



Full wwPDB EM Validation Report ⓘ

Dec 18, 2022 – 05:11 am GMT

PDB ID : 6ZYY
EMDB ID : EMD-11581
Title : Outer Dynein Arm-Shulin complex - Dyh3 motor region (Tetrahymena thermophila)
Authors : Mali, G.R.; Abid Ali, F.; Lau, C.K.; Begum, F.; Boulanger, J.; Howe, J.D.; Chen, Z.A.; Rappsilber, J.; Skehel, M.; Carter, A.P.
Deposited on : 2020-08-03
Resolution : 4.40 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.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

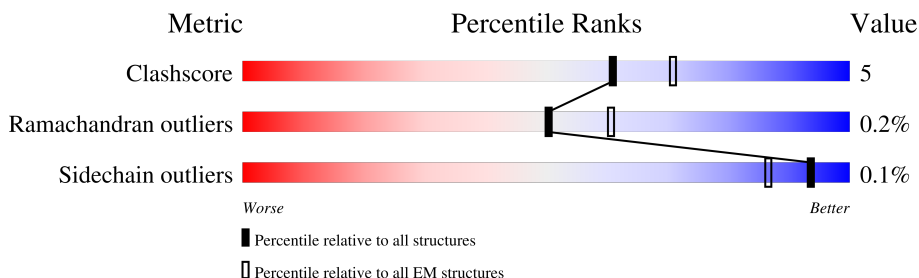
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	C	4620	
2	Y	1200	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 22453 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 Dynein heavy chain, outer arm protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	2901	Total	C	N	O	S	0	0
			21875	13931	3736	4092	116		

- Molecule 2 is a protein called Shulin.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	Y	66	Total	C	N	O	0	0
			466	303	89	74		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



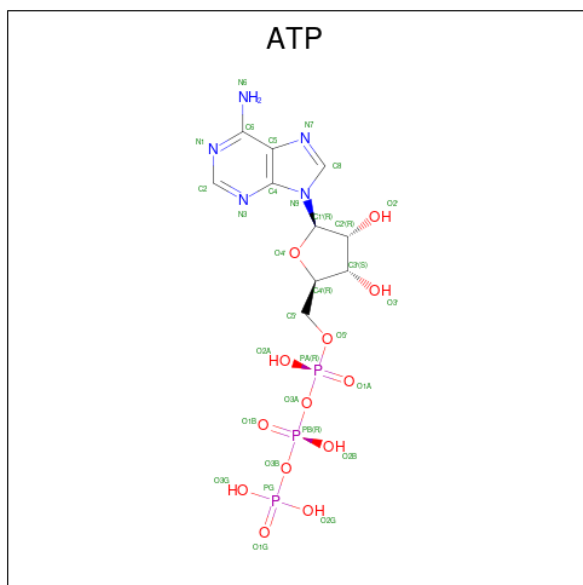
Mol	Chain	Residues	Atoms					AltConf
3	C	1	Total	C	N	O	P	0
			81	30	15	30	6	
3	C	1	Total	C	N	O	P	0
			81	30	15	30	6	

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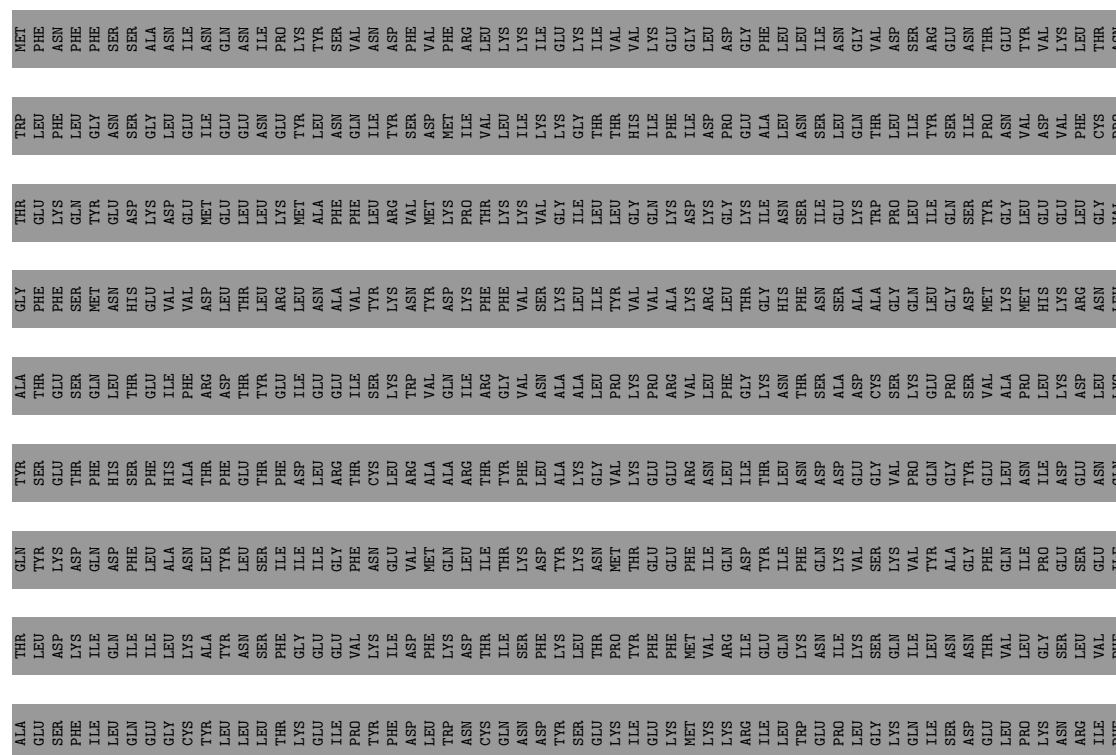
Mol	Chain	Residues	Atoms					AltConf
3	C	1	Total	C	N	O	P	0
			81	30	15	30	6	

