



## Full wwPDB EM Validation Report ⓘ

May 5, 2025 – 10:32 PM 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

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

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

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

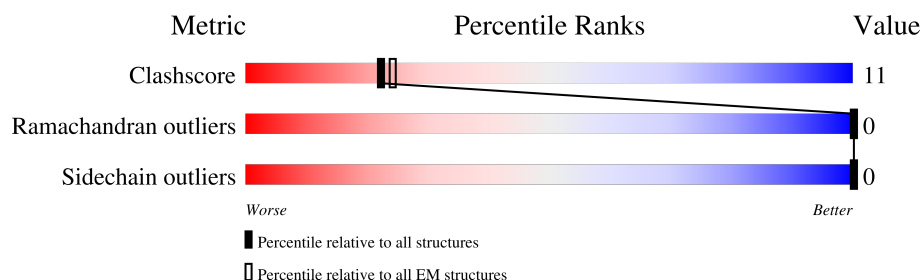
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.30 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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	4646	

## 2 Entry composition [i](#)

There are 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	C	N	O	P	0
			31	10	5	13	3	

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

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



Y1990	L1811	E1683	S1583	M1507	K1441	VAL	TRP	ARG	GLU	ALA	ASN	GLU	ASN	PHE
D1991	I1812	V1684	K1584	L1508	N1442	ALA	GLU	PHE	LEU	LEU	LYS	LEU	LYS	ASN
K1992	L1815	H1695	M1589	L1509	E1443	GLU	GLU	PHE	THR	THR	GLN	ASP	ASP	PHE
T1993	V1816	L1698	D1590	S1510	A1444	LEU	LEU	GLN	THR	THR	GLN	MET	GLY	GLY
S1994	L1831	I1699	V1591	P1511	I1445	Q1327	VAL	PRO	ASN	PRO	ASN	ILE	GLY	VAL
A1995	N1832	M1698	L1592	V1512	V1446	D1328	THR	TRP	VAL	ASP	GLY	VAL	GLY	VAL
M2018	M1842	E1700	N1593	Y1513	K1447	L1329	GLY	LEU	THR	GLY	ASP	ILE	ILE	ASP
N2019	L1843	W1701	I1594	K1514	D1448	K1330	ASN	TYR	LEU	ARG	PRO	ILE	GLY	LEU
G2020	F1844	L1713	G1595	V1515	V1449	G1331	ARG	ASP	GLU	THR	ALA	GLY	GLY	LEU
G2021	Y1845	L1717	G1596	F1516	L1450	V1332	PRO	ASN	LEU	PHE	LEU	VAL	VAL	ILE
THR				E1517	L1451	W1333	GLU	ILE	PRO	ASP	GLY	ARG	ARG	GLY
ALA				E1518	V1452	S1334	GLU	GLY	ILE	ASN	GLY	LEU	LEU	GLY
GLY				D1519	A1453	E1335	ALA	GLY	ALA	SER	GLY	ALA	ALA	GLY
ARG				A1520	Q1454	L1336	GLN	GLY	VAL	THR	GLY	LEU	LEU	ASP
S2026	L1857	V1724	L1604	L1521	G1455	S1337	ALA	GLY	ASP	VAL	ALA	ARG	ARG	LEU
D2030	A1864	E1725	L1607	S1522	E1456	K1338	LEU	PHE	TYR	VAL	LYS	LYS	LYS	GLY
K2033	Y1868	I1726	L1607	W1523	M1457	V1339	THR	PHE	ALA	THR	GLY	ALA	ALA	VAL
L2039	G1728	F1727	K1610	E1524	A1458	W1340	THR	ASP	PHE	GLY	THR	THR	THR	ARG
A2040	K1729	K1627	I1611	D1525	L1459	E1341	GLY	ILE	THR	VAL	VAL	VAL	VAL	GLY
M2041	W1741	F1627	R1623	K1526	E1460	Q1342	LYS	ARG	ALA	ASP	GLY	GLY	GLY	THR
D2045	K1744	S1625	S1624	L1527	E1461	I1343	PHE	ARG	VAL	VAL	VAL	VAL	VAL	LEU
I2049	Y1745	F1626	S1624	M1528	A1462	D1344	LYS	LYS	TRP	TRP	TRP	TRP	TRP	GLY
V2052	Q1748	L1636	V1632	W1537	E1466	Q1345	ILE	ILE	VAL	VAL	VAL	VAL	VAL	MET
M2053	L1749	L1637	G1633	I1538	I1466	M1346	THR	ILE	GLN	GLN	GLN	GLN	GLN	LEU
L2054	V1750	L1638	D1634	D1539	R1467	K1347	VAL	GLN	VAL	VAL	VAL	VAL	VAL	LEU
S2055	M1769	E1635	G1634	W1536	E1468	Q1349	GLY	GLN	GLY	GLY	GLY	GLY	GLY	GLY
S2056	G1770	L1636	E1635	V1537	E1469	P1350	ASP	ALA	LYS	ASN	ASN	ASN	ASN	ASP
L2065	G1771	L1637	L1636	W1537	W1470	W1351	VAL	ALA	LYS	LEU	LEU	LEU	LEU	LEU
A2066	G1772	L1638	L1637	I1538	Y1473	V1352	VAL	ALA	LYS	ASN	ASN	ASN	ASN	ASP
I2069	K1917	L1638	L1637	D1539	E1474	S1353	GLN	GLN	LYS	LYS	LYS	LYS	LYS	THR
G1920	G1920	I1641	I1641	Q1541	L1475	V1354	GLY	LYS	GLN	ASP	ASP	ASP	ASP	ALA
H1921	H1921	K1645	K1645	R1542	D1476	Q1355	ALA	ILE	LYS	TRP	TRP	TRP	TRP	ALA
Q1922	Q1922	N1646	N1646	R1543	L1477	P1356	VAL	VAL	GLY	MET	MET	MET	MET	GLN
L1927	L1927	V1647	V1647	Y1546	L1477	R1357	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA
L1928	L1928	L1650	L1650	L1547	N1482	K1358	THR	THR	THR	THR	THR	THR	THR	VAL
D1937	D1937	F1658	F1658	I1550	K1483	L1359	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
A1940	A1940	V1661	V1661	F1551	C1484	R1360	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
L1948	L1948	V1661	V1661	T1552	R1485	Q1361	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
W1954	W1954	I1665	I1665	G1553	L1486	N1362	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU
N1961	N1961	E1668	E1668	S1554	R1488	L1363	THR	THR	THR	THR	THR	THR	THR	THR
P1968	P1968	L1674	L1674	L1561	G1489	D1364	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
N1989	N1989	G1675	G1675	L1561	W1490	A1365	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
R2105	R2105	L1676	L1676	E1564	D1491	L1366	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
E2106	E2106	S1677	S1677	F1568	D1492	L1367	THR	THR	THR	THR	THR	THR	THR	THR
R2107	R2107	R1678	R1678	I1571	N1495	N1368	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU
K2110	K2110	R1679	R1679	A1577	K1496	Q1369	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
				L1578	V1497	L1370	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU
				K1579	K1498	K1371	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
				M1579	E1499	S1372	THR	THR	THR	THR	THR	THR	THR	THR
				K1580	H1500	F1373	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
				K1581	I1501	P1374	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU
				V1582	N1502	A1375	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
						R1376	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
						L1377	THR	THR	THR	THR	THR	THR	THR	THR
						R1378	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
						Q1379	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN
						Y1380	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN



