LYS:HE2	1:A:4442:LYS:HB3	1.82	0.45
1:A:1665:ILE:HD11	1:A:1683:GLU:HB2	1.99	0.45
1:A:1792:LEU:HD12	1:A:1815:LEU:HD12	1.99	0.45
1:A:1792:LEU:HD22	1:A:1808:LEU:HD22	1.99	0.45
1:A:1568:PHE:HB2	1:A:1611:ILE:CD1	2.46	0.45
1:A:1698:ILE:HD13	1:A:1701:TRP:NE1	2.23	0.45
1:A:1665:ILE:O	1:A:1674:LEU:N	2.49	0.45
1:A:3073:GLU:HG2	1:A:3074:GLY:N	2.31	0.45
1:A:3563:GLN:HE22	1:A:3569:ALA:HB2	1.82	0.45
1:A:1397:ASN:O	1:A:1401:ILE:HG13	2.18	0.44
1:A:2110:LYS:HA	1:A:2113:ARG:NH2	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2517:TYR:CE1	1:A:2521:ILE:HD13	2.53	0.44
1:A:3488:ARG:HH22	1:A:3773:LEU:HD21	1.81	0.44
1:A:3705:ARG:HG2	1:A:3813:PHE:CD2	2.52	0.44
1:A:2979:VAL:HG13	1:A:2980:LEU:HD12	2.00	0.44
1:A:3567:LEU:HD12	1:A:3568:PRO:HD2	1.98	0.44
1:A:2651:ALA:HB1	1:A:2705:ARG:NH2	2.32	0.44
1:A:2393:GLU:O	1:A:2397:ARG:NH1	2.51	0.44
1:A:2994:MET:O	1:A:3067:THR:OG1	2.26	0.44
1:A:3705:ARG:HA	1:A:3813:PHE:HE2	1.82	0.44
1:A:3913:GLU:N	1:A:3913:GLU:OE1	2.51	0.44
1:A:1961:ASN:HB3	1:A:2018:MET:HE1	2.00	0.44
1:A:2827:HIS:CG	1:A:2873:TYR:HD2	2.36	0.44
1:A:3534:HIS:O	1:A:3537:GLN:HG2	2.17	0.44
1:A:4489:LEU:HD23	1:A:4492:ILE:HD12	2.00	0.44
1:A:1537:TRP:HZ2	1:A:1579:MET:HE2	1.82	0.44
1:A:1725:GLU:O	1:A:1729:LYS:HG2	2.18	0.44
1:A:2123:ASP:O	1:A:2127:ILE:HG13	2.18	0.44
1:A:2273:ARG:HA	1:A:2273:ARG:NE	2.32	0.44
1:A:4601:LYS:HB2	1:A:4604:VAL:HG23	1.99	0.44
1:A:1647:VAL:HA	1:A:1650:LEU:HD13	1.99	0.44
1:A:3028:THR:O	1:A:3032:GLN:OE1	2.35	0.44
1:A:3780:VAL:O	1:A:3784:VAL:HG23	2.17	0.44
1:A:1676:ILE:HB	1:A:1684:VAL:HG22	1.99	0.44
1:A:2715:PRO:HA	1:A:2720:ARG:HB2	2.00	0.44
1:A:2784:PHE:HB3	1:A:2792:TYR:CD2	2.53	0.44
1:A:3123:PRO:HB3	1:A:3540:ASN:OD1	2.18	0.44
1:A:3654:ARG:HH21	1:A:3661:LEU:HG	1.82	0.44
1:A:4025:LEU:HD22	1:A:4027:LEU:HD22	2.00	0.44
1:A:4460:LEU:HD12	1:A:4461:PRO:HD2	2.00	0.44
1:A:1695:HIS:HB3	1:A:1700:GLU:HG2	2.00	0.43
1:A:1917:LYS:HG2	1:A:1921:HIS:CD2	2.53	0.43
1:A:2324:LEU:HD23	1:A:2334:SER:HA	2.00	0.43
1:A:1748:GLN:NE2	1:A:1868:TYR:OH	2.39	0.43
1:A:2605:LEU:HD13	1:A:2662:PHE:HE2	1.82	0.43
1:A:2737:ASP:OD1	1:A:2738:TYR:N	2.48	0.43
1:A:3048:GLU:O	1:A:3052:LYS:HG2	2.18	0.43
1:A:4260:PHE:CE2	1:A:4608:PRO:HB3	2.53	0.43
1:A:1440:GLN:HA	1:A:1443:GLU:HG3	2.01	0.43
1:A:2460:SER:OG	1:A:2589:LYS:HD2	2.19	0.43
1:A:2464:GLN:HG2	1:A:2583:THR:HG23	2.01	0.43
1:A:3661:LEU:HD12	1:A:3668:ASP:HB3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1678:SER:OG	1:A:1679:ARG:N	2.51	0.43
1:A:1786:GLU:OE1	1:A:1786:GLU:HA	2.18	0.43
1:A:2396:ARG:O	1:A:2399:LYS:HG2	2.18	0.43
1:A:2802:TRP:O	1:A:2806:ILE:HG12	2.18	0.43
1:A:4398:LEU:HG	1:A:4417:VAL:HG21	2.00	0.43
1:A:1880:VAL:HG23	1:A:2052:VAL:HG11	2.01	0.43
1:A:2889:LEU:HG	1:A:2916:LEU:HD11	2.00	0.43
1:A:3600:ILE:HD11	1:A:3634:LEU:HD13	2.00	0.43
1:A:2049:ILE:HG21	1:A:2090:LEU:HD11	2.00	0.43
1:A:2242:GLU:HG3	1:A:2248:GLU:HA	2.00	0.43
1:A:2658:TRP:CE2	1:A:2705:ARG:HG2	2.54	0.43
1:A:3555:ASN:HB2	1:A:3558:GLU:OE1	2.18	0.43
1:A:1547:LEU:HD12	1:A:1551:PHE:CE2	2.54	0.43
1:A:2156:LEU:O	1:A:2160:LEU:HD13	2.19	0.43
1:A:1393:TYR:HA	1:A:1396:ILE:HG12	2.01	0.43
1:A:1405:SER:OG	1:A:1406:GLU:N	2.52	0.43
1:A:1812:ILE:HG21	1:A:2056:SER:HA	2.01	0.43
1:A:3103:TYR:CE2	1:A:3107:LYS:HD2	2.54	0.43
1:A:3146:SER:O	1:A:3150:VAL:HG23	2.18	0.43
1:A:4332:LEU:HD23	1:A:4332:LEU:HA	1.89	0.43
1:A:2072:PHE:CE2	1:A:2141:VAL:HG11	2.54	0.43
1:A:2683:ILE:O	1:A:2687:VAL:HG22	2.19	0.43
1:A:3736:GLY:O	1:A:3740:LEU:N	2.43	0.43
1:A:3865:GLN:NE2	1:A:3869:ASN:OD1	2.51	0.43
1:A:2218:HIS:HA	1:A:2340:ARG:HD3	2.01	0.42
1:A:2395:GLN:HB3	1:A:2398:ARG:NH2	2.34	0.42
1:A:3924:ILE:HD12	1:A:3952:GLN:NE2	2.34	0.42
1:A:4031:VAL:O	1:A:4123:ARG:NH1	2.52	0.42
1:A:4423:LEU:HD13	1:A:4466:HIS:HD2	1.84	0.42
1:A:4577:LEU:HD13	1:A:4638:ARG:HD2	1.99	0.42
1:A:2079:GLN:HB2	1:A:2160:LEU:HD21	2.01	0.42
1:A:2206:LYS:HD3	1:A:2206:LYS:HA	1.86	0.42
1:A:2581:LEU:HD13	1:A:2591:LEU:CD2	2.48	0.42
1:A:2972:PHE:CZ	1:A:3004:PHE:HB3	2.53	0.42
1:A:3802:LEU:N	1:A:3803:PRO:HD2	2.35	0.42
1:A:3873:ARG:HD3	1:A:4025:LEU:HG	2.01	0.42
1:A:4560:VAL:N	1:A:4588:THR:O	2.52	0.42
1:A:1463:LEU:O	1:A:1467:ARG:NE	2.48	0.42
1:A:2660:VAL:HG22	1:A:2707:GLN:HB2	2.02	0.42
1:A:3069:ASN:ND2	1:A:3690:PRO:HB2	2.29	0.42
1:A:3079:ALA:HB2	1:A:3086:PHE:CE2	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3722:PRO:O	1:A:3725:ASP:N	2.52	0.42
1:A:3909:LEU:HD12	1:A:4344:LEU:HB2	2.00	0.42
1:A:4183:LEU:HD11	1:A:4215:ALA:HB1	2.02	0.42
1:A:2522:THR:OG1	1:A:2524:VAL:HG12	2.19	0.42
1:A:4084:ILE:HD11	1:A:4096:LEU:HD11	2.00	0.42
1:A:2992:PHE:HD2	1:A:3064:VAL:HG13	1.83	0.42
1:A:3576:ASN:ND2	1:A:3700:ASN:O	2.37	0.42
1:A:4423:LEU:HD13	1:A:4466:HIS:CD2	2.54	0.42
1:A:1792:LEU:HD23	1:A:1792:LEU:HA	1.87	0.42
1:A:2257:LYS:O	1:A:2678:ARG:HG3	2.20	0.42
1:A:2263:HIS:HD2	1:A:2695:THR:HB	1.85	0.42
1:A:3620:ARG:O	1:A:3624:GLU:HG2	2.19	0.42
1:A:1601:LEU:HD12	1:A:1601:LEU:HA	1.92	0.42