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



G2178	S2179	P2180	H2181	I2185	L2203	D2206	G2210	V2211	T2214	E2242	N2243	L2244	V2247	L2248	D2249	E2273	A2317	K2322	L2323	G2324	N2325	L2326	L2327	R2328	K2329	F2336	T2337	Q2340	E2343	D2350	F2353	S2356	V2357	L2361	L2378	Q2381	G2397	T2398	V2399													
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N1460	T1466	I1467	L1468	E1469	R1470	L1471	E1472	Q1475	L1476	Q1477	L1478	S1479	T1480	F1481	N1482	S1483	Q1484	R1485	H1486	V1487	T1488	K1491	A1492	L1497	F1501	V1504	N1505	D1506	V1518	L1521	E1522	P1523	T1526	G1527	G1528	A1531	R1532	A1538	K1539	Q1540	F1541	T1544	D1545	K1546	I1551	M1552						
I1383	K1384	E1385	I1386	T1387	M1388	I1389	K1390	Y1393	E1394	M1395	P1396	D1397	Q1398	F1399	Y1400	I1401	E1402	E1403	I1404	R1405	G1406	A1407	K1408	L1409	L1410	D1411	F1412	R1413	E1414	D1415	I1416	E1417	D1418	I1419	K1425	Q1426	I1427	L1433	Y1439	M1443	Q1444	F1445	Q1446	F1447	G1448	I1449	W1450	R1453	D1454	V1455	P1456	G1457
D1321	D1322	L1323	A1324	K1325	M1326	E1327	D1328	ALA	GLY	LYS	TRP	GLY	GLU	GLN	CYS	SER	ARG	PRO	GLU	LEU	PRO	TRP	GLN	ALA	TRP	ARG	ASP	ASN	LEU	TRP	ILE	ASP	SER	ARG	E1362	Q1363	L1364	P1365	L1366	I1367	I1368	S1369	L1370	K1371	S1374	I1375	M1376	P1377	R1378	H1379	K1382	
GLN	MET	TYR	LYS	ILE	ASN	ALA	ARG	GLY	PHE	LEU	GLN	LYS	GLN	ASN	CYS	THR	PRO	GLU	LEU	ASP	PRO	TRP	GLN	ALA	TRP	ARG	GLN	GLN	PHE	K1311	E1312	K1313	S1314	W1315	Q1316	D1317	V1318	S1319	K1320													
TYR	GLN	HIS	LYS	GLN	ALA	ILE	TYR	LEU	GLY	GLU	MET	LYS	LEU	LYS	GLN	PHE	THR	SER	GLN	VAL	GLN	VAL	ILE	ASP	GLY	ILE	GLU	PRO	ALA	GLU	ARG	ILE	GLN	TRP	GLU	TRP	LYS	VAL	GLY	GLN	GLY	GLY	GLY	GLY	GLY	GLY	GLY					
GLN	ILE	ARG	LYS	GLN	GLU	ALA	GLU	PHE	ASN	PRO	VAL	GLN	GLU	GLN	MET	TYR	SER	GLN	LEU	PRO	GLY	ILE	THR	ASP	GLN	LEU	GLU	ALA	ARG	GLU	ARG	ILE	GLN	TRP	GLU	TRP	LYS	VAL	GLY	GLN	GLY	GLY	GLY	GLY	GLY	GLY	GLY					
ILE	CYS	THR	SER	LEU	THR	TRP	ALA	THR	TRP	LEU	GLN	ILE	SER	ILE	GLN	ASP	HEU	ASN	GLY	PRO	MET	ILE	ASP	GLN	LEU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU				
THR	LYS	PHE	GLU	TRP	CYS	LYS	GLU	ILE	GLU	TRP	GLN	ILE	PHE	LYS	ASP	HEU	ASN	GLY	PRO	MET	ILE	ASP	GLN	LEU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU			
ALA	VAL	LEU	ARG	CYS	LEU	HIS	LYS	THR	TRP	ASP	GLN	ILE	THR	ARG	ILE	GLN	ALA	THR	GLN	VAL	GLN	VAL	THR	GLN	LEU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU			
SER	THR	GLN	ASN	SER	LEU	ASN	ALA	THR	VAL	VAL	CYS	GLY	GLU	LYS	ARG	ILE	GLN	PRO	GLY	ALA	ASN	LYS	THR	GLN	LEU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU			
ILE	ASN	SER	LYS	THR	PHE	LEU	THR	SER	VAL	VAL	GLU	VAL	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU				