I4619	F4620	E4625	I4626	A4627	T4628	E4629	E4630	D4631	S4634	E4637	R4638	V4642	E4646	F4482	R4485	I4486	L4489	I4492	A4495	E4503	L4504	K4505	H4508	L4511	G4512	G4513	V4528	T4547	S4548	Q4549	G4550	L4553	D4554	V4560	K4564	K4574	L4577	I4581	P4586	L4587	T4588	V4592	K4593	K4594	N4597	T4598	E4599	K4600	K4601	V4604	P4608	V4609					
ALA	GLU	THR	GLU	LYS	LYS	THR	THR	ASP	SER	THR	SER	THR	ALA	ALA	THR	GLU	LYS	THR	ASP	THR	SER	ASP	GLY	ARG	PRO	A4375	H4381	I4391	L4398	E4414	V4417	K4418	L4423	R4428	A4432	D4433	V4434	V4435	Q4436	V4437	C4438	K4442	K4443	Q4444	T4445	L4448	R4449	I4452	L4460	P4461	H4466	V4475	I4476				
D4217	D4220	D4224	D4225	T4226	P4239	L4243	M4247	F4260	D4261	L4264	T4267	F4268	L4269	E4270	R4271	H4291	M4296	P4297	D4298	E4303	E4304	F4305	V4306	V4309	P4324	M4325	M4326	L4332	M4339	M4343	L4344	K4345	K4346	Q4347	M4348	L4349	GLU	ASP	GLU	ASP	ASP	LEU	ALA														
R4098	V4099	G4104	W4105	L4106	M4107	Q4108	K4112	L4116	Q4117	P4118	H4119	A4120	R4123	T4127	M4128	N4131	P4132	K4133	V4134	R4140	T4144	V4153	K4154	M4157	L4158	R4168	R4176	Y4180	F4181	L4182	L4183	A4184	W4185	T4189	E4192	R4193	S4202	Y4205	E4206	A4215	G4216																
E3967	I3835	S3975	E3976	E3977	F3996	D3999	R4000	M4007	L4013	F3864	Q3865	N3869	R3870	R3873	L3886	K3891	V3896	L3909	R3910	E3913	I3914	V3915	L3916	S3917	A3918	Q3919	K3923	I3924	E3933	K3934	V3935	V3936	R3937	K3945	D3946	L3947	I3948	A3949	K3950	V3951	Q3952	A3953	D3954	E3955													
V3756	K3757	G3758	R3759	L3760	L3761	D3762	D3763	D3764	T3765	I3766	I3767	T3768	T3769	L3770	E3771	N3772	L3773	K3774	R3775	E3776	A3777	A3778	E3779	V3780	R3782	K3783	V3784	E3785	E3786	T3787	D3788	I3789	V3790	M3791	Q3792	E3793	V3794	E3795	T3796	Y3801	L3802	P3803	S3809	S3810	I3811	F3812	F3813	T3814	M3815	E3816	S3817	L3818	L3824	S3828			
D3668	I3669	D3670	L3671	L3679	S3680	T3681	R3682	D3683	P3689	P3690	D3691	L3692	C3693	S3694	N3700	R3705	L3708	V3716	P3722	D3723	V3724	E3726	K3727	R3728	S3729	D3730	L3731	L3732	K3733	L3734	Q3735	G3736	E3737	F3738	Q3739	L3740	R3741	L3742	R3743	Q3744	L3745	E3746	K3747	S3748	L3749	L3750	Q3751	A3752	L3753	N3754	E3755						
F3496	K3497	N3498	Q3499	M3500	T3502	G3505	D3506	C3507	L3508	S3510	T3514	A3515	Y3516	A3517	G3518	W3522	S3523	H3534	H3535	L3536	Q3537	N3540	I3541	F3542	Q3543	R3544	T3545	D3546	E3551	Y3552	L3553	S3554	N3555	A3556	D3557	E3558	R3559	L3560	R3561	W3562	Q3563	A3564	L3567	P3568	A3569	N3576	M3579	L3580	K3581								
MET	ILE	ARG	ASP	LEU	GLU	ALA	SER	ILE	ALA	ALA	TYR	LYS	GLU	TYR	VAL	LEU	ILE	SER	GLU	ALA	GLN	ALA	ILE	LYS	ALA	ASP	LEU	ALA	ALA	VAL	GLU	A3470	K3471	V3472	K3473	R3474	S3475	T3476	A3477	L3478	L3479	K3480	S3481	L3482	S3483	A3484	E3485	R3486	E3487	R3488	K3489	E3490	K3491	T3492	S3493	E3494	T3495



## 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 ( $\text{\AA}$ )	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 ( $\text{\AA}$ )	1.0312, 1.0312, 1.0312	Depositor

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ATP, 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	0.16	0/25022	0.34	1/33900 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	1409	LYS	CB-CA-C	-5.03	110.39	117.23

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	24503	0	24573	550	0
2	A	81	0	36	4	0
3	A	31	0	12	2	0
4	A	2	0	0	0	0
All	All	24617	0	24621	550	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 (550) 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:3601:MET:HE2	1:A:3634:LEU:HD23	1.64	0.79
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:4153:VAL:HG12	1:A:4157:MET:HE2	1.69	0.75
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:2755:MET:HE1	1:A:2803:VAL:HG13	1.70	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:1961:ASN:HB3	1:A:2018:MET:HE1	1.74	0.69
1:A:2386:PRO:HA	1:A:2416:GLN:HE22	1.56	0.69
1:A:1769:MET:HE2	1:A:1775:ALA:HA	1.74	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:1486:LEU:HD23	1:A:1579:MET:HE3	1.76	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:2189:MET:HE1	1:A:2239:LYS:HD3	1.77	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:2053:MET:HE1	1:A:2094:LYS:HE3	1.78	0.65
1:A:3518:GLY:HA3	1:A:3579:MET:HE1	1.77	0.65
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1857:LEU:HD22	1:A:1868:TYR:HB2	1.80	0.64
1:A:4631:ASP:O	1:A:4634:SER:OG	2.16	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
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:4339:MET:SD	1:A:4343:MET:HE2	2.40	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:3030:MET:HE1	1:A:3050:LEU:HB2	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:2747:ILE:O	1:A:2750:THR:OG1	2.21	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:4104:GLY:HA2	1:A:4107:MET:HE3	1.86	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:2370:SER:H	1:A:2373:MET:HE2	1.71	0.55
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2603:MET:HE1	2:A:4703:ADP:C4	2.42	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
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:1744:LYS:C	1:A:1745:TYR:HD2	2.16	0.53
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:2773:MET:HE2	1:A:2799:MET:SD	2.49	0.53
1:A:3194:LEU:HD22	1:A:3500:MET:HE3	1.91	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:2603:MET:HE1	2:A:4703:ADP:C5	2.44	0.52
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:4202:SER:OG	1:A:4261:ASP:OD2	2.24	0.51
1:A:1476:ASP:HB3	1:A:1488:ARG:NH1	2.26	0.51
1:A:1888:CYS:HB2	1:A:2041:MET:HE1	1.92	0.51
1:A:2039:LEU:HD23	1:A:2041:MET:HE2	1.92	0.51
1:A:2369:LEU:HD12	1:A:2373:MET:HE3	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1842:MET:HE3	1:A:1922:GLN:HG2	1.92	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: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:3612:THR:HG22	1:A:3619:PHE:HD1	1.78	0.49
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:4205:TYR:OH	1:A:4261:ASP:OD2	2.23	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2444:GLU:HG3	1:A:2510:MET:HE1	1.96	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:3967:GLU:HG2	1:A:4007:MET:CE	2.45	0.46
1:A:1363:LEU:HD11	1:A:1435:TRP:CH2	2.50	0.46
1:A:2370:SER:N	1:A:2373:MET:HE2	2.30	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
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:2936:ILE:HG21	1:A:3093:TRP:CZ3	2.50	0.45
1:A:2972:PHE:CZ	1:A:3008:MET:HE3	2.51	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:2221:MET:HE1	1:A:2348:LEU:HD21	1.98	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:4182:LEU:HD21	1:A:4296:MET:HE1	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:4020:ILE:HG23	1:A:4021:MET:HE3	1.99	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:2686:MET:HE2	1:A:2686:MET:HB3	1.62	0.45
1:A:1665:ILE:O	1:A:1674:LEU:N	2.49	0.45
1:A:2953:MET:HE2	1:A:2953:MET:HB3	1.86	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
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:2683:ILE:HA	1:A:2686:MET:HE2	1.99	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:1725:GLU:O	1:A:1729:LYS:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:3113:MET:HE2	1:A:3115:LEU:HD11	1.99	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:4128:MET:HE1	1:A:4134:VAL:HG11	1.99	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2755:MET:CE	1:A:2803:VAL:HG13	2.45	0.43
1:A:3817:SER:C	1:A:4346:MET:HE1	2.43	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:2972:PHE:HZ	1:A:3008:MET:HE3	1.84	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:3191:ARG:NE	1:A:3500:MET:HE2	2.34	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
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:2206:LYS:NZ	1:A:2363:TRP:O	2.41	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:1769:MET:HE1	1:A:1778:LEU:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2220:LEU:HD11	1:A:2342:MET:HE2	2.02	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:4055:VAL:HB	1:A:4095:MET:HE1	2.01	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: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
1:A:4037:PRO:HB2	1:A:4118:PRO:HB2	2.02	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

*Continued on next page...*



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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:4247:MET:HE2	1:A:4247:MET:HB3	1.90	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

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%)	2706 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1421	HIS
1	A	1440	GLN
1	A	1500	HIS
1	A	1593	ASN
1	A	1755	GLN
1	A	1850	GLN
1	A	1876	GLN
1	A	1894	GLN
1	A	1931	ASN
1	A	2130	ASN
1	A	2209	GLN
1	A	2217	ASN
1	A	2416	GLN
1	A	2577	HIS
1	A	2588	HIS
1	A	2621	ASN
1	A	2637	HIS
1	A	2685	GLN
1	A	2913	ASN
1	A	3197	GLN
1	A	3820	GLN
1	A	3845	ASN
1	A	4114	HIS
1	A	4506	ASN
1	A	4508	HIS
1	A	4573	ASN
1	A	4579	ASN

### 5.3.3 RNA ⓘ

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	4704	-	24,29,29	0.85	0	29,45,45	1.25	2 (6%)
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%)