1:A:1789:LEU:HD23	1:A:1789:LEU:HA	1.85	0.42
1:A:2443:LEU:HD23	1:A:2510:MET:HG2	2.02	0.42
1:A:2667:ASN:OD1	1:A:2712:CYS:HB3	2.20	0.42
1:A:2828:GLU:OE2	1:A:2924:ARG:NH2	2.53	0.42
1:A:2944:THR:O	1:A:2948:ARG:HG3	2.20	0.42
1:A:3172:THR:HG21	1:A:3694:SER:HB2	2.01	0.42
1:A:3502:THR:HB	1:A:3543:PHE:HA	2.02	0.42
1:A:4594:LYS:HE3	1:A:4594:LYS:HB2	1.93	0.42
1:A:2630:LEU:HA	1:A:2633:LYS:HD2	2.01	0.42
1:A:3815:MET:O	1:A:3818:LEU:HB2	2.19	0.42
1:A:4033:THR:HG22	1:A:4034:GLU:N	2.35	0.42
1:A:4448:LEU:HD12	1:A:4448:LEU:HA	1.81	0.42
1:A:1351:TRP:CH2	1:A:1400:VAL:HG13	2.55	0.41
1:A:2406:GLU:HG2	1:A:2409:ALA:HB2	2.02	0.41
1:A:2440:ALA:HB3	1:A:2502:LEU:HD12	2.02	0.41
1:A:2446:ILE:HD11	1:A:2714:PRO:HG3	2.01	0.41
1:A:2789:GLN:HG3	1:A:2838:VAL:HG21	2.02	0.41
1:A:3150:VAL:HG13	1:A:3532:TRP:CE2	2.55	0.41
1:A:3638:VAL:HG23	1:A:3679:LEU:HD22	2.02	0.41
1:A:3767:ILE:HG13	1:A:3771:GLU:OE2	2.20	0.41
1:A:3100:GLU:HA	1:A:3130:TYR:CE1	2.55	0.41
1:A:3510:SER:OG	1:A:3553:LEU:HD11	2.20	0.41
1:A:1469:VAL:O	1:A:1473:TYR:HB2	2.20	0.41
1:A:1607:LEU:HA	1:A:1610:LYS:HD2	2.02	0.41
1:A:1803:LEU:HG	1:A:1807:LYS:HE3	2.02	0.41
1:A:2065:LEU:HD21	1:A:2134:GLN:HG2	2.01	0.41
1:A:2445:HIS:NE2	1:A:2449:LEU:HD22	2.35	0.41
1:A:2836:ARG:HB2	1:A:3091:LEU:HD11	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3589:ILE:N	1:A:3679:LEU:O	2.42	0.41
1:A:4432:ALA:O	1:A:4436:GLN:HG2	2.20	0.41
1:A:2458:LEU:O	1:A:2462:LEU:HG	2.21	0.41
1:A:2898:LYS:HE2	1:A:2898:LYS:HA	2.02	0.41
1:A:3122:VAL:HG21	1:A:3136:PRO:HB2	2.01	0.41
1:A:3781:THR:HG22	1:A:3785:GLU:OE1	2.19	0.41
1:A:2268:LEU:H	1:A:2268:LEU:HD23	1.85	0.41
1:A:2845:TRP:CE2	1:A:2849:ASN:ND2	2.88	0.41
1:A:3607:ARG:O	1:A:3632:PRO:HD2	2.20	0.41
1:A:3766:ILE:HD12	1:A:3766:ILE:HA	1.92	0.41
1:A:4269:LEU:HD23	1:A:4269:LEU:HA	1.90	0.41
1:A:1638:LEU:HA	1:A:1641:ILE:HG12	2.03	0.41
1:A:2135:GLU:O	1:A:2138:ILE:HG22	2.21	0.41
1:A:2203:TRP:CH2	1:A:2236:VAL:HG11	2.55	0.41
1:A:2465:ALA:HB2	1:A:2493:TYR:CD1	2.55	0.41
1:A:2472:TYR:HE1	1:A:2481:MET:HB2	1.85	0.41
1:A:3759:ARG:H	1:A:3759:ARG:HG3	1.64	0.41
1:A:4205:TYR:OH	1:A:4261:ASP:OD2	2.23	0.41
1:A:4243:LEU:O	1:A:4247:MET:HG3	2.21	0.41
1:A:1350:PRO:O	1:A:1354:VAL:HG23	2.21	0.41
1:A:4482:PHE:HE2	1:A:4486:ILE:HD11	1.86	0.41
1:A:1466:ILE:HG23	1:A:1500:HIS:NE2	2.36	0.41
1:A:1538:ILE:HG13	1:A:1539:ASP:N	2.35	0.41
1:A:1579:MET:HA	1:A:1582:VAL:HG12	2.03	0.41
1:A:1625:SER:CB	1:A:1699:ASN:HD21	2.32	0.41
1:A:2200:GLY:O	1:A:2204:VAL:HG23	2.21	0.41
1:A:2306:ASP:OD2	1:A:2676:THR:OG1	2.31	0.41
1:A:2446:ILE:HD11	1:A:2714:PRO:HB3	2.02	0.41
1:A:2802:TRP:CZ2	1:A:2829:ALA:HB2	2.56	0.41
1:A:3186:LEU:HD23	1:A:3186:LEU:HA	1.87	0.41
1:A:3508:LEU:HD13	1:A:3536:LEU:HD21	2.03	0.41
1:A:3510:SER:O	1:A:3514:ILE:HG12	2.21	0.41
1:A:3767:ILE:HA	1:A:3770:LEU:HG	2.03	0.41
1:A:3846:LEU:HB3	1:A:3855:ARG:NH1	2.36	0.41
1:A:3916:LEU:HD23	1:A:3916:LEU:HA	1.91	0.41
1:A:1390:LEU:HD23	1:A:1390:LEU:HA	1.90	0.41
1:A:1477:LEU:HB3	1:A:1485:ARG:HG3	2.03	0.41
1:A:2972:PHE:HE1	1:A:2976:LEU:HD11	1.86	0.41
1:A:3597:THR:O	1:A:3601:MET:HG2	2.21	0.41
1:A:3641:TYR:CD2	1:A:3692:LEU:HD12	2.56	0.41
1:A:3792:GLN:O	1:A:3796:THR:HG23	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4037:PRO:HB2	1:A:4118:PRO:HB2	2.02	0.41
1:A:4153:VAL:HG12	1:A:4157:MET:HE1	2.03	0.41
1:A:4324:PRO:HB3	1:A:4638:ARG:HH12	1.83	0.41
1:A:1508:LYS:HG3	1:A:1513:TYR:CZ	2.55	0.40
1:A:1880:VAL:HG12	2:A:4701:ADP:N1	2.35	0.40
1:A:2138:ILE:HG13	1:A:2161:LEU:HD11	2.03	0.40
1:A:4495:ALA:HB1	1:A:4503:GLU:HG3	2.03	0.40
1:A:1665:ILE:HG22	1:A:1674:LEU:HB2	2.04	0.40
1:A:1849:LYS:HE2	1:A:1849:LYS:HB3	1.93	0.40
1:A:2030:ASP:OD2	1:A:4131:ASN:ND2	2.55	0.40
1:A:2072:PHE:CZ	1:A:2161:LEU:HD13	2.57	0.40
1:A:2086:TYR:CZ	1:A:2149:LEU:HD23	2.56	0.40
1:A:2491:GLN:HB3	1:A:2524:VAL:HG21	2.02	0.40
1:A:2090:LEU:O	1:A:2094:LYS:HG3	2.21	0.40
1:A:2577:HIS:HE1	1:A:2736:VAL:HA	1.87	0.40
1:A:2922:ILE:HG22	1:A:2950:VAL:HG11	2.04	0.40
1:A:1477:LEU:HB3	1:A:1485:ARG:CG	2.52	0.40
1:A:1678:SER:HB2	1:A:1872:TYR:OH	2.21	0.40
1:A:3506:ASP:OD1	1:A:3544:ARG:HG3	2.22	0.40
1:A:4087:ALA:HB1	1:A:4092:ARG:O	2.21	0.40
1:A:1451:LEU:HD12	1:A:3656:THR:HG21	2.04	0.40
1:A:2962:LYS:CE	1:A:3665:GLY:H	2.35	0.40
1:A:2972:PHE:CZ	1:A:3008:MET:HE3	2.56	0.40
1:A:3835:ILE:O	1:A:3839:VAL:HG23	2.22	0.40
1:A:4086:THR:HA	1:A:4089:LYS:NZ	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	3035/4646 (65%)	2967 (98%)	68 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2706/4125 (66%)	2705 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3078	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2416	GLN
1	A	2577	HIS
1	A	2588	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\# Z > 2$
2	ADP	A	4701	-	24,29,29	0.85	0	29,45,45	1.24	2 (6%)
3	ATP	A	4702	4	28,33,33	0.70	0	34,52,52	0.59	1 (2%)
2	ADP	A	4703	-	24,29,29	0.87	0	29,45,45	1.25	2 (6%)
2	ADP	A	4704	-	24,29,29	0.85	0	29,45,45	1.25	2 (6%)