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LYS	PRO	LYS	ARG	ILE	GLN	VAL	ALA	ILE	ALA	GLU	ARG	GLN	ILE	ALA	LEU	LYS	GLU	GLU	ALA	ARG	GLU	ASP	ILE	PRO	GLU	ARG	CYS	I3555	T3556	T3557	L3558	S3559	H3560	P3561	K3562	F3563	K3564	D3565	K3566	F3567	L3568	K3569	M3572	E3573	S3574	G3575	L3576	T3577	L3578	I3583	E3584	V3587	D3588	P3589
LEU	LYS	GLU	PHE	ILE	LYS	ASP	SER	MET	ALA	ASN	VAL	LEU	THR	ILE	GLU	LEU	PRO	TYR	LEU	ASN	GLN	ILE	GLU	TRP	ASP	GLU	ALA	ARG	GLU	ILE	PHE	VAL	GLU	ALA	GLN	THR	TYR	GLU	TYR	GLU	ASP	MET	ASN	LYS	ASP	GLU	LEU	ALA	ASN	GLN	PRO			
GLY	ASP	GLU	ILE	VAL	ALA	THR	ASN	ILE	ALA	CYS	GLU	VAL	PHE	GLU	ALA	ARG	ILE	SER	PRO	GLU	ILE	GLU	ARG	GLU	VAL	ASN	GLU	ALA	GLN	VAL	GLU	THR	ASP	VAL	GLU	ALA	THR	ASP	SER	ILE	GLU	VAL	GLU	ASP	GLU	LEU	ALA	ASN	GLN	PRO				
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R2851	S2853	R2857	L2864	Q2872	K2873	Q2874	T2877	R2878	T2883	G2884	T2888	Q2889	I2891	T2894	K2895	T2896	D2901	F2910	D2911	D2912	A2913	G2914	K2918	Q2919	L2923	M2924	T2925	E2928	V2929	K2930	K2931	E2932	E2933	F2934	L2935	E2936	Y2937	L2938	M2939	M2940	V2941	L2942	S2943	T2944	G2945									
R2851	S2853	R2857	L2864	Q2872	K2873	Q2874	T2877	R2878	T2883	G2884	T2888	Q2889	I2891	T2894	K2895	T2896	D2901	F2910	D2911	D2912	A2913	G2914	K2918	Q2919	L2923	M2924	T2925	E2928	V2929	K2930	K2931	E2932	E2933	F2934	L2935	E2936	Y2937	L2938	M2939	M2940	V2941	L2942	S2943	T2944	G2945									
R2851	S2853	R2857	L2864	Q2872	K2873	Q2874	T2877	R2878	T2883	G2884	T2888	Q2889	I2891	T2894	K2895	T2896	D2901	F2910	D2911	D2912	A2913	G2914	K2918	Q2919	L2923	M2924	T2925	E2928	V2929	K2930	K2931	E2932	E2933	F2934	L2935	E2936	Y2937	L2938	M2939	M2940	V2941	L2942	S2943	T2944	G2945									
R2851	S2853	R2857	L2864	Q2872	K2873	Q2874	T2877	R2878	T2883	G2884	T2888	Q2889	I2891	T2894	K2895	T2896	D2901	F2910	D2911	D2912	A2913	G2914	K2918	Q2919	L2923	M2924	T2925	E2928	V2929	K2930	K2931	E2932	E2933	F2934	L2935	E2936	Y2937	L2938	M2939	M2940	V2941	L2942	S2943	T2944	G2945									
R2851	S2853	R2857	L2864	Q2872	K2873	Q2874	T2877	R2878	T2883	G2884	T2888	Q2889	I2891	T2894	K2895	T2896	D2901	F2910	D2911	D2912	A2913	G2914	K2918	Q2919	L2923	M2924	T2925	E2928	V2929	K2930	K2931	E2932	E2933	F2934	L2935	E2936	Y2937	L2938	M2939	M2940	V2941	L2942	S2943	T2944	G2945									
R2851	S2853	R2857	L2864	Q2872	K2873	Q2874	T2877	R2878	T2883	G2884	T2888	Q2889	I2891	T2894	K2895	T2896	D2901	F2910	D2911	D2912	A2913	G2914	K2918	Q2919	L2923	M2924	T2925	E2928	V2929	K2930	K2931	E2932	E2933	F2934	L2935	E2936	Y2937	L2938	M2939	M2940	V2941	L2942	S2943	T2944	G2945									
R2851	S2853	R2857	L2864	Q2872	K2873	Q2874	T2877	R2878	T2883	G2884	T2888	Q2889	I2891	T2894	K2895	T2896	D2901	F2910	D2911	D2912	A2913	G2914	K2918	Q2919	L2923	M2924	T2925	E2928	V2929	K2930	K2931	E2932	E2933	F2934	L2935	E2936	Y2937	L2938	M2939	M2940	V2941	L2942	S2943	T2944	G2945									
R2851	S2853	R2857	L2864	Q2872	K2873	Q2874	T2877	R2878	T2883	G2884	T2888	Q2889	I2891	T2894	K2895	T2896	D2901	F2910	D2911	D2912	A2913	G291																																



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	49397	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	52	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.082	Depositor
Minimum map value	-0.069	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	499.5, 499.5, 499.5	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.11, 1.11, 1.11	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: 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	C	0.37	1/22277 (0.0%)	0.65	18/30197 (0.1%)
2	Y	0.37	0/477	0.60	0/648
All	All	0.37	1/22754 (0.0%)	0.65	18/30845 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	2857	ARG	CB-CG	-5.58	1.37	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2857	ARG	NE-CZ-NH2	-25.58	107.51	120.30
1	C	2857	ARG	NH1-CZ-NH2	8.53	128.78	119.40
1	C	3069	MET	CB-CG-SD	-7.32	90.44	112.40
1	C	3069	MET	CG-SD-CE	-6.80	89.32	100.20
1	C	4182	PRO	N-CA-CB	6.65	111.28	103.30
1	C	4188	PRO	N-CA-CB	6.65	111.28	103.30
1	C	2857	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	C	3744	ARG	NE-CZ-NH2	-6.53	117.03	120.30
1	C	2978	PRO	N-CA-CB	6.33	110.89	103.30
1	C	4180	PRO	N-CA-CB	6.29	110.85	103.30
1	C	4546	PRO	N-CA-CB	6.21	110.75	103.30
1	C	2979	PRO	N-CA-CB	6.20	110.73	103.30
1	C	2857	ARG	CG-CD-NE	-6.06	99.07	111.80
1	C	4433	PRO	CA-N-CD	-6.02	103.07	111.50
1	C	2805	PRO	N-CA-CB	5.63	110.06	103.30
1	C	3483	PRO	N-CA-CB	5.61	110.03	103.30
1	C	2327	LEU	CA-CB-CG	5.25	127.39	115.30
1	C	3744	ARG	NE-CZ-NH1	5.22	122.91	120.30