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	4704	-	-	4/12/32/32	0/3/3/3
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

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

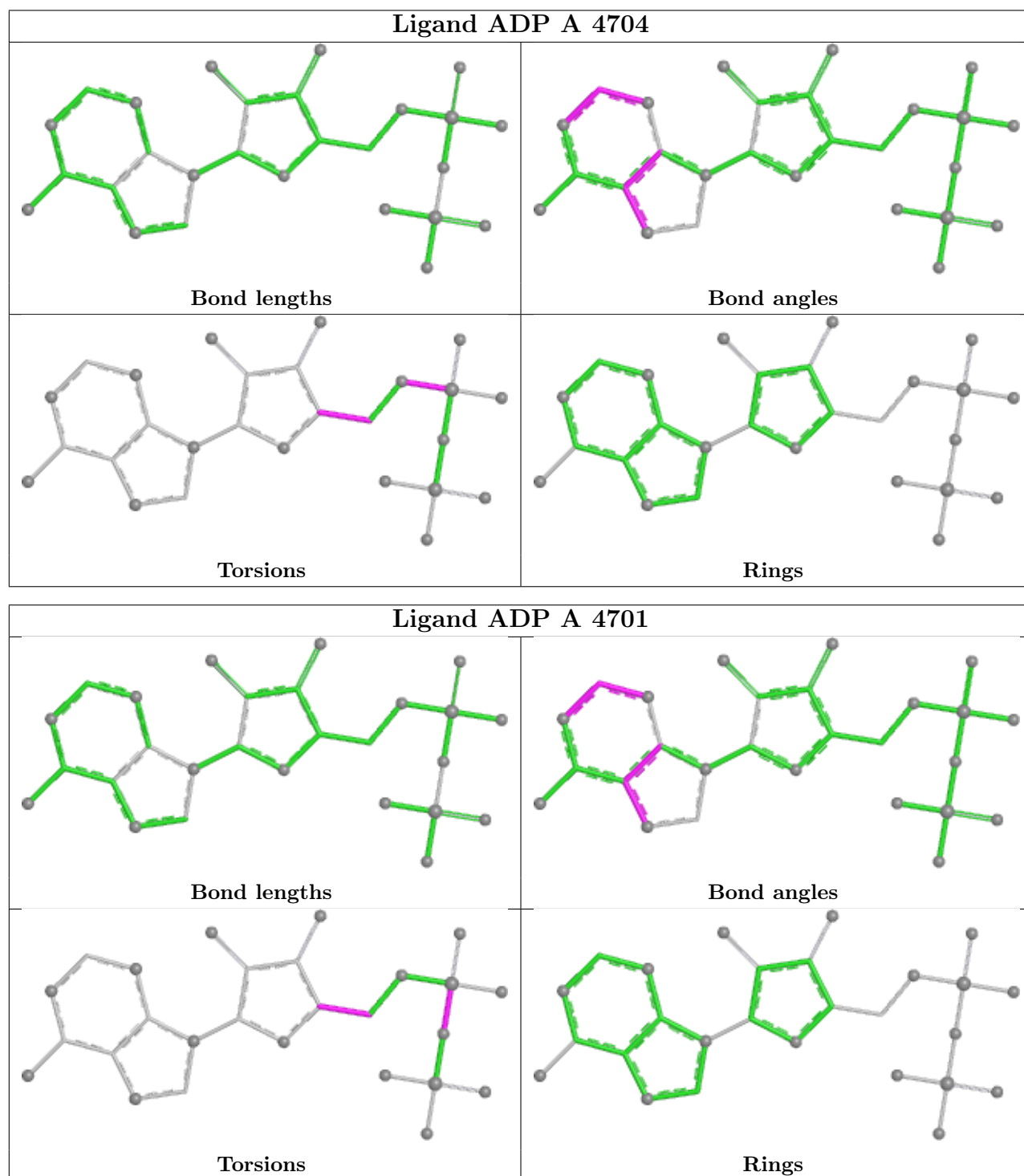
There are no ring outliers.

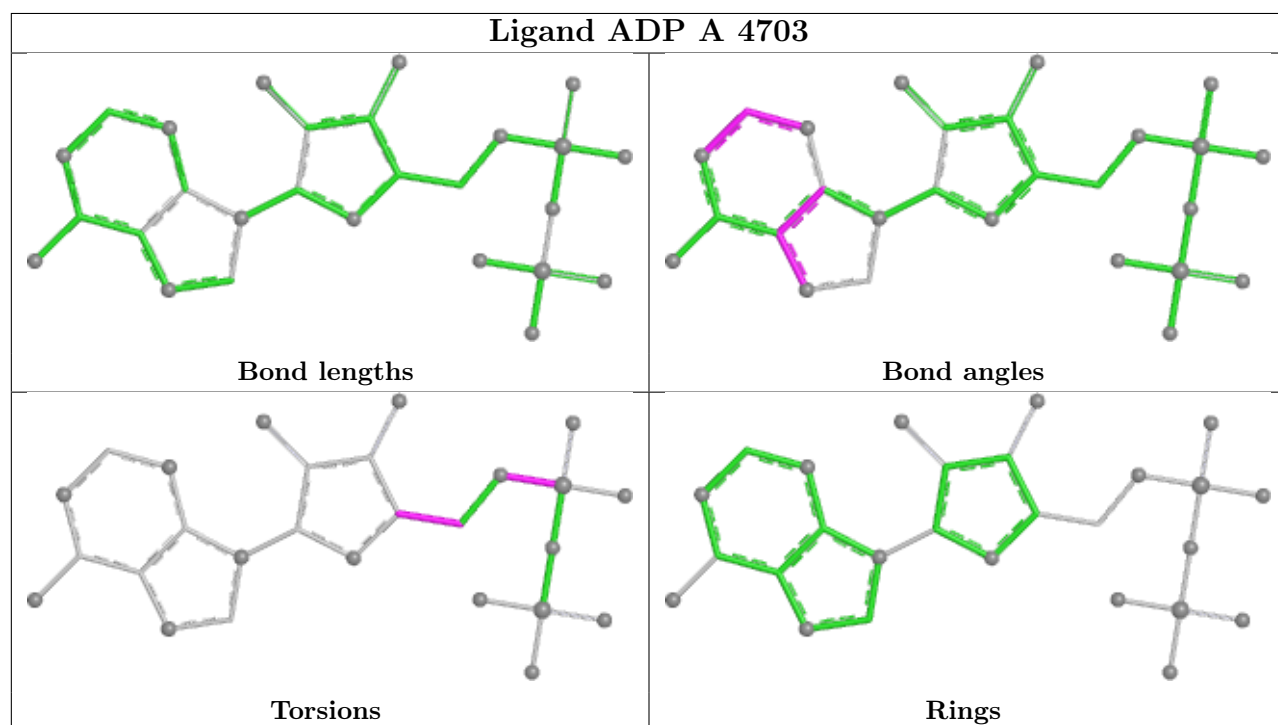
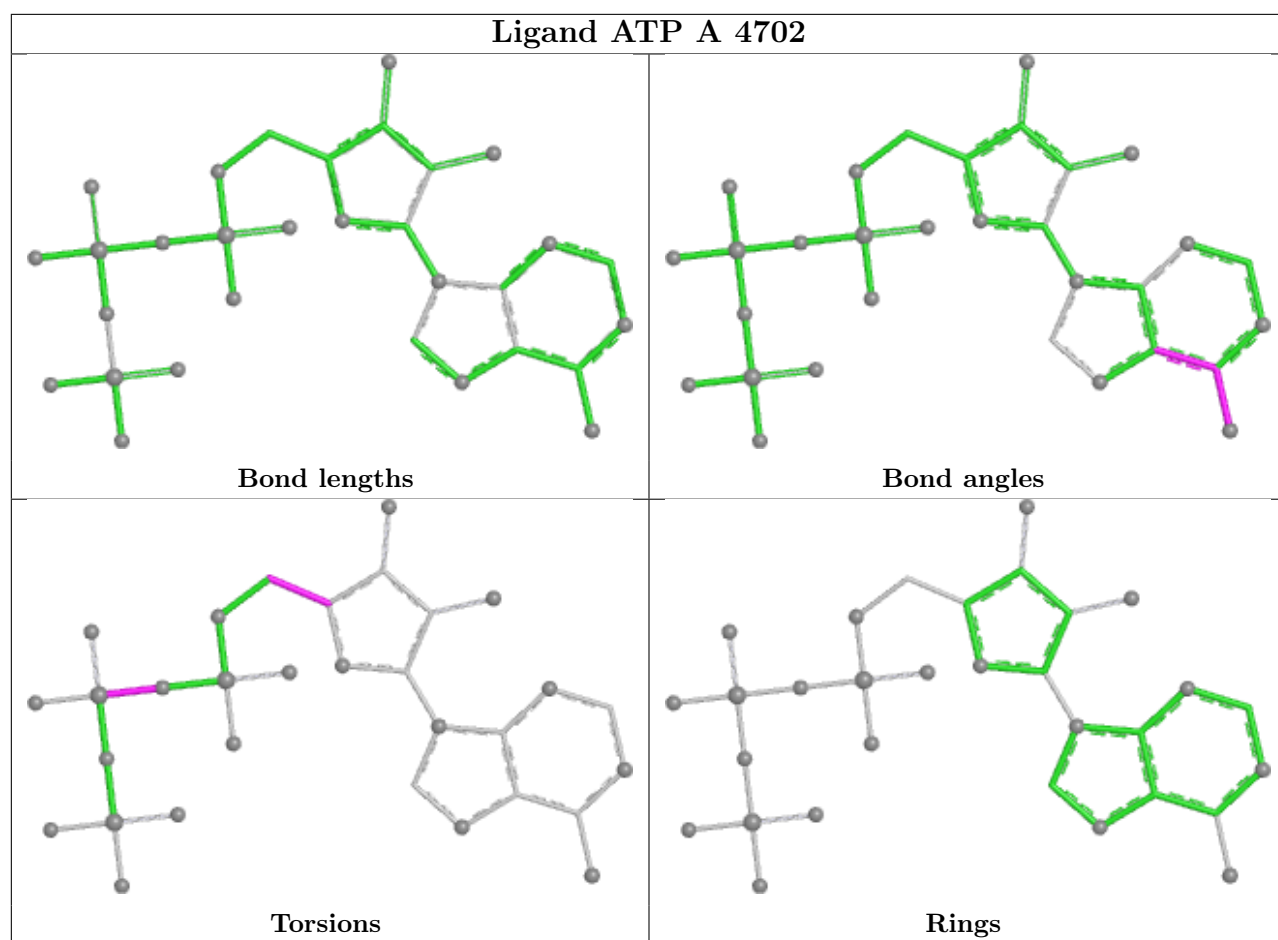
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4704	ADP	1	0
2	A	4701	ADP	1	0
3	A	4702	ATP	2	0
2	A	4703	ADP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