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	-	-	3/12/32/32	0/3/3/3
3	ATP	A	4702	4	-	3/18/38/38	0/3/3/3
2	ADP	A	4703	-	-	5/12/32/32	0/3/3/3
2	ADP	A	4704	-	-	4/12/32/32	0/3/3/3

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4701	ADP	N3-C2-N1	-3.85	123.45	128.67
2	A	4704	ADP	N3-C2-N1	-3.73	123.61	128.67
2	A	4703	ADP	N3-C2-N1	-3.69	123.67	128.67
2	A	4704	ADP	C4-C5-N7	-2.43	106.77	109.34
2	A	4703	ADP	C4-C5-N7	-2.42	106.78	109.34
3	A	4702	ATP	C5-C6-N6	2.33	123.86	120.31
2	A	4701	ADP	C4-C5-N7	-2.31	106.90	109.34

There are no chirality outliers.

All (15) torsion outliers are listed below:

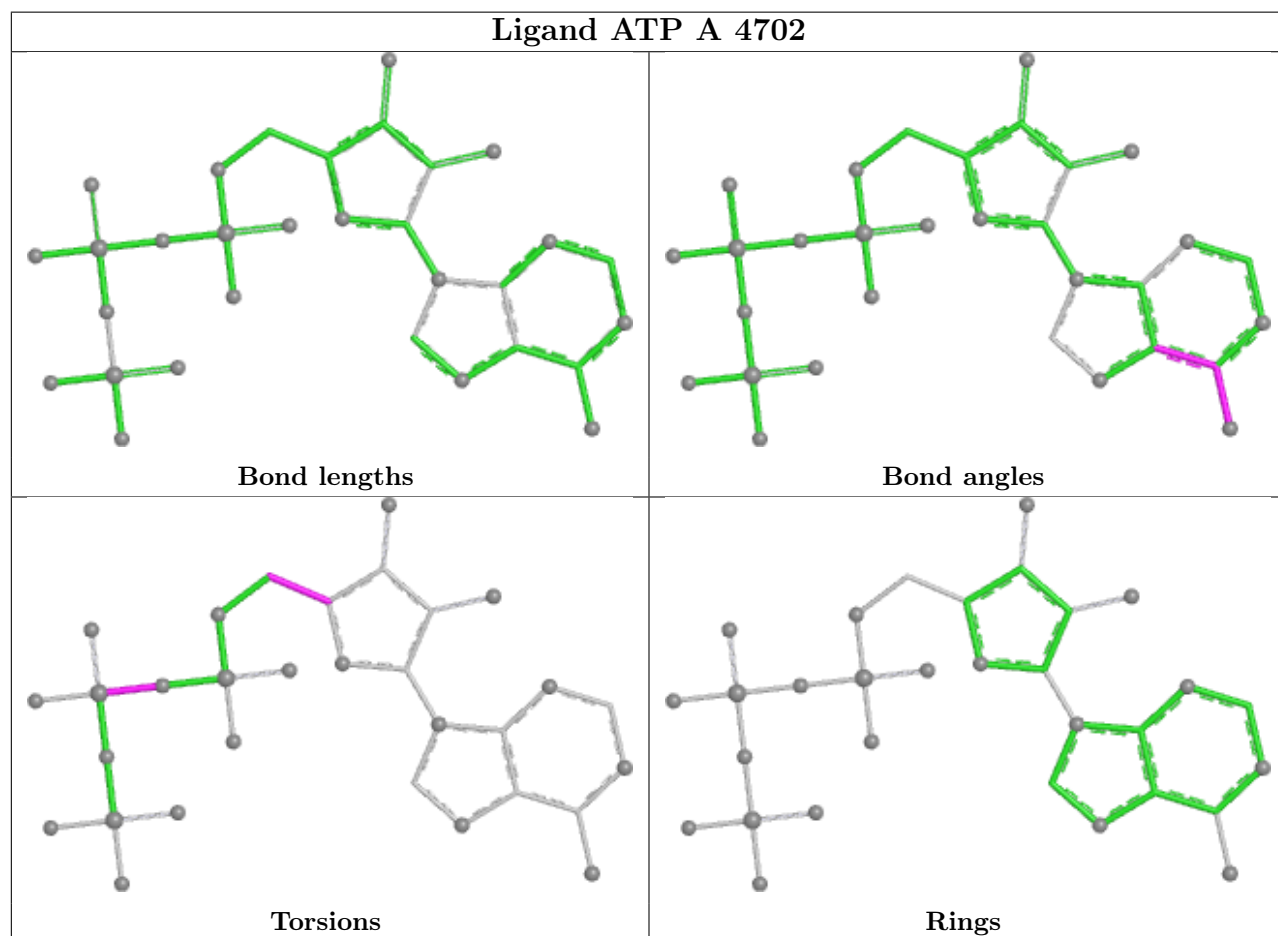
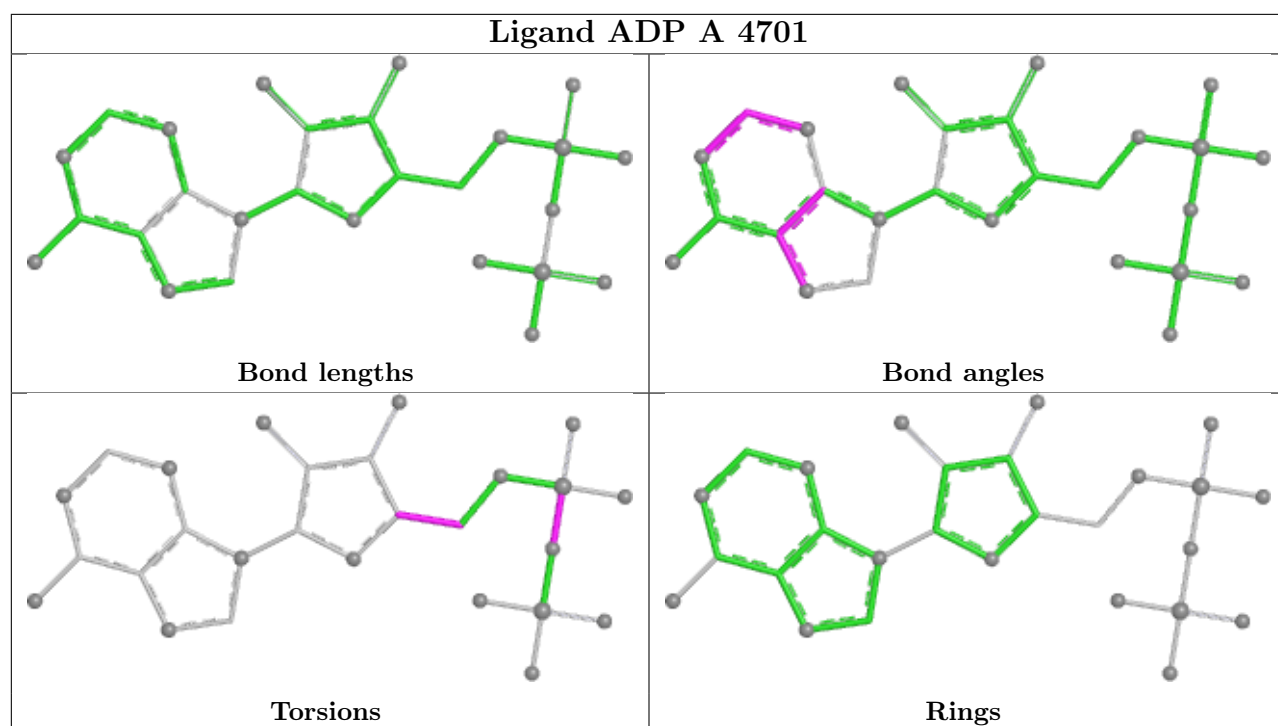
Mol	Chain	Res	Type	Atoms
2	A	4703	ADP	C5'-O5'-PA-O1A
2	A	4703	ADP	C5'-O5'-PA-O2A
2	A	4703	ADP	C5'-O5'-PA-O3A
2	A	4704	ADP	C5'-O5'-PA-O2A
2	A	4704	ADP	C5'-O5'-PA-O3A
2	A	4704	ADP	C3'-C4'-C5'-O5'
2	A	4704	ADP	O4'-C4'-C5'-O5'
3	A	4702	ATP	O4'-C4'-C5'-O5'
2	A	4701	ADP	PB-O3A-PA-O1A
2	A	4703	ADP	O4'-C4'-C5'-O5'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