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	C	21875	0	20694	197	0
2	Y	466	0	390	5	0
3	C	81	0	36	0	0
4	C	31	0	12	0	0
All	All	22453	0	21132	202	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (202) 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:C:2499:LYS:NZ	1:C:2611:MET:O	2.11	0.83
1:C:1314:SER:O	1:C:1318:VAL:N	2.14	0.79
1:C:4125:ASN:O	1:C:4128:SER:OG	2.00	0.77
1:C:2776:LYS:O	1:C:2781:LYS:NZ	2.18	0.76
1:C:3636:PRO:O	1:C:3639:SER:OG	2.03	0.74
1:C:2943:SER:O	1:C:2992:ARG:NH2	2.21	0.73
1:C:1986:LEU:O	1:C:1991:LYS:NZ	2.24	0.71
2:Y:1148:ASN:OD1	2:Y:1149:ILE:N	2.23	0.71
1:C:2843:ASP:OD2	1:C:2847:LYS:NZ	2.25	0.70
1:C:1862:MET:SD	1:C:1971:SER:OG	2.48	0.69
1:C:2322:LYS:NZ	1:C:2378:LEU:O	2.26	0.69
1:C:1932:GLU:O	1:C:1935:SER:OG	2.10	0.69
1:C:3664:SER:OG	1:C:3671:GLU:OE2	2.07	0.69
1:C:3789:SER:O	1:C:3798:ARG:NH2	2.26	0.68
1:C:2164:SER:OG	1:C:2273:GLU:OE2	2.12	0.67
1:C:3741:ASN:O	1:C:3745:GLU:N	2.27	0.67
1:C:4215:LEU:O	1:C:4218:THR:OG1	2.11	0.67
1:C:2434:SER:OG	1:C:2437:TYR:O	2.12	0.67
1:C:2595:GLN:N	1:C:2595:GLN:OE1	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2027:PHE:CZ	1:C:2074:LEU:HD21	2.30	0.67
1:C:2340:GLN:NE2	1:C:2343:GLU:O	2.28	0.66
1:C:2894:THR:OG1	1:C:2896:THR:O	2.12	0.66
1:C:2850:LEU:O	1:C:2853:SER:OG	2.12	0.66
1:C:2888:ILE:HG23	1:C:2923:LEU:HD23	1.78	0.65
1:C:2936:GLU:N	1:C:2936:GLU:OE1	2.30	0.65
1:C:4113:ILE:HG22	1:C:4117:PHE:CE2	2.32	0.65
1:C:2492:ILE:O	1:C:2634:MET:N	2.29	0.65
1:C:3037:SER:O	1:C:3041:THR:HG23	1.98	0.64
1:C:4461:LEU:CD2	1:C:4553:LEU:HD11	2.26	0.64
1:C:2890:GLN:NE2	1:C:2928:GLU:OE2	2.31	0.63
1:C:3776:GLU:OE1	1:C:3776:GLU:N	2.32	0.63
1:C:2768:GLN:N	1:C:2768:GLN:OE1	2.32	0.63
1:C:4022:GLY:O	1:C:4023:GLN:NE2	2.32	0.63
1:C:3870:GLU:O	1:C:3874:TRP:N	2.31	0.62
1:C:2910:PHE:O	1:C:2914:GLY:N	2.31	0.62
2:Y:1147:ARG:HD3	2:Y:1151:GLY:HA2	1.81	0.62
2:Y:1148:ASN:HB3	2:Y:1154:LEU:HD21	1.82	0.62
1:C:2543:VAL:HG12	1:C:2548:ALA:CB	2.29	0.62
1:C:2940:MET:SD	1:C:2944:THR:OG1	2.58	0.61
1:C:1589:GLU:OE1	1:C:1589:GLU:N	2.32	0.61
1:C:2543:VAL:HG12	1:C:2548:ALA:HB3	1.81	0.61
1:C:2211:VAL:O	1:C:2214:THR:OG1	2.13	0.61
1:C:2353:PRO:O	1:C:2356:SER:OG	2.16	0.61
1:C:1902:HIS:O	1:C:1903:ARG:NE	2.34	0.60
1:C:4209:ASP:OD1	1:C:4210:ASP:N	2.35	0.60
1:C:2621:ILE:O	1:C:2626:LYS:NZ	2.34	0.60
1:C:4537:SER:OG	1:C:4538:LYS:NZ	2.34	0.60
1:C:1801:LYS:N	1:C:1805:ASP:OD2	2.35	0.60
1:C:2443:CYS:SG	1:C:2444:SER:N	2.75	0.59
1:C:2925:THR:OG1	1:C:2928:GLU:OE1	2.12	0.59
1:C:2560:ASP:OD1	1:C:2561:ASP:N	2.35	0.59
1:C:2008:ILE:HD11	1:C:2051:ILE:CG2	2.32	0.59
1:C:1487:VAL:O	1:C:1491:LYS:NZ	2.36	0.59
1:C:4143:ARG:NH1	1:C:4219:TYR:OH	2.35	0.59
1:C:3057:GLN:N	1:C:3057:GLN:OE1	2.35	0.59
1:C:1855:TYR:OH	1:C:1884:ASP:OD2	2.19	0.59
1:C:2685:PRO:O	1:C:4396:GLN:NE2	2.36	0.59
1:C:2912:ASP:O	1:C:2918:LYS:N	2.37	0.58
1:C:3069:MET:CE	1:C:3472:ARG:HB3	2.34	0.57
1:C:2175:THR:HG22	1:C:2180:PRO:HA	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3095:TYR:HE1	1:C:3451:THR:HG23	1.68	0.57
1:C:1827:ILE:HG22	1:C:1828:THR:H	1.70	0.56
1:C:4109:PHE:O	1:C:4113:ILE:HG21	2.05	0.56
1:C:3627:CYS:SG	1:C:3628:ARG:N	2.78	0.56
1:C:3949:ASP:OD1	1:C:3950:ARG:N	2.37	0.56
1:C:2490:LEU:HD21	1:C:2611:MET:HG2	1.86	0.56
1:C:3117:PHE:CB	1:C:3433:ALA:HB2	2.36	0.56
1:C:2477:LEU:HD12	1:C:2606:GLN:OE1	2.06	0.56
1:C:1700:SER:O	1:C:1704:GLN:NE2	2.39	0.55
1:C:2420:GLN:OE1	1:C:2420:GLN:N	2.38	0.55
1:C:4067:HIS:ND1	1:C:4068:GLU:O	2.40	0.55
1:C:4320:VAL:HG21	1:C:4411:TYR:CE2	2.42	0.55
1:C:4024:GLU:N	1:C:4024:GLU:OE1	2.40	0.55
1:C:1376:MET:O	1:C:1379:HIS:N	2.40	0.54
1:C:2452:GLN:O	1:C:2458:GLN:NE2	2.41	0.54
1:C:4522:GLU:OE1	1:C:4522:GLU:N	2.41	0.54
1:C:1925:GLU:OE1	1:C:1983:ARG:NH2	2.40	0.53
1:C:2439:ASP:OD1	1:C:2440:TRP:N	2.41	0.53
1:C:2625:LEU:HD21	1:C:2629:PHE:CE2	2.43	0.53
1:C:2008:ILE:HD11	1:C:2051:ILE:HG21	1.91	0.53
1:C:2324:GLY:O	1:C:2327:LEU:N	2.41	0.53
1:C:2490:LEU:HD22	1:C:2631:ILE:HG22	1.90	0.53
1:C:1501:PHE:O	1:C:1504:VAL:HG12	2.09	0.52
1:C:1929:ILE:HG21	1:C:1934:LEU:HD21	1.91	0.52
1:C:3777:GLN:O	1:C:3781:LEU:HD23	2.09	0.52
1:C:1995:ARG:NH2	1:C:4161:ASP:OD1	2.42	0.52
1:C:2493:GLY:O	1:C:2499:LYS:NZ	2.42	0.52
1:C:2840:VAL:HG11	1:C:3038:VAL:HG22	1.91	0.52
1:C:1916:GLN:HG2	1:C:1964:ILE:HD11	1.92	0.52
1:C:2023:LEU:HD22	1:C:2074:LEU:HD23	1.92	0.51
1:C:3790:GLU:O	1:C:3798:ARG:NE	2.38	0.51
1:C:3801:ASN:O	1:C:3801:ASN:ND2	2.42	0.51
1:C:4163:GLU:O	1:C:4167:LEU:HD23	2.11	0.51
1:C:3520:MET:HG2	1:C:3645:ILE:HD11	1.93	0.51
1:C:4531:LEU:HD21	1:C:4534:CYS:SG	2.51	0.51
1:C:1970:VAL:O	1:C:1971:SER:OG	2.29	0.51
1:C:2787:ASP:OD1	1:C:2788:PHE:N	2.41	0.51
1:C:2397:GLY:O	1:C:2633:ASN:N	2.43	0.50
1:C:2919:GLN:N	1:C:2919:GLN:OE1	2.44	0.50
2:Y:1156:HIS:ND1	2:Y:1157:HIS:O	2.44	0.50