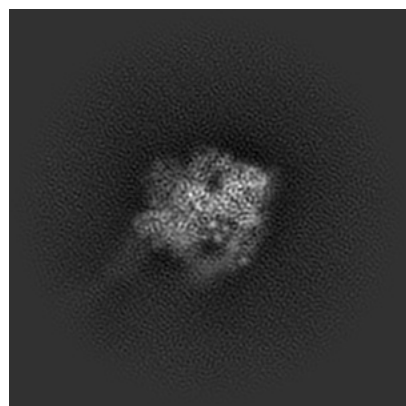
## 6 Map visualisation [i](#)

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

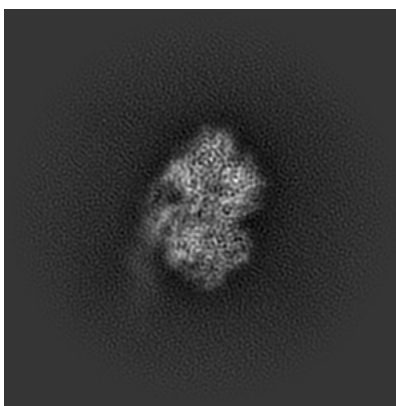
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

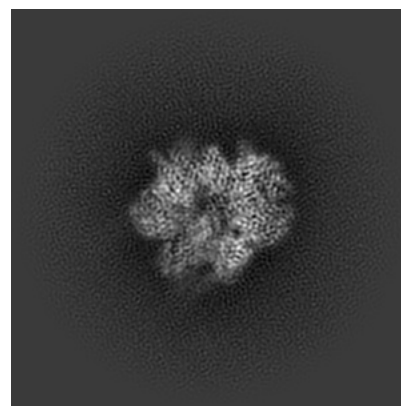
#### 6.1.1 Primary map



X

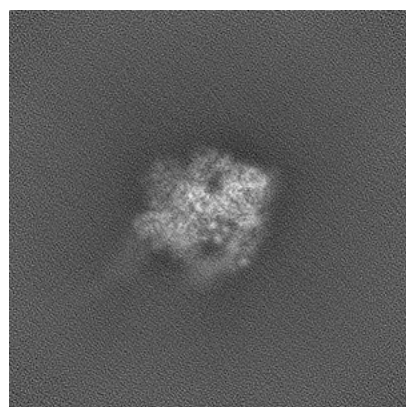


Y

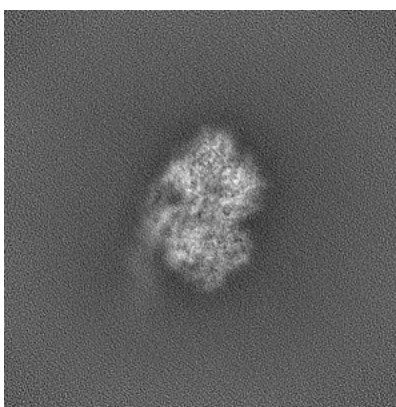


Z

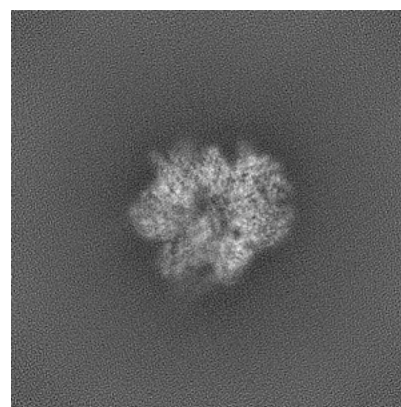
#### 6.1.2 Raw map



X



Y



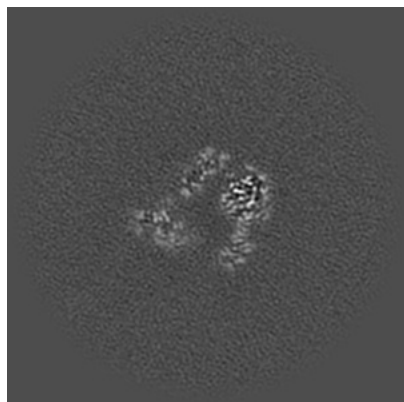
Z

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

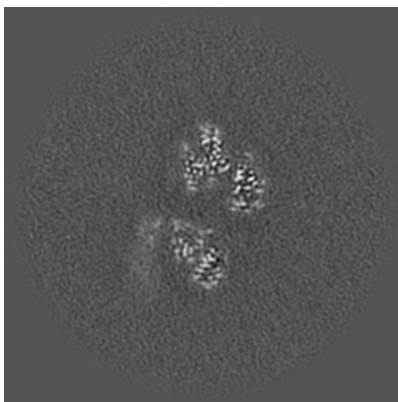


## 6.2 Central slices [i](#)

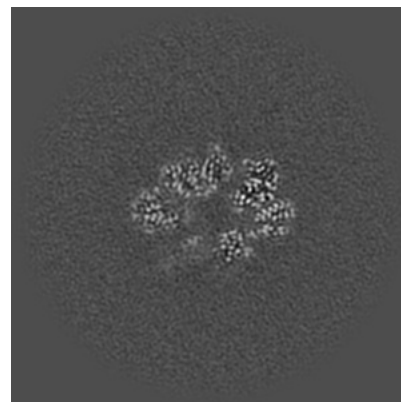
### 6.2.1 Primary map



X Index: 160

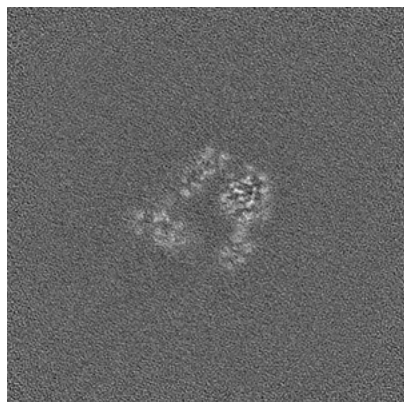


Y Index: 160

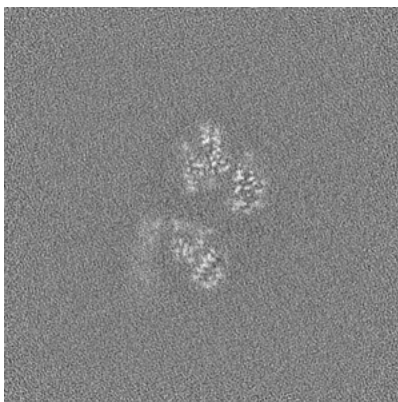


Z Index: 160

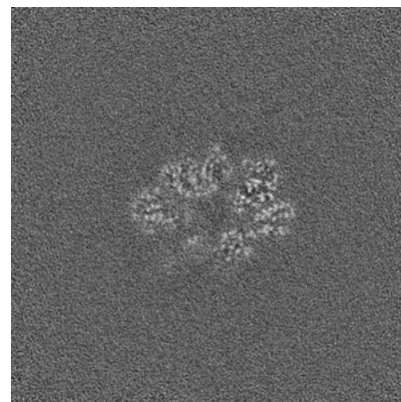
### 6.2.2 Raw map



X Index: 160



Y Index: 160



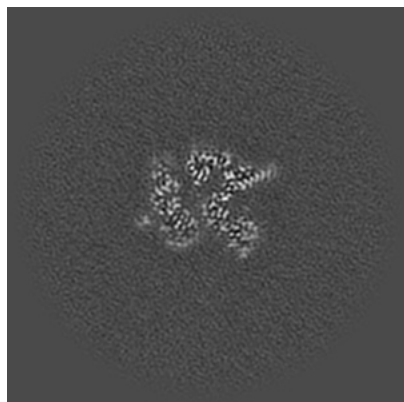
Z Index: 160

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

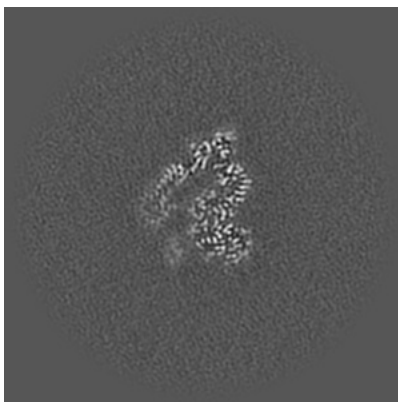