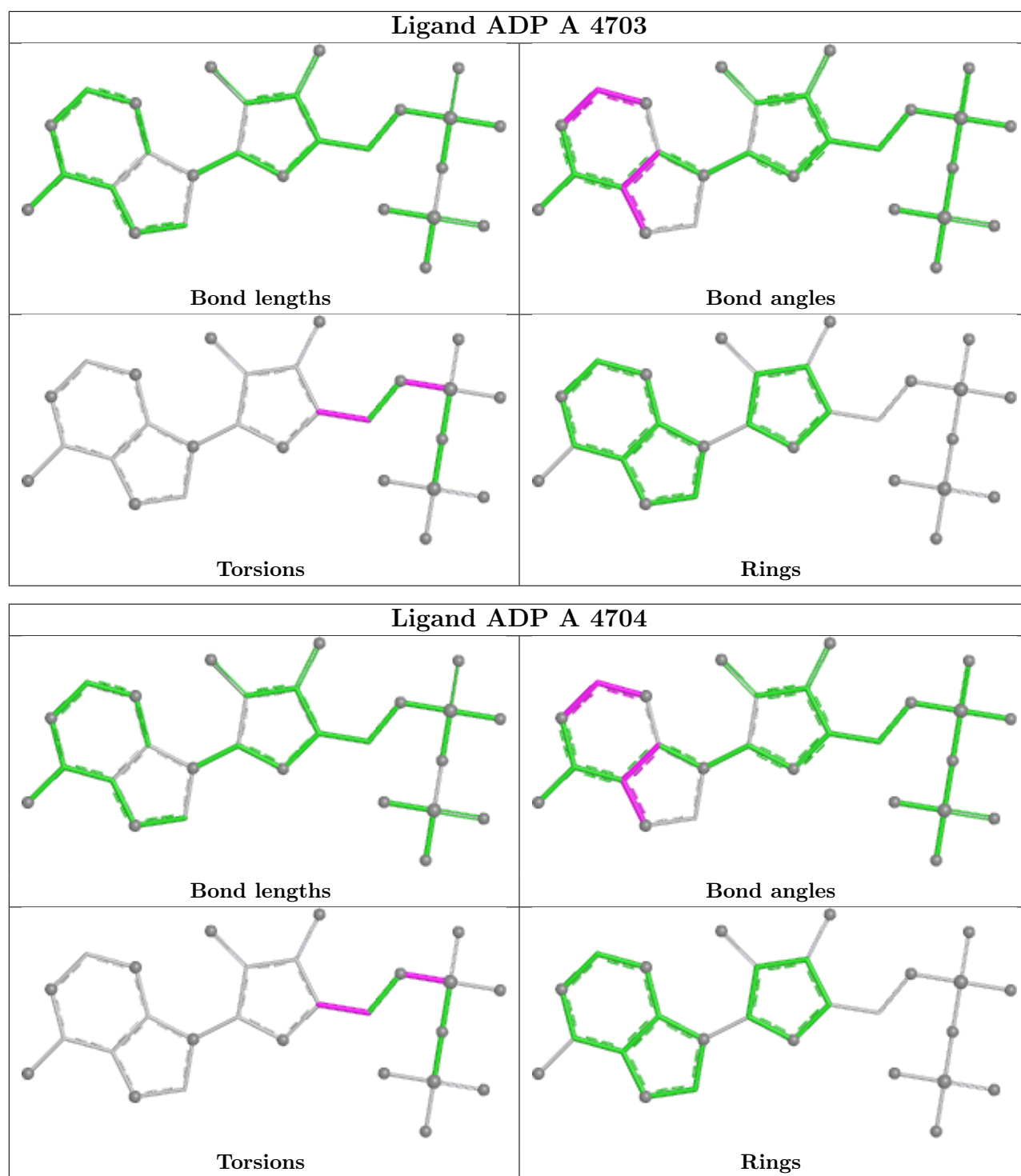
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4701	ADP	1	0
3	A	4702	ATP	2	0
2	A	4704	ADP	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

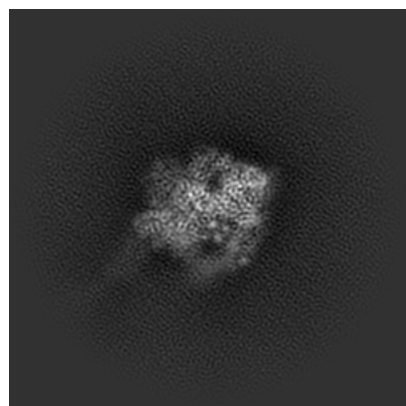
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44713. These allow visual inspection of the internal detail of the map and identification of artifacts.

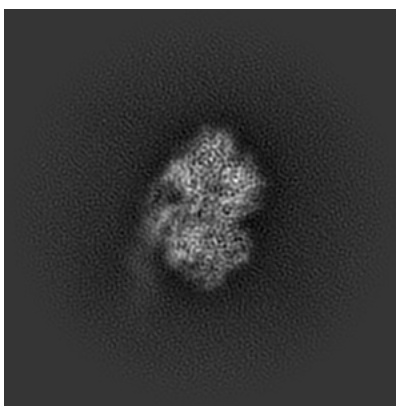
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

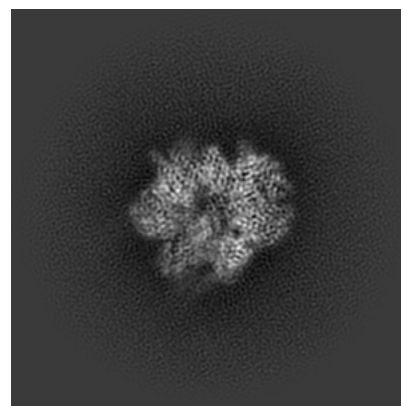
6.1.1 Primary map



X

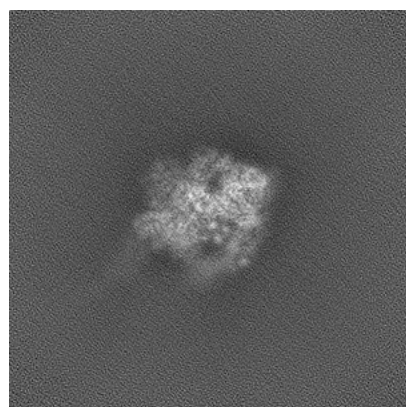


Y

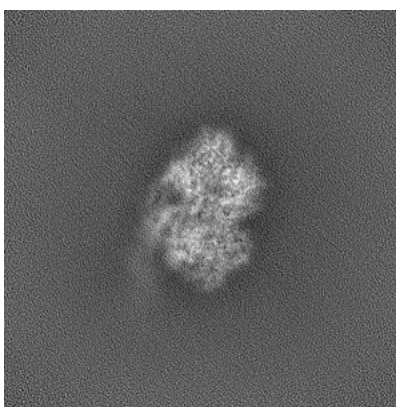


Z

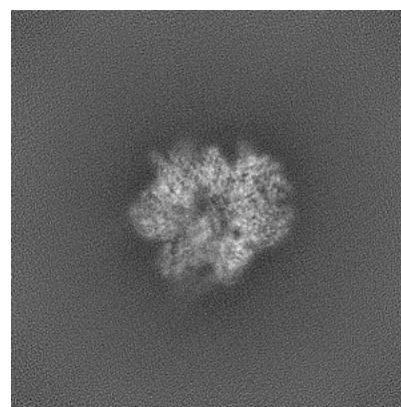
6.1.2 Raw map



X



Y

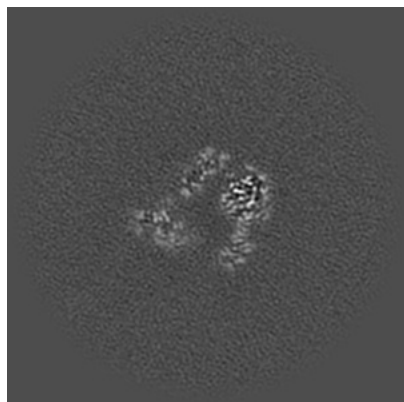


Z

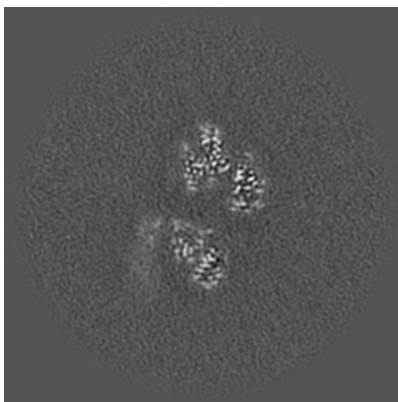
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