1:C:2185:ILE:O	1:C:2589:TYR:OH	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2483:HIS:O	1:C:2484:THR:OG1	2.21	0.50
1:C:3529:LEU:HD13	1:C:3625:MET:HG3	1.93	0.50
1:C:2748:ASN:O	1:C:2748:ASN:ND2	2.39	0.49
1:C:2590:MET:SD	1:C:2590:MET:N	2.85	0.49
1:C:3095:TYR:CE1	1:C:3451:THR:HG23	2.47	0.49
1:C:4465:THR:HG1	1:C:4617:CYS:HG	1.60	0.49
1:C:2932:GLU:O	1:C:2935:LEU:N	2.42	0.49
1:C:2178:GLY:O	1:C:2179:SER:OG	2.30	0.48
1:C:2928:GLU:OE1	1:C:2928:GLU:N	2.47	0.48
1:C:4276:GLU:N	1:C:4276:GLU:OE1	2.46	0.48
1:C:2864:LEU:N	1:C:3023:THR:O	2.45	0.48
1:C:2180:PRO:O	1:C:2181:HIS:ND1	2.47	0.48
1:C:4304:ARG:NH2	1:C:4305:PRO:O	2.47	0.48
1:C:2357:VAL:O	1:C:2361:LEU:HD23	2.14	0.48
1:C:3592:ASP:O	1:C:3595:LEU:N	2.47	0.48
1:C:4385:THR:HG21	1:C:4419:TRP:HE1	1.78	0.47
1:C:2490:LEU:HD21	1:C:2611:MET:CG	2.43	0.47
1:C:4122:ASP:OD1	1:C:4124:SER:OG	2.32	0.47
1:C:1944:ILE:HG21	1:C:1972:TYR:OH	2.15	0.47
1:C:3098:SER:OG	1:C:3451:THR:OG1	2.30	0.47
1:C:2709:CYS:CB	1:C:2713:THR:HG23	2.45	0.47
1:C:2748:ASN:C	1:C:2748:ASN:HD22	2.11	0.47
1:C:1877:GLY:O	1:C:1881:THR:OG1	2.28	0.46
1:C:3744:ARG:O	1:C:3748:ARG:N	2.43	0.46
1:C:1857:THR:HG21	1:C:1997:VAL:HG22	1.97	0.46
1:C:4117:PHE:O	1:C:4120:LYS:NZ	2.40	0.46
1:C:4526:ILE:O	1:C:4553:LEU:HD13	2.16	0.46
1:C:2115:ASP:OD1	1:C:2116:VAL:N	2.48	0.46
1:C:3770:MET:N	1:C:3772:ASN:OD1	2.47	0.46
1:C:1819:ASP:OD1	1:C:1820:ILE:N	2.47	0.46
1:C:3069:MET:HE1	1:C:3472:ARG:HB3	1.97	0.46
1:C:3520:MET:HG2	1:C:3645:ILE:CD1	2.46	0.46
1:C:2381:GLN:N	1:C:2381:GLN:OE1	2.49	0.46
1:C:2244:LEU:O	1:C:2247:VAL:HG12	2.16	0.45
1:C:2709:CYS:HB3	1:C:2713:THR:HG23	1.98	0.45
1:C:2738:GLU:O	1:C:2742:ALA:N	2.49	0.45
1:C:4214:GLU:O	1:C:4218:THR:HG23	2.17	0.45
1:C:1765:SER:HA	1:C:1769:LEU:HD13	1.99	0.45
1:C:2324:GLY:HA2	1:C:2327:LEU:HB2	1.99	0.45
1:C:3464:TYR:CD1	1:C:3468:LEU:HD22	2.52	0.45
1:C:1735:VAL:HG11	1:C:1808:TRP:CZ3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1320:LYS:HA	1:C:1324:ALA:HB1	1.99	0.45
1:C:2003:ASP:OD1	1:C:2004:ARG:N	2.50	0.44
1:C:2477:LEU:HD13	1:C:2487:ASN:OD1	2.17	0.44
1:C:2325:ASN:OD1	1:C:2328:ARG:NH2	2.48	0.44
1:C:3955:THR:HA	1:C:3958:PHE:CE1	2.52	0.44
1:C:4382:VAL:O	1:C:4386:LEU:HD23	2.18	0.44
1:C:2120:ILE:HG22	1:C:2124:ILE:HD12	2.00	0.44
1:C:2697:ARG:NH1	1:C:3020:ASN:OD1	2.51	0.44
1:C:2938:ILE:O	1:C:2942:LEU:HD12	2.18	0.44
1:C:3439:GLN:O	1:C:3443:LEU:N	2.42	0.44
2:Y:1147:ARG:HD3	2:Y:1151:GLY:CA	2.46	0.43
1:C:2418:ILE:HB	1:C:2419:PRO:HD2	2.00	0.43
1:C:2901:ASP:N	1:C:2901:ASP:OD1	2.52	0.43
1:C:4218:THR:HG21	1:C:4609:LYS:HG2	2.00	0.43
1:C:3811:TYR:CE1	1:C:3815:ASN:ND2	2.82	0.43
1:C:2206:ASP:N	1:C:2206:ASP:OD1	2.51	0.43
1:C:1917:SER:OG	1:C:1918:GLY:N	2.51	0.43
1:C:1983:ARG:NH2	1:C:2242:GLU:OE2	2.46	0.43
1:C:1400:TYR:O	1:C:1403:GLU:N	2.47	0.43
1:C:2788:PHE:HE1	1:C:2853:SER:HB2	1.84	0.43
1:C:3503:TRP:O	1:C:3506:GLN:N	2.52	0.43
1:C:2177:LEU:HD12	1:C:2177:LEU:O	2.19	0.43
1:C:3790:GLU:OE1	1:C:3802:ILE:HG12	2.19	0.43
1:C:1521:LEU:HD12	1:C:1581:LEU:HD22	2.01	0.43
1:C:2874:GLN:O	1:C:2878:ARG:NH1	2.51	0.43
1:C:1772:LEU:HD23	1:C:1778:ARG:HA	2.01	0.42
1:C:1896:THR:OG1	1:C:1897:ASN:N	2.50	0.42
1:C:2877:THR:HG21	1:C:2923:LEU:CD1	2.49	0.42
1:C:3726:VAL:O	1:C:3730:LEU:N	2.44	0.42
1:C:3911:ILE:O	1:C:3947:ARG:NH2	2.53	0.42
1:C:4015:GLU:OE1	1:C:4015:GLU:N	2.51	0.42
1:C:3540:TRP:O	1:C:3544:LYS:N	2.50	0.42
1:C:4105:LEU:O	1:C:4108:THR:OG1	2.34	0.42
1:C:2210:GLY:O	1:C:2214:THR:HG23	2.20	0.42
1:C:2244:LEU:HD22	1:C:2247:VAL:HG11	2.01	0.42
1:C:3659:LEU:HD21	1:C:3744:ARG:HD2	2.02	0.42
1:C:2664:VAL:O	1:C:2667:SER:OG	2.38	0.42
1:C:2824:LEU:HD21	1:C:2883:ILE:CG2	2.50	0.42
1:C:2051:ILE:O	1:C:2055:LEU:HD23	2.20	0.42
1:C:3784:GLU:O	1:C:3787:ASP:N	2.53	0.42
1:C:2124:ILE:HG21	1:C:2132:ASN:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4461:LEU:HD23	1:C:4553:LEU:HD11	2.01	0.41
1:C:1518:TRP:NE1	1:C:1522:GLU:OE2	2.53	0.41
1:C:3470:GLN:HG3	1:C:3471:GLN:N	2.34	0.41
1:C:3471:GLN:O	1:C:3475:VAL:HG13	2.20	0.41
1:C:2064:GLN:OE1	1:C:2066:ILE:HG23	2.20	0.41
1:C:4498:LEU:O	1:C:4501:VAL:HG22	2.20	0.41
1:C:2659:ASP:N	1:C:2659:ASP:OD1	2.54	0.41
1:C:4156:GLU:N	1:C:4156:GLU:OE1	2.53	0.41
1:C:2399:TYR:N	1:C:2633:ASN:OD1	2.54	0.41
1:C:3637:GLU:HB3	1:C:3641:LYS:HZ3	1.86	0.41
1:C:3440:LYS:O	1:C:3444:VAL:HG23	2.21	0.41
1:C:3447:VAL:O	1:C:3451:THR:HG22	2.21	0.41
1:C:3496:ASP:OD1	1:C:3496:ASP:N	2.54	0.41
1:C:3654:LEU:HD11	1:C:3775:LEU:HD11	2.03	0.41
1:C:4158:ASN:OD1	1:C:4160:SER:OG	2.32	0.40
1:C:2336:PHE:CZ	1:C:2337:ILE:HD11	2.56	0.40
1:C:2914:GLY:O	1:C:2990:ARG:NH1	2.54	0.40
1:C:3069:MET:HE2	1:C:3472:ARG:HB3	2.03	0.40
1:C:3789:SER:O	1:C:3789:SER:OG	2.34	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	2877/4620 (62%)	2606 (91%)	265 (9%)	6 (0%)	47 81
2	Y	64/1200 (5%)	55 (86%)	9 (14%)	0	100 100
All	All	2941/5820 (50%)	2661 (90%)	274 (9%)	6 (0%)	50 81