## 6.3 Largest variance slices [i](#)

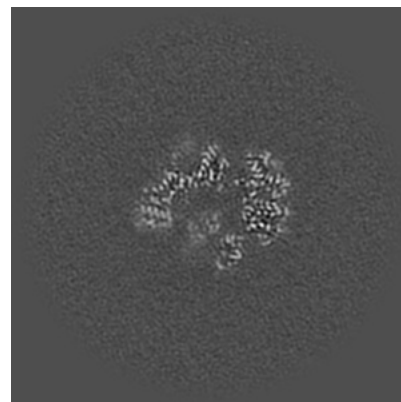
### 6.3.1 Primary map



X Index: 183

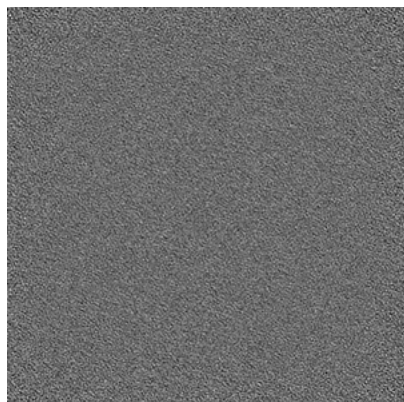


Y Index: 181

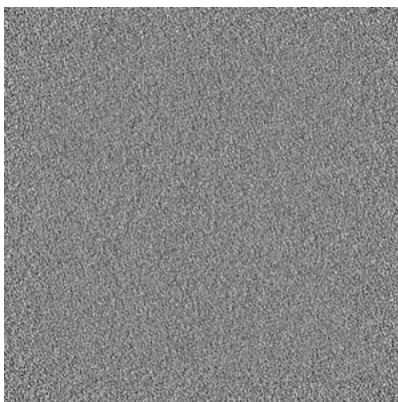


Z Index: 172

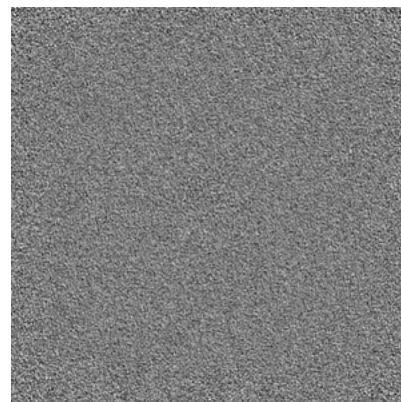
### 6.3.2 Raw map



X Index: 0



Y Index: 0

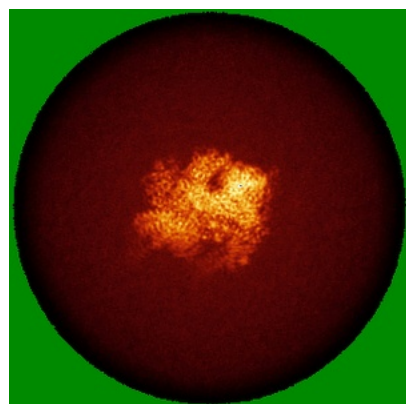


Z Index: 0

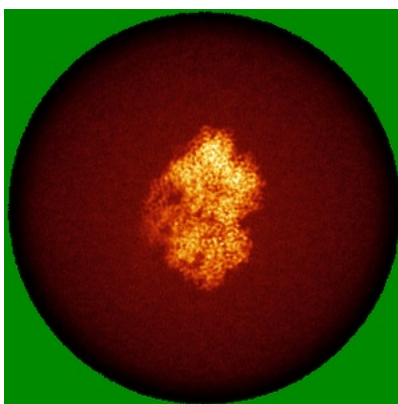
The images above show the largest variance slices of the map in three orthogonal directions.

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

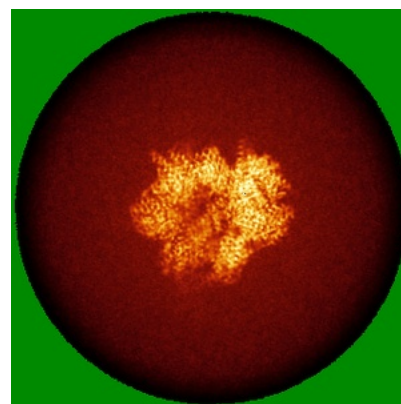
### 6.4.1 Primary map



X

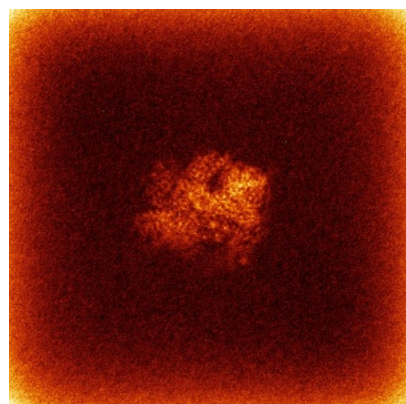


Y

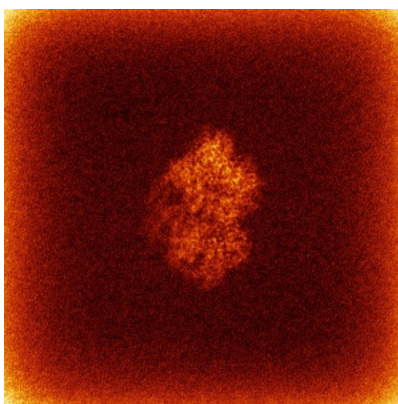


Z

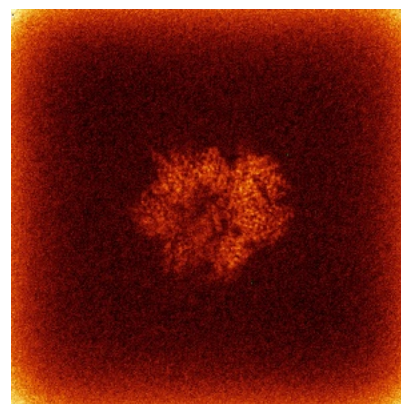
### 6.4.2 Raw map



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](#)

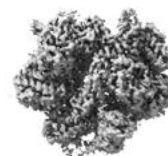
### 6.5.1 Primary map



X



Y



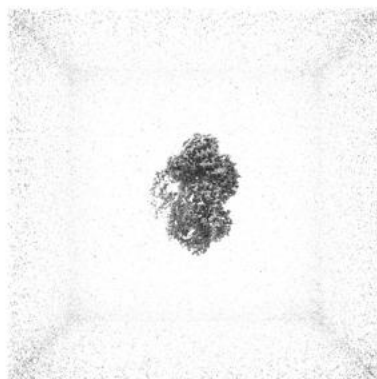
Z

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.

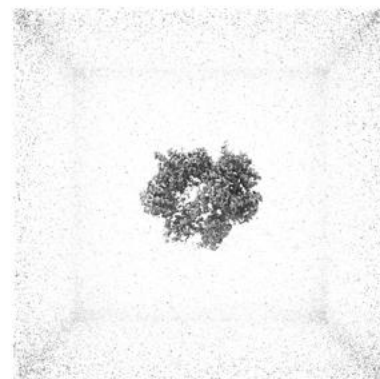
### 6.5.2 Raw map



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.