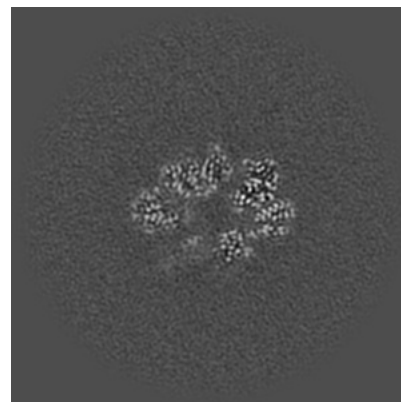
6.2.1 Primary map



X Index: 160

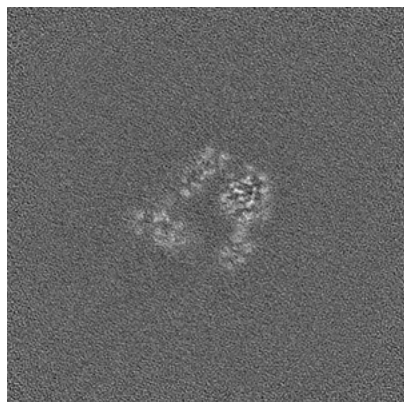


Y Index: 160

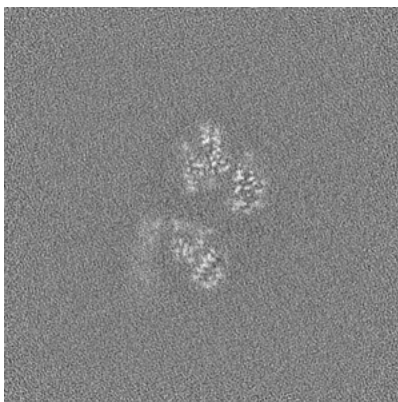


Z Index: 160

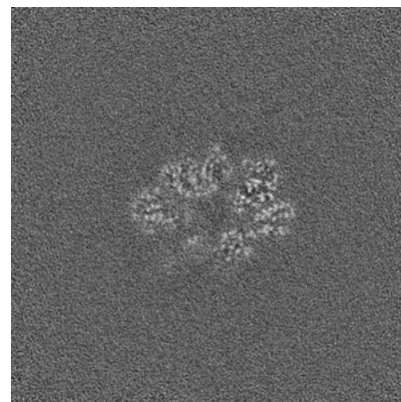
6.2.2 Raw map



X Index: 160



Y Index: 160

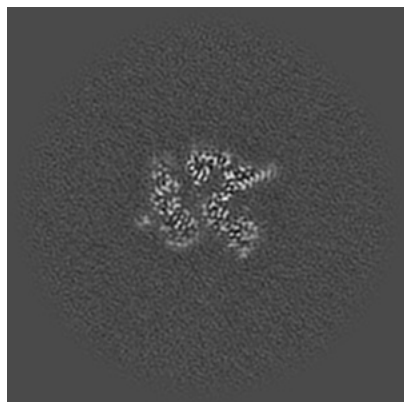


Z Index: 160

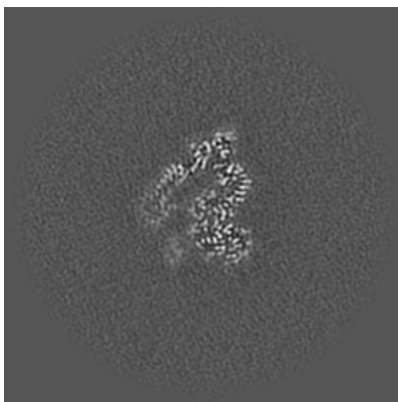
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

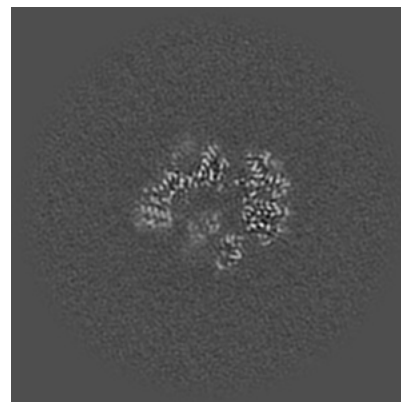
6.3.1 Primary map



X Index: 183

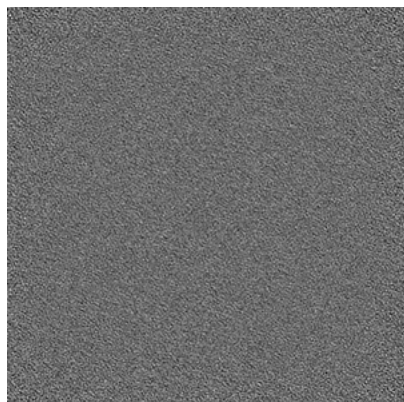


Y Index: 181

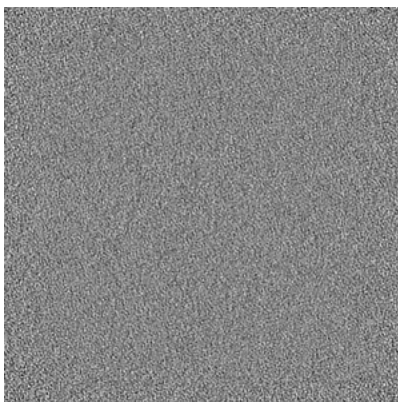


Z Index: 172

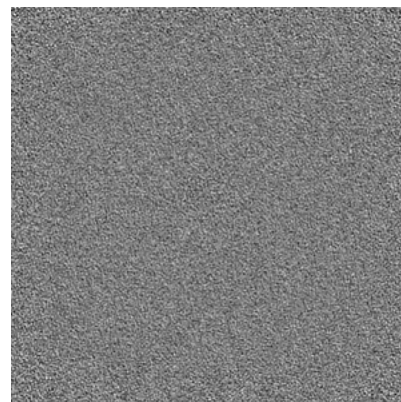
6.3.2 Raw map



X Index: 0



Y Index: 0

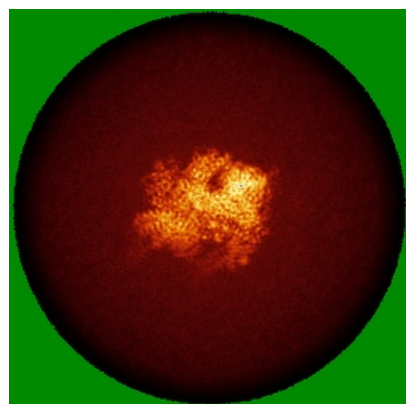


Z Index: 0

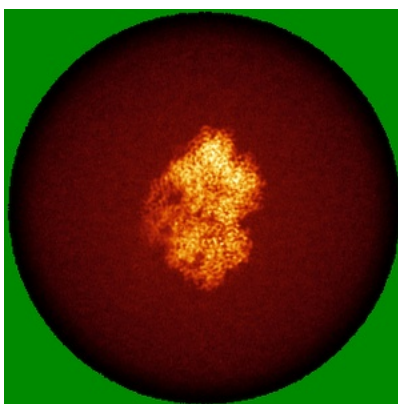
The images above show the largest variance slices of the map in three orthogonal directions.

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

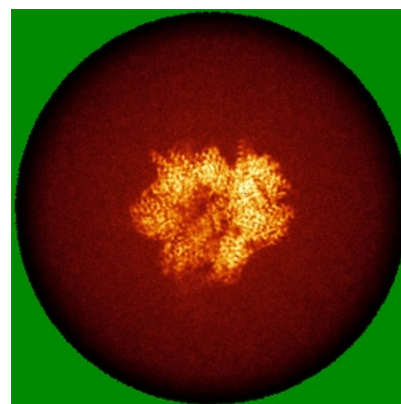
6.4.1 Primary map



X

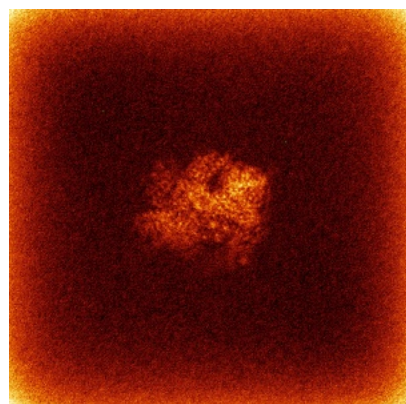


Y

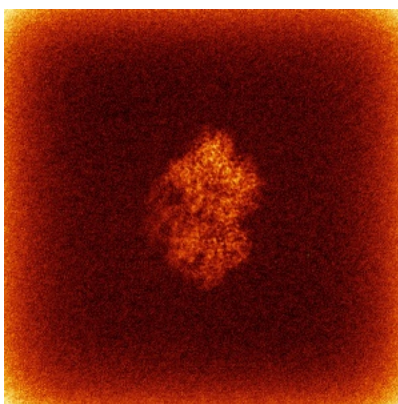


Z

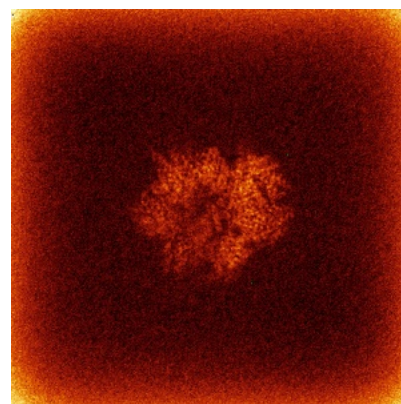
6.4.2 Raw map



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



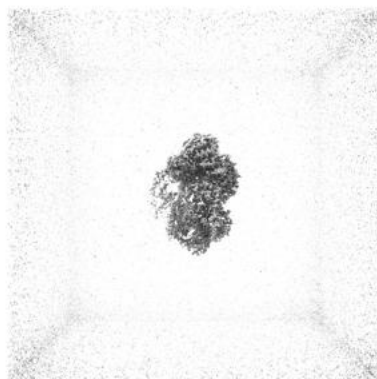
Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

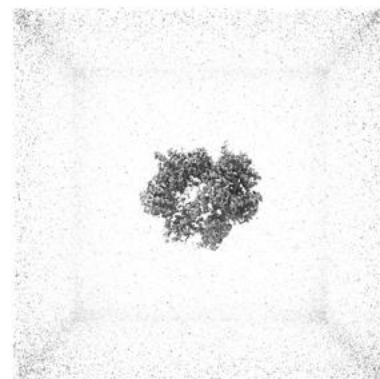
6.5.2 Raw map



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.