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	2978	PRO
1	C	2979	PRO
1	C	4182	PRO
1	C	4188	PRO
1	C	4546	PRO
1	C	4121	VAL

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	C	2182/4196 (52%)	2179 (100%)	3 (0%)	93	97
2	Y	33/1102 (3%)	33 (100%)	0	100	100
All	All	2215/5298 (42%)	2212 (100%)	3 (0%)	93	97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	2329	LYS
1	C	2748	ASN
1	C	3801	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	C	4703	-	24,29,29	0.93	1 (4%)	29,45,45	1.54	4 (13%)
4	ATP	C	4702	-	26,33,33	0.87	1 (3%)	31,52,52	1.68	5 (16%)
3	ADP	C	4701	-	24,29,29	0.96	1 (4%)	29,45,45	1.49	3 (10%)
3	ADP	C	4704	-	24,29,29	0.92	1 (4%)	29,45,45	1.49	4 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	C	4703	-	-	4/12/32/32	0/3/3/3
4	ATP	C	4702	-	-	4/18/38/38	0/3/3/3
3	ADP	C	4701	-	-	1/12/32/32	0/3/3/3
3	ADP	C	4704	-	-	3/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	4704	ADP	C5-C4	2.25	1.46	1.40
3	C	4701	ADP	C5-C4	2.18	1.46	1.40
3	C	4703	ADP	C5-C4	2.13	1.46	1.40
4	C	4702	ATP	C5-C4	2.03	1.46	1.40