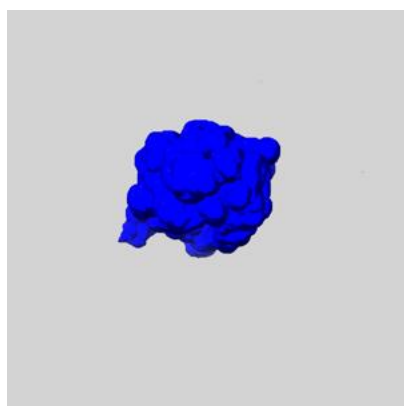
## 6.6 Mask visualisation [i](#)

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

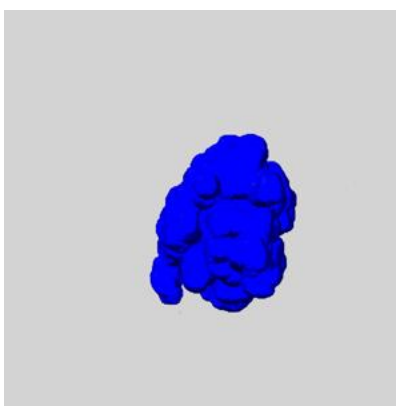
A mask typically either:

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

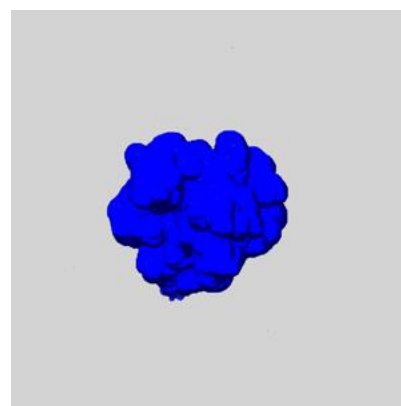
### 6.6.1 emd\_44713\_msk\_1.map [i](#)



X



Y

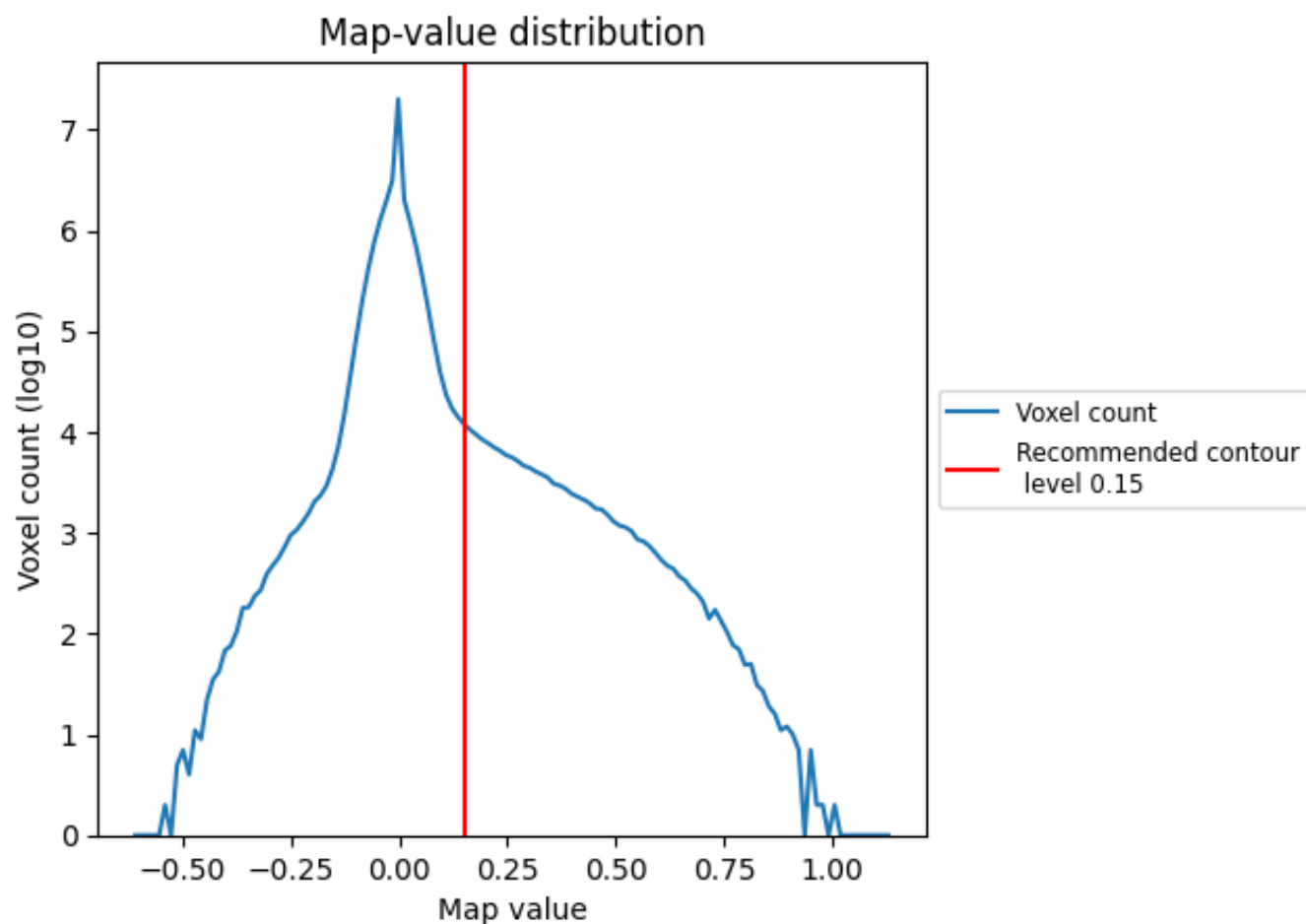


Z

## 7 Map analysis [i](#)

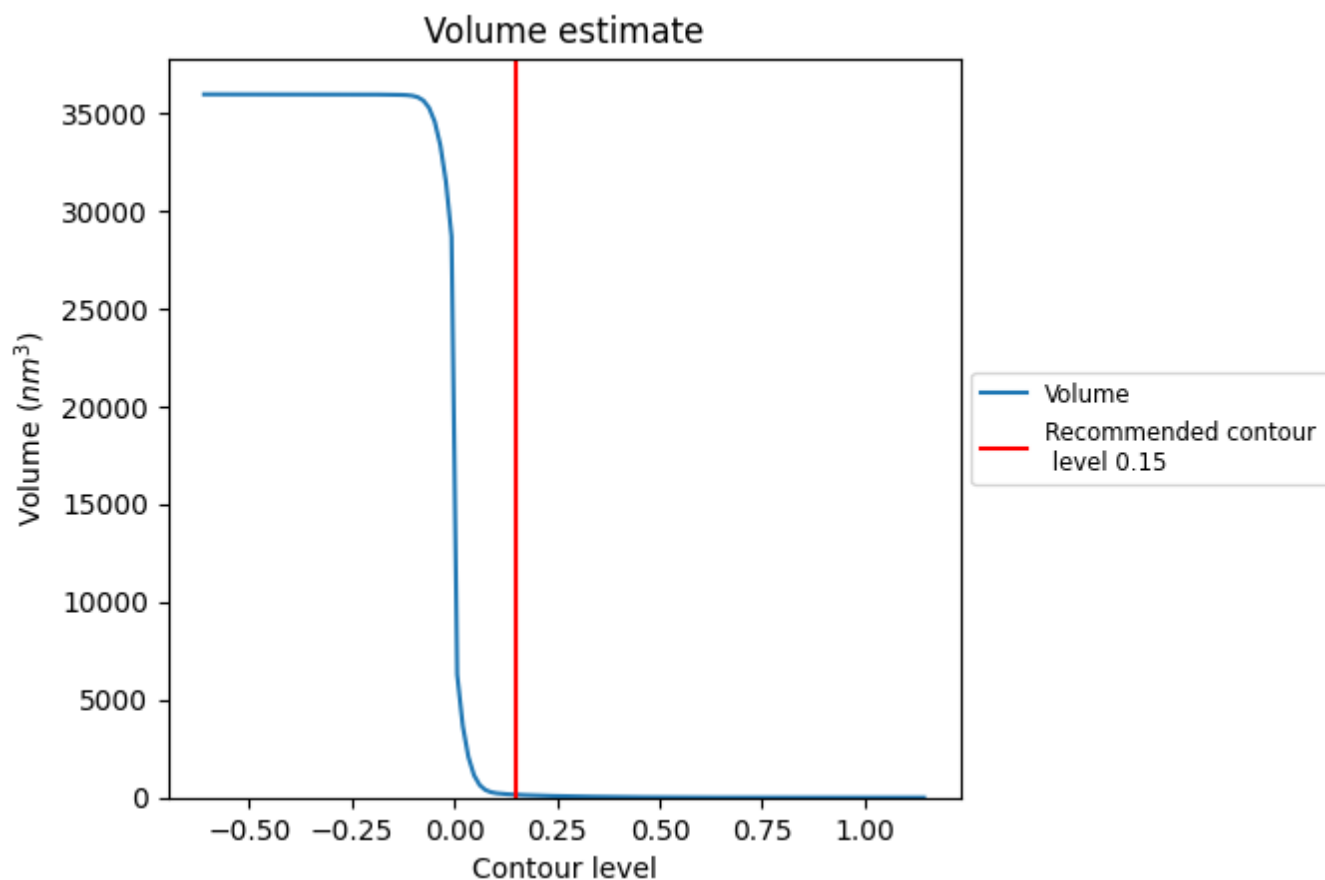
This section contains the results of statistical analysis of the map.