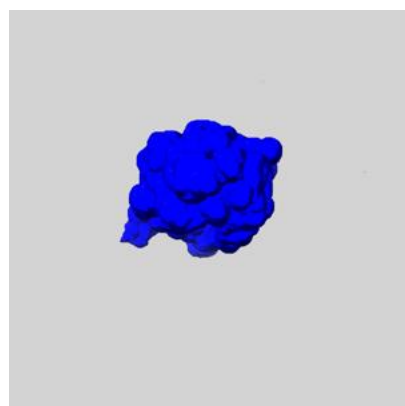
6.6 Mask visualisation [i](#)

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

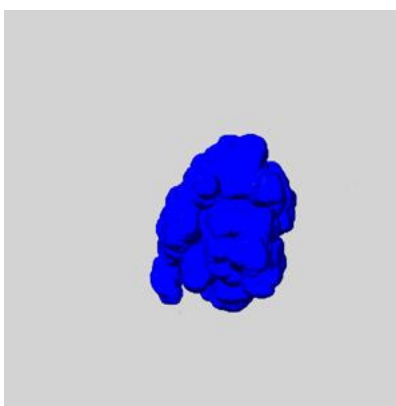
A mask typically either:

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

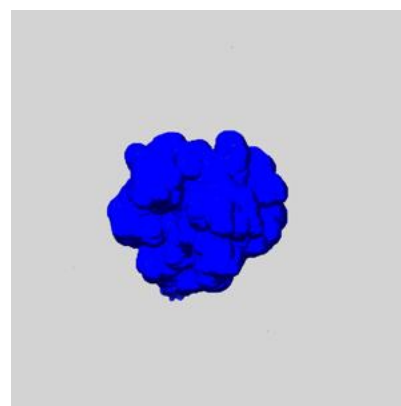
6.6.1 emd_44713_msk_1.map [i](#)



X



Y

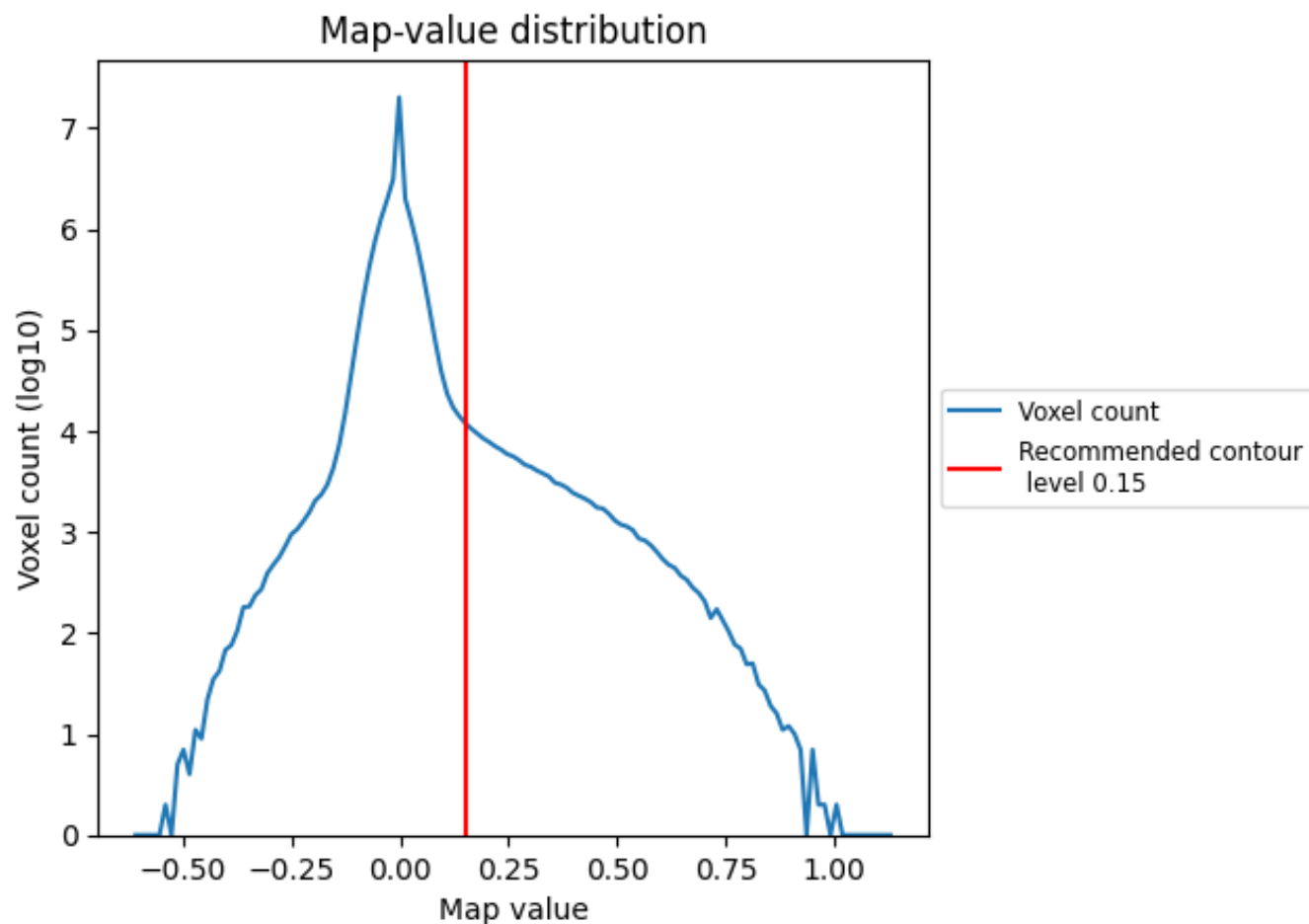


Z

7 Map analysis [i](#)

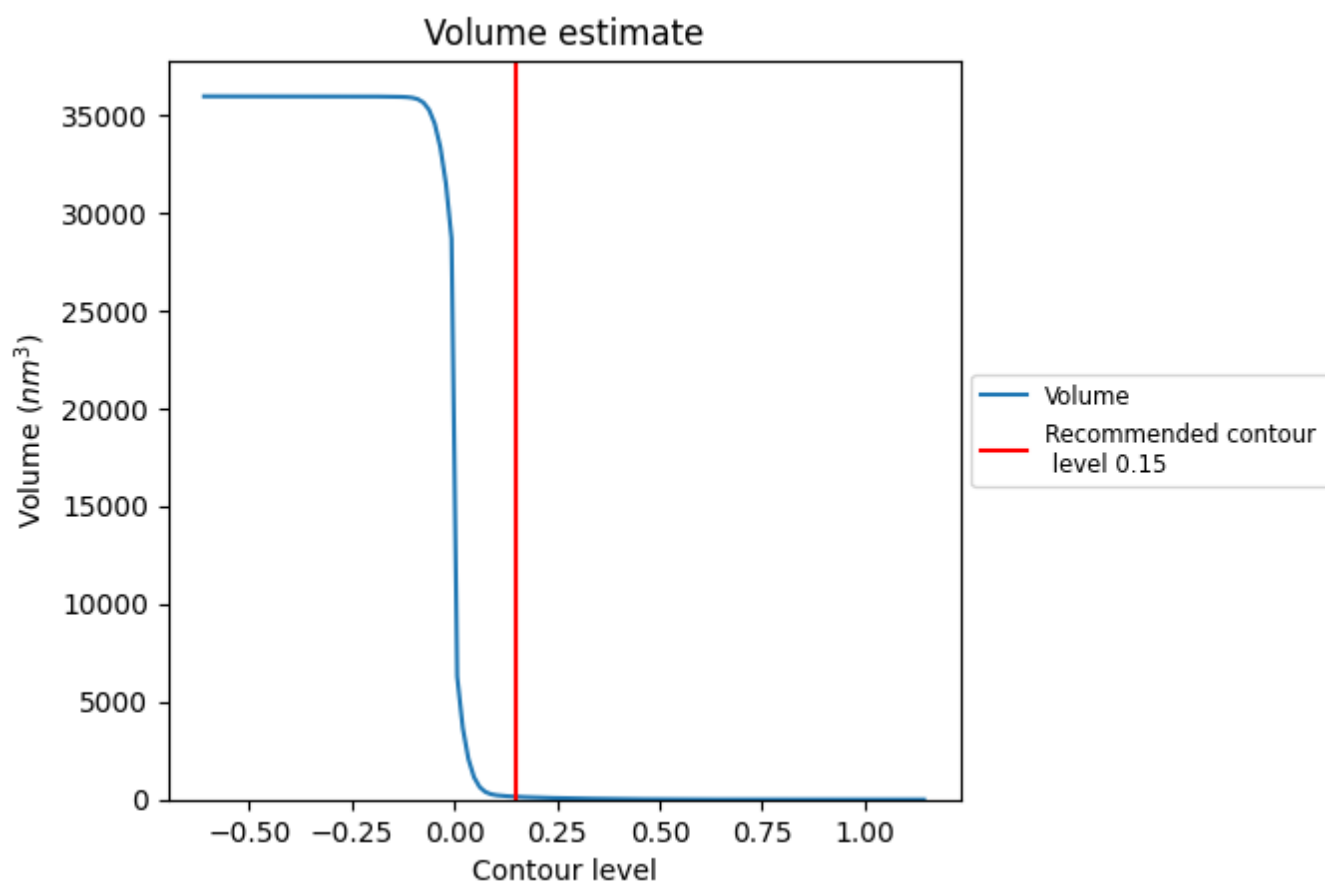
This section contains the results of statistical analysis of the map.