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	4702	ATP	PA-O3A-PB	-5.12	115.25	132.83
3	C	4701	ADP	PA-O3A-PB	-4.56	117.17	132.83
3	C	4704	ADP	PA-O3A-PB	-4.21	118.36	132.83
4	C	4702	ATP	PB-O3B-PG	-4.13	118.64	132.83
3	C	4703	ADP	PA-O3A-PB	-4.13	118.66	132.83
3	C	4703	ADP	N3-C2-N1	-3.65	122.97	128.68
4	C	4702	ATP	N3-C2-N1	-3.65	122.97	128.68
3	C	4704	ADP	N3-C2-N1	-3.52	123.17	128.68
3	C	4703	ADP	C3'-C2'-C1'	3.17	105.76	100.98
3	C	4701	ADP	N3-C2-N1	-3.13	123.78	128.68
3	C	4701	ADP	C4-C5-N7	-2.94	106.34	109.40
3	C	4704	ADP	C3'-C2'-C1'	2.79	105.18	100.98
3	C	4704	ADP	C4-C5-N7	-2.54	106.75	109.40
4	C	4702	ATP	C4-C5-N7	-2.15	107.16	109.40
4	C	4702	ATP	N6-C6-N1	2.15	123.03	118.57
3	C	4703	ADP	C4-C5-N7	-2.09	107.22	109.40

There are no chirality outliers.

All (12) torsion outliers are listed below:

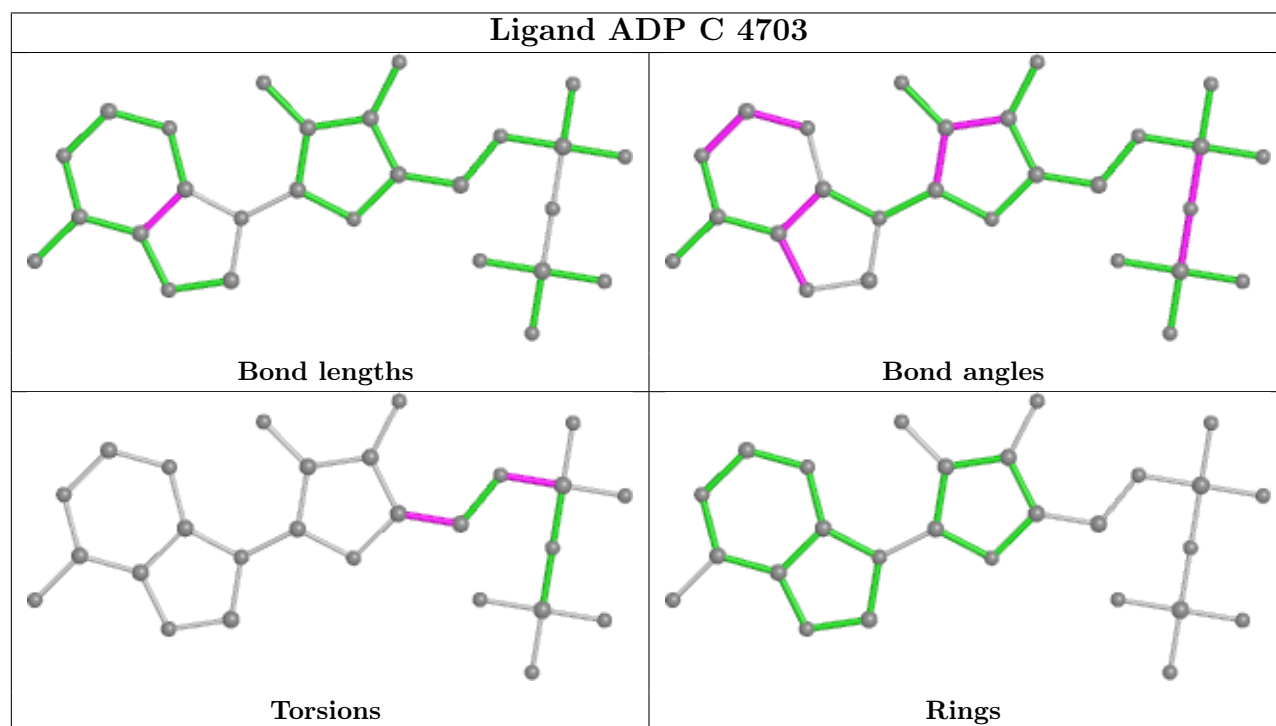
Mol	Chain	Res	Type	Atoms
3	C	4703	ADP	C5'-O5'-PA-O1A
3	C	4703	ADP	C5'-O5'-PA-O2A
3	C	4704	ADP	C5'-O5'-PA-O2A
4	C	4702	ATP	C5'-O5'-PA-O1A
4	C	4702	ATP	C5'-O5'-PA-O3A
4	C	4702	ATP	C3'-C4'-C5'-O5'
4	C	4702	ATP	O4'-C4'-C5'-O5'
3	C	4704	ADP	C5'-O5'-PA-O3A
3	C	4704	ADP	C5'-O5'-PA-O1A
3	C	4703	ADP	C5'-O5'-PA-O3A
3	C	4701	ADP	C5'-O5'-PA-O1A
3	C	4703	ADP	O4'-C4'-C5'-O5'