### 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.

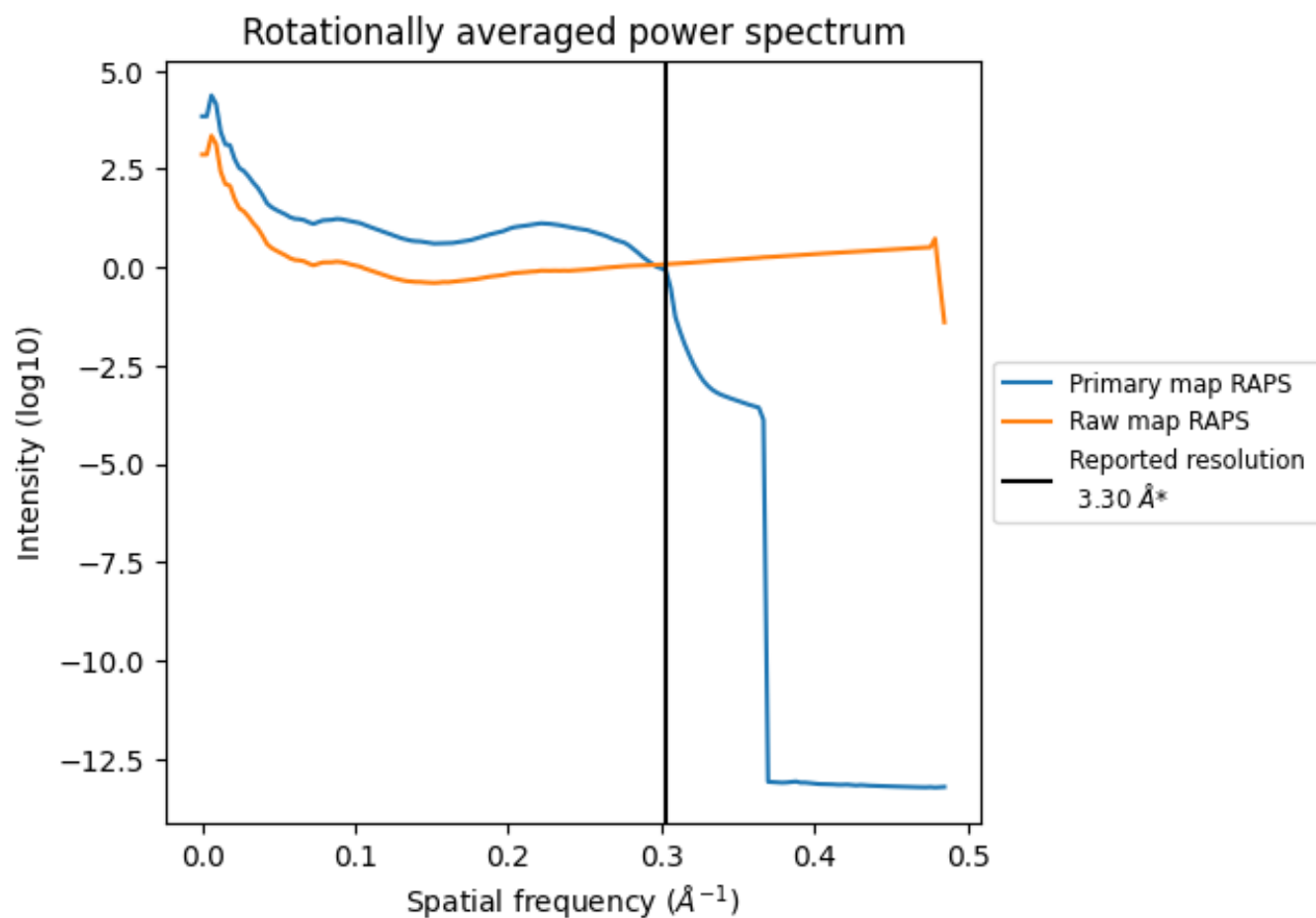
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 146 nm<sup>3</sup>; 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 ⓘ



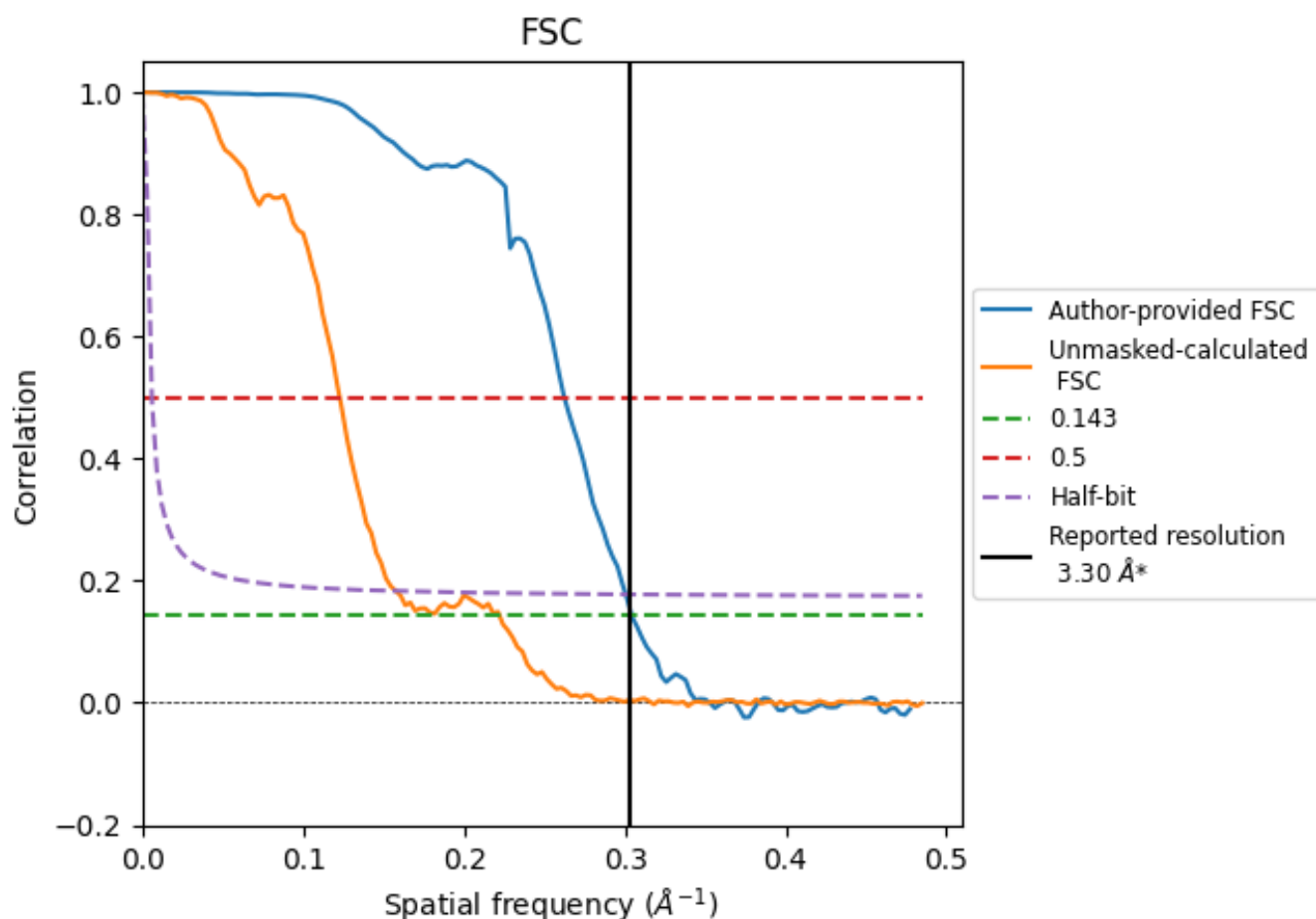
\*Reported resolution corresponds to spatial frequency of 0.303 Å<sup>-1</sup>



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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.303  $\text{\AA}^{-1}$