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.

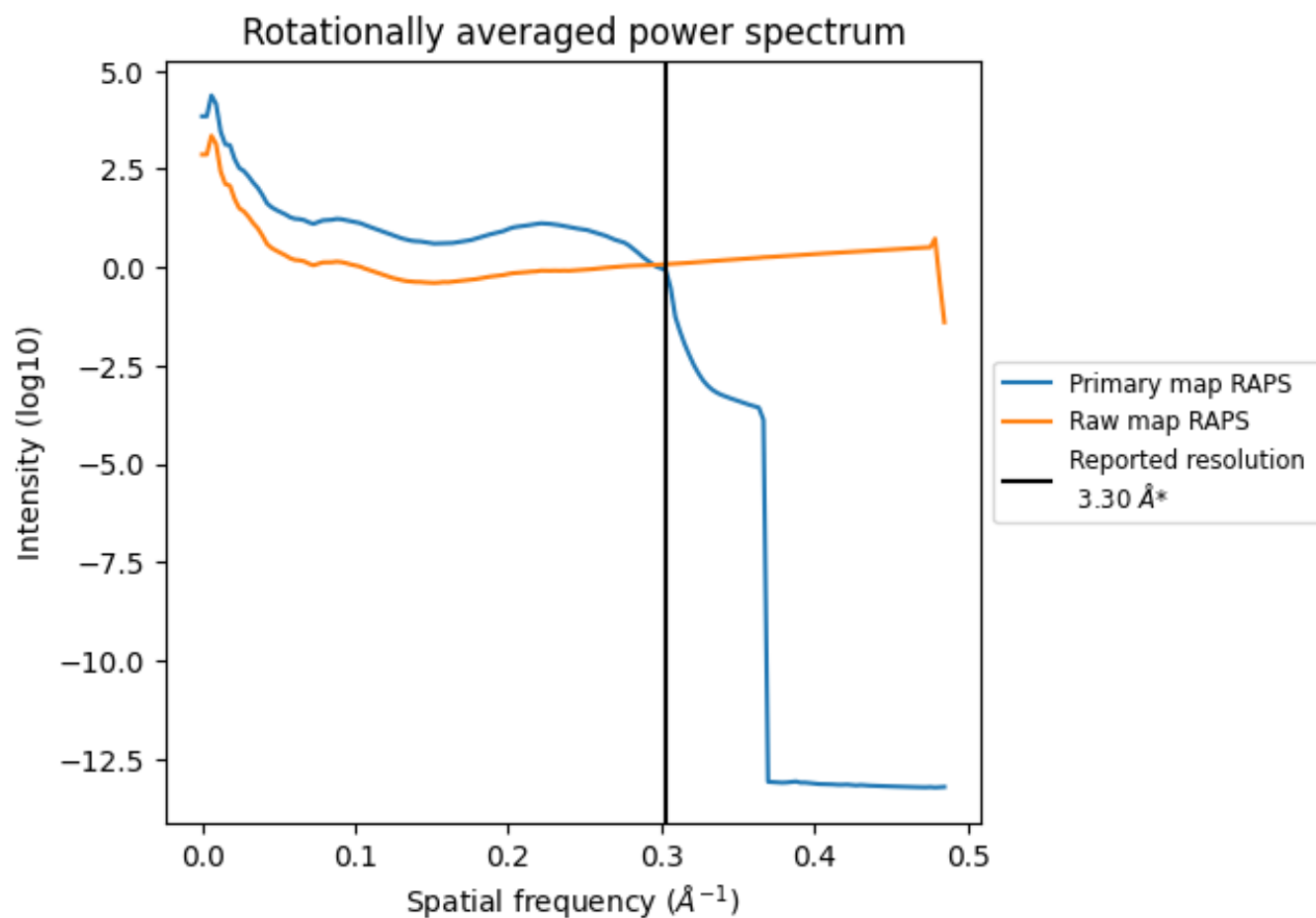
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 146 nm³; this corresponds to an approximate mass of 132 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 ⓘ

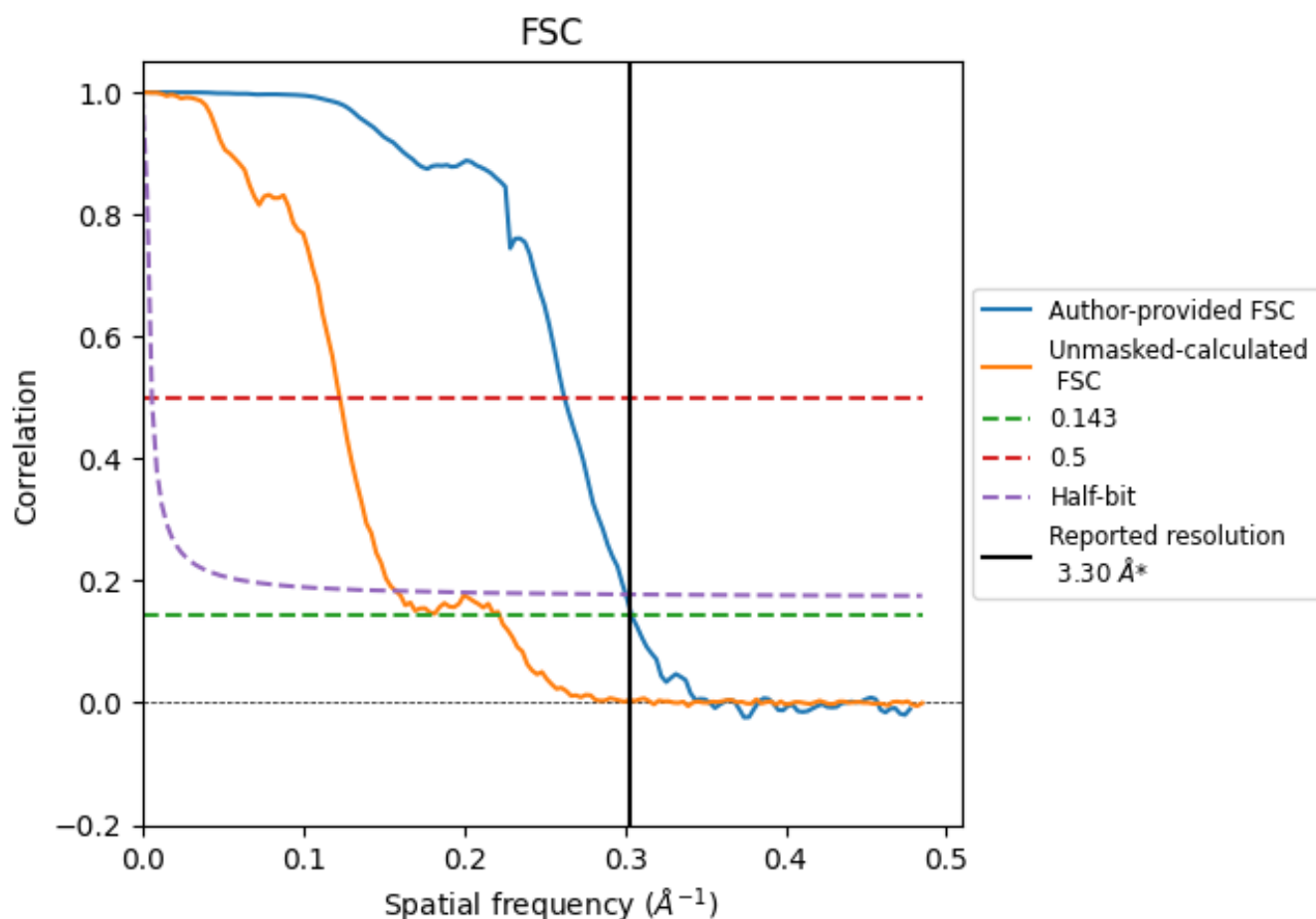


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 \AA^{-1}

8.2 Resolution estimates [i](#)

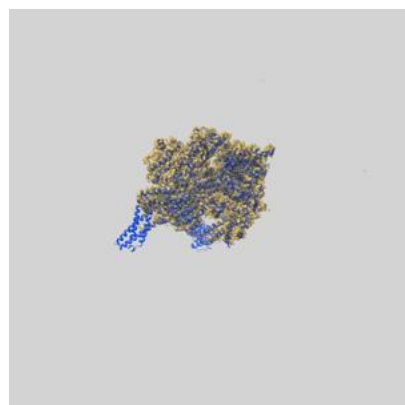
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.29	3.81	3.33
Unmasked-calculated*	4.50	8.14	6.34

*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 4.50 differs from the reported value 3.3 by more than 10 %

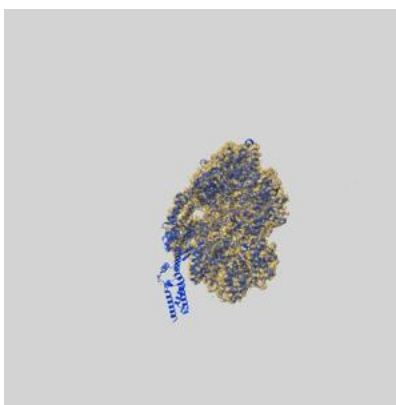
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44713 and PDB model 9BMW. Per-residue inclusion information can be found in section 3 on page 5.

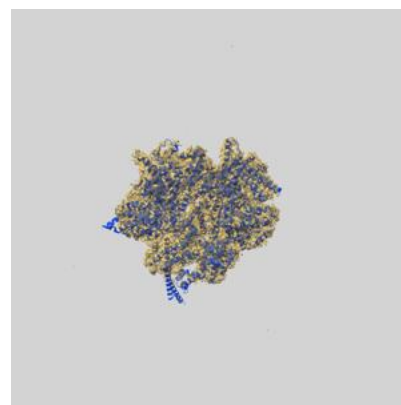
9.1 Map-model overlay [i](#)



X



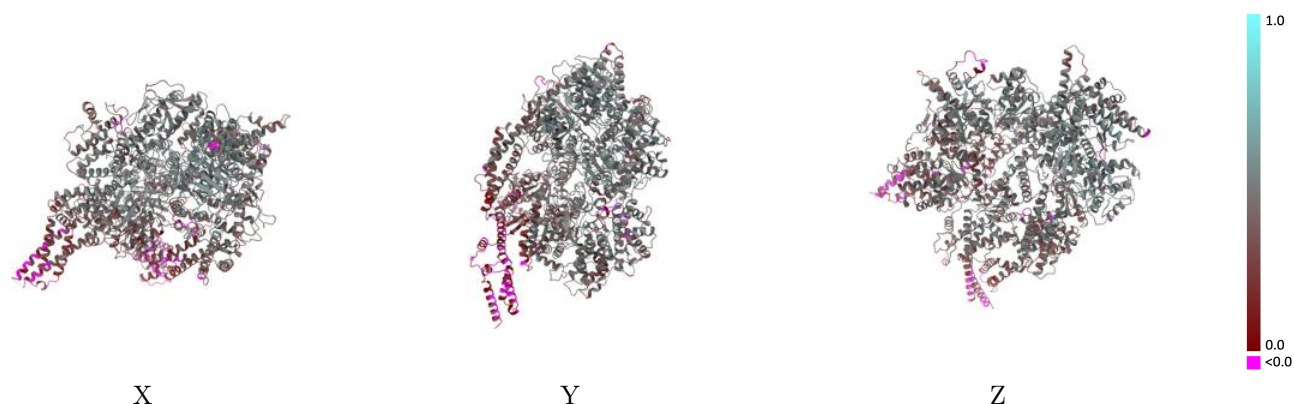
Y



Z

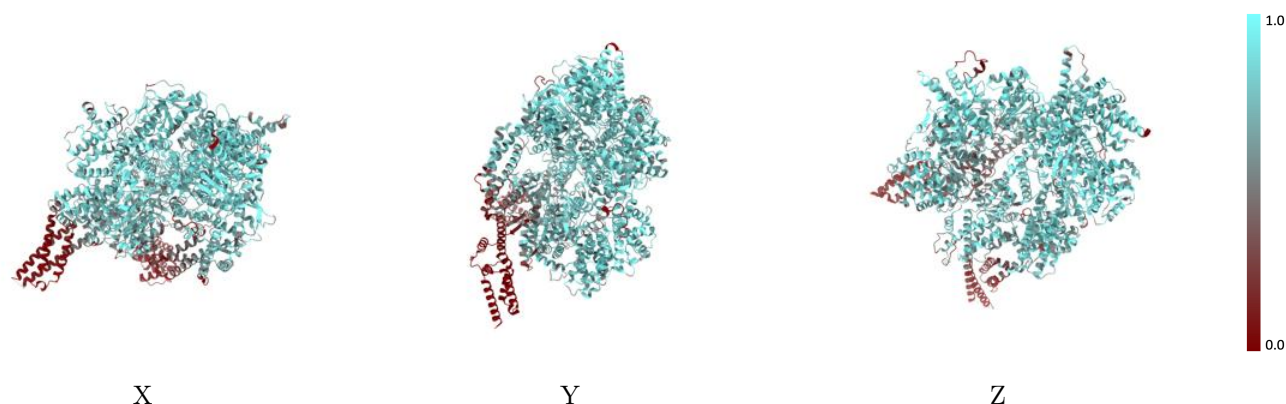
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



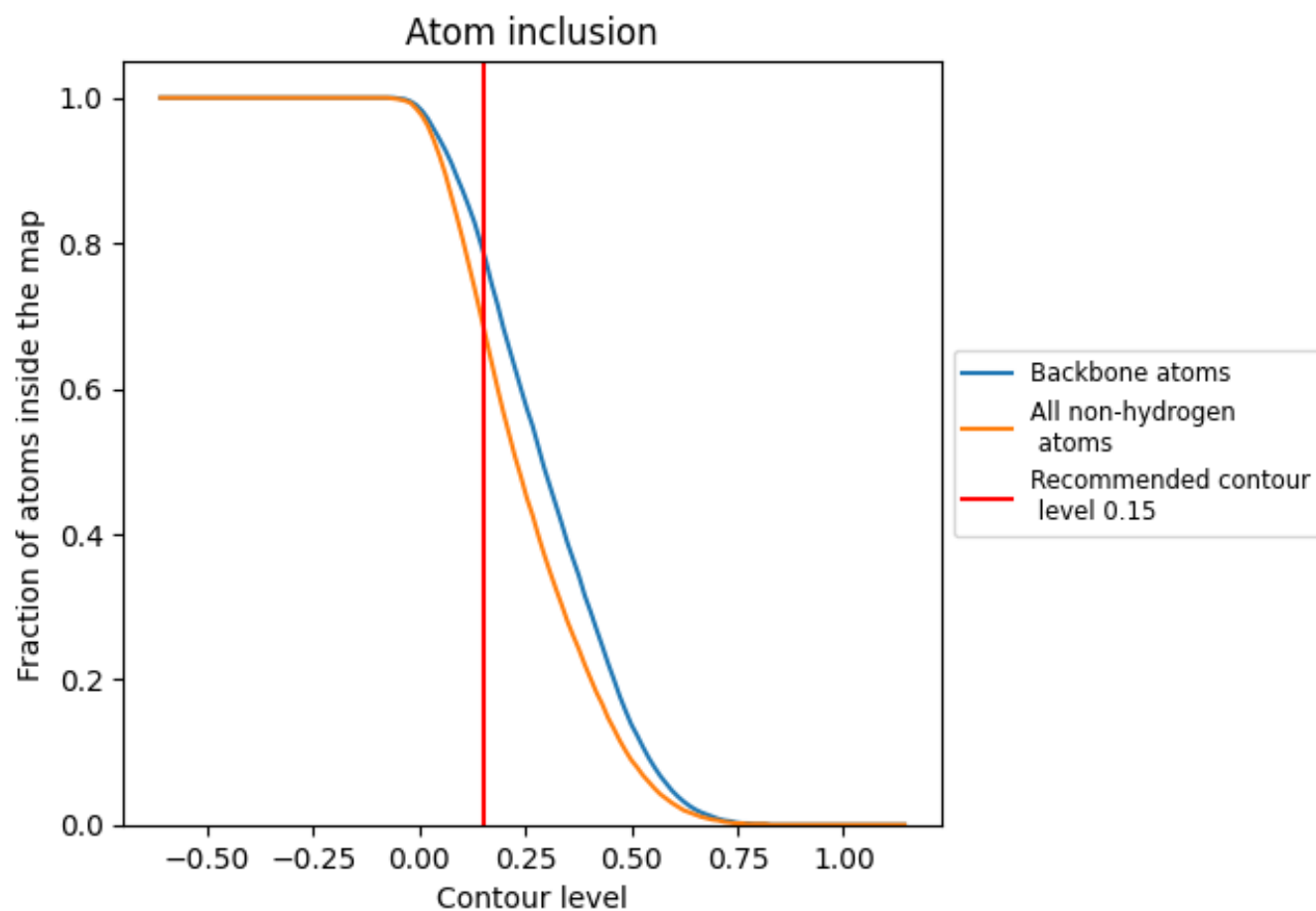
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 69% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6880	<div></div> 0.4110
A	<div></div> 0.6880	<div></div> 0.4110