## 8.2 Resolution estimates [i](#)

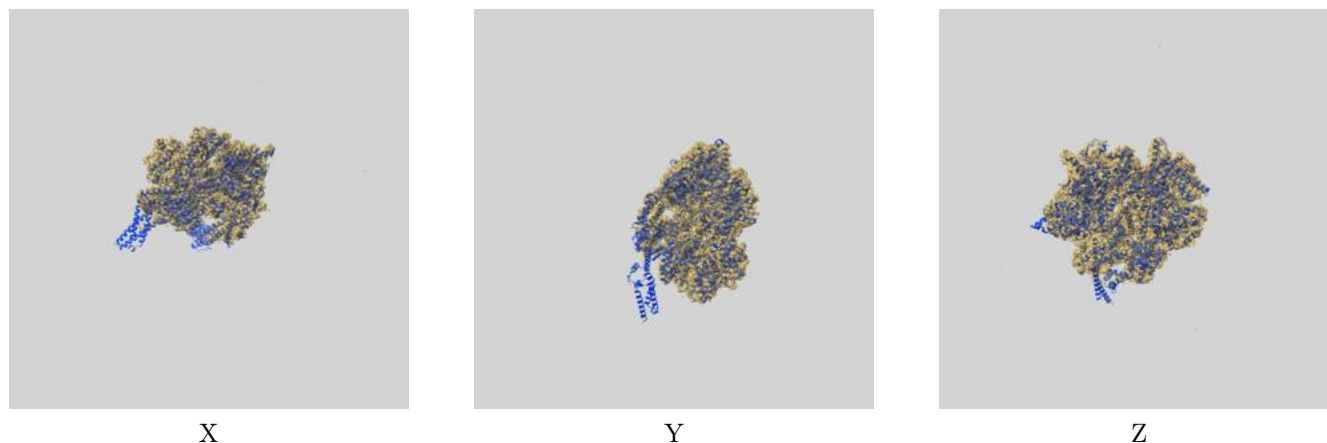
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.29	3.81	3.33
Unmasked-calculated*	4.50	8.14	6.34

\*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](#)

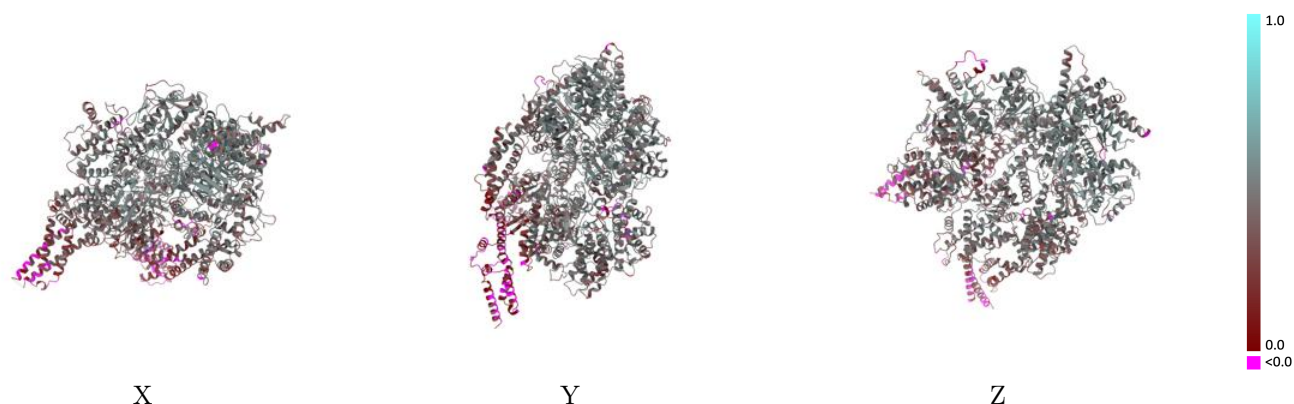
This section contains information regarding the fit between EMDB map EMD-44713 and PDB model 9BMW. Per-residue inclusion information can be found in section 3 on page 5.

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



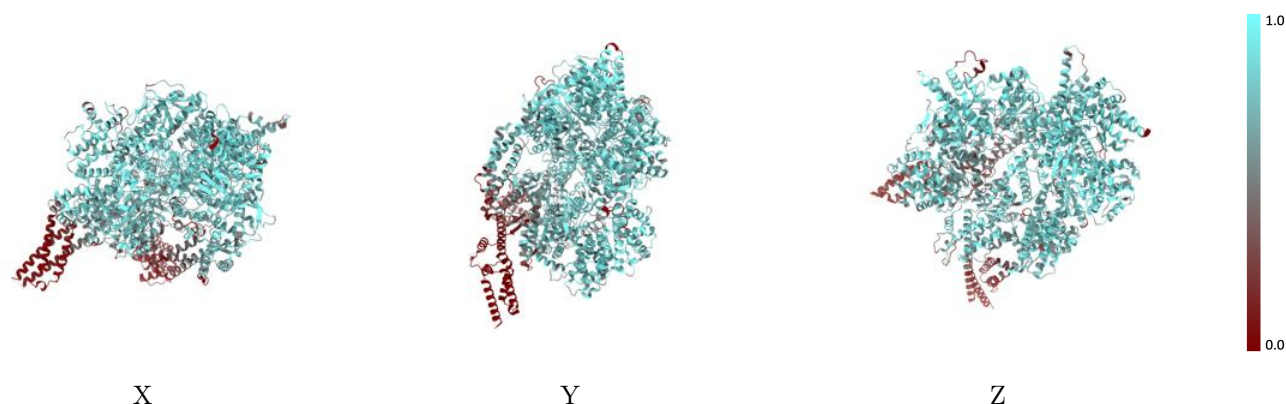
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



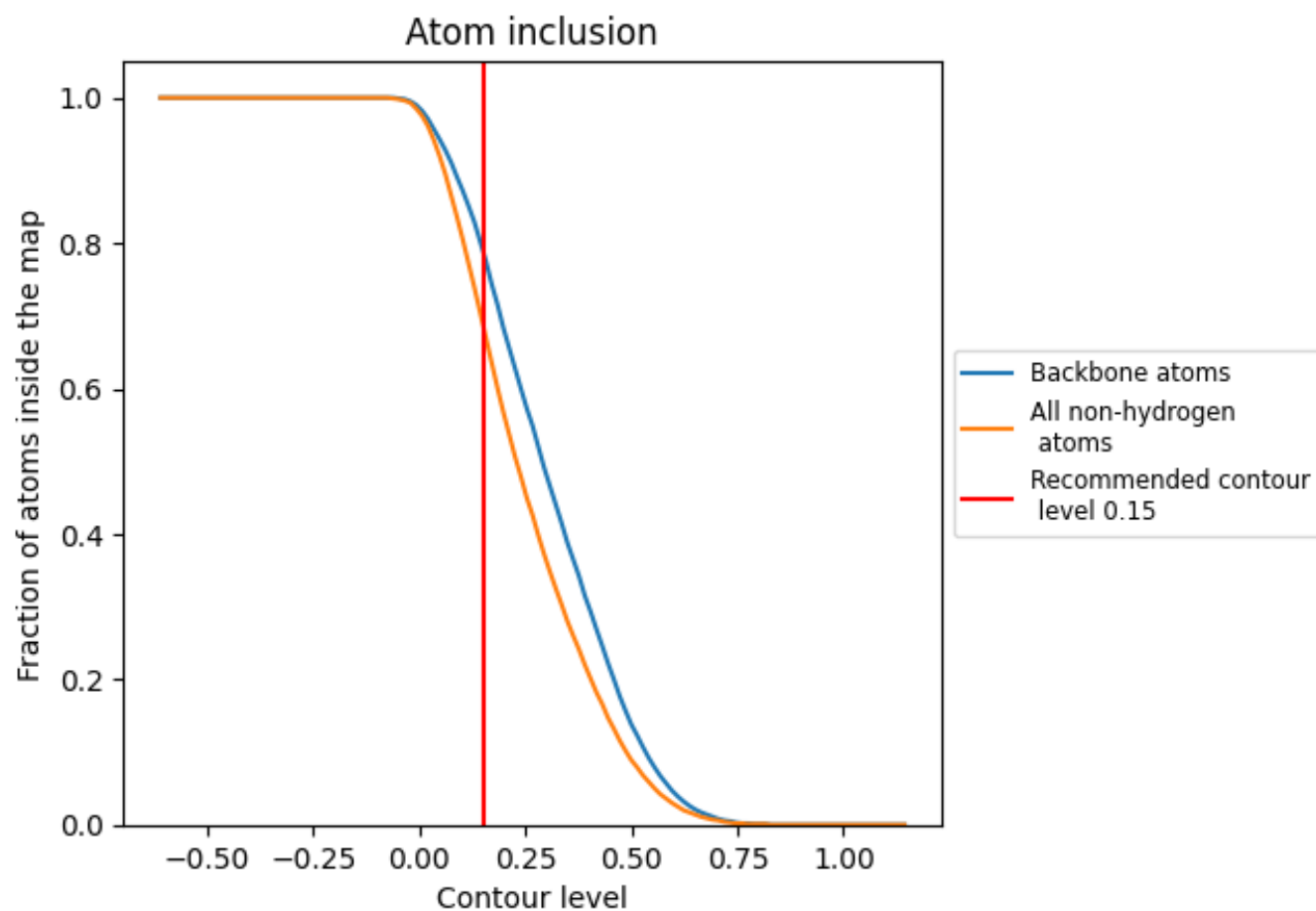
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

## 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