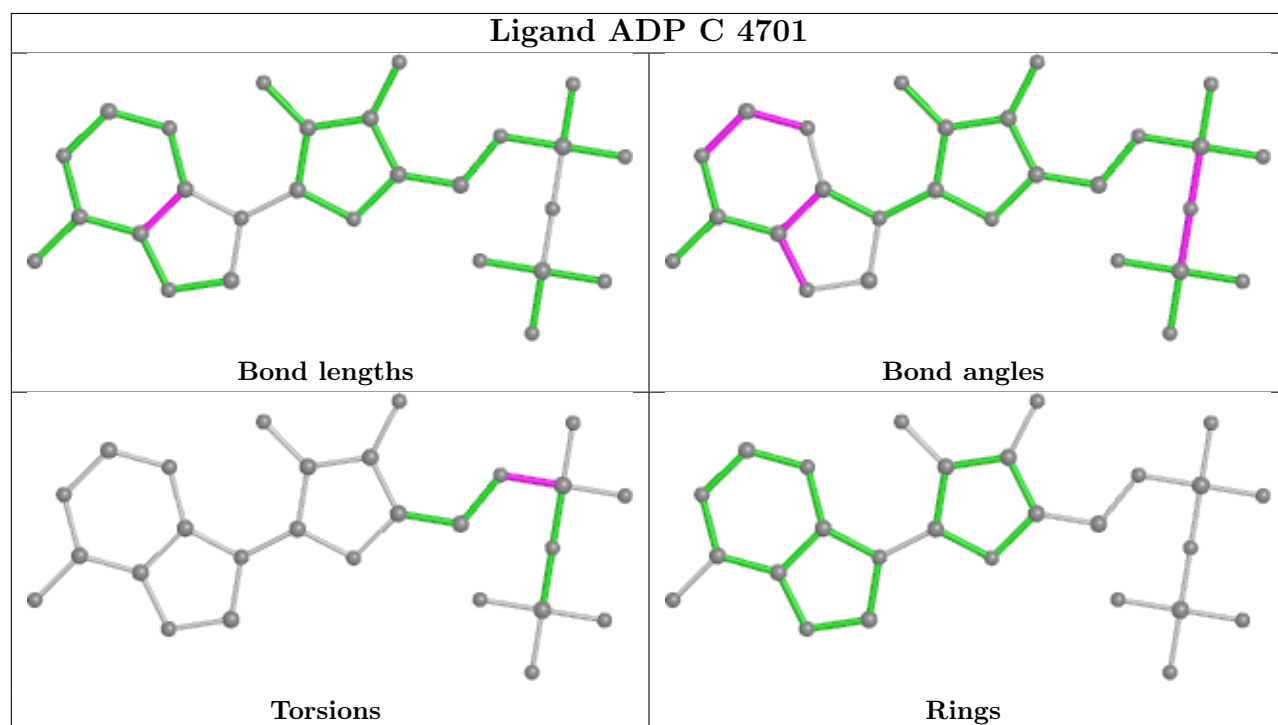
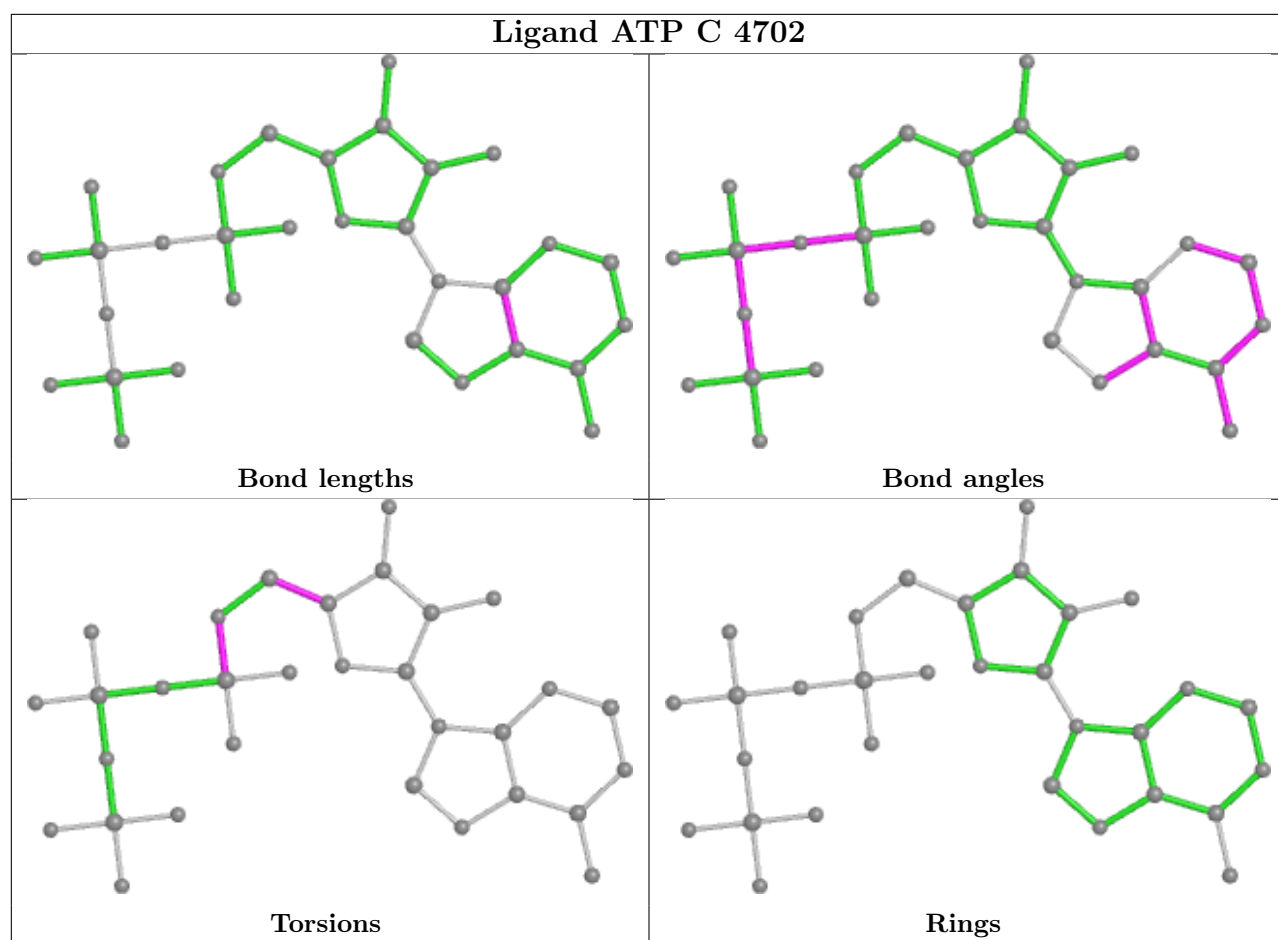
There are no ring outliers.

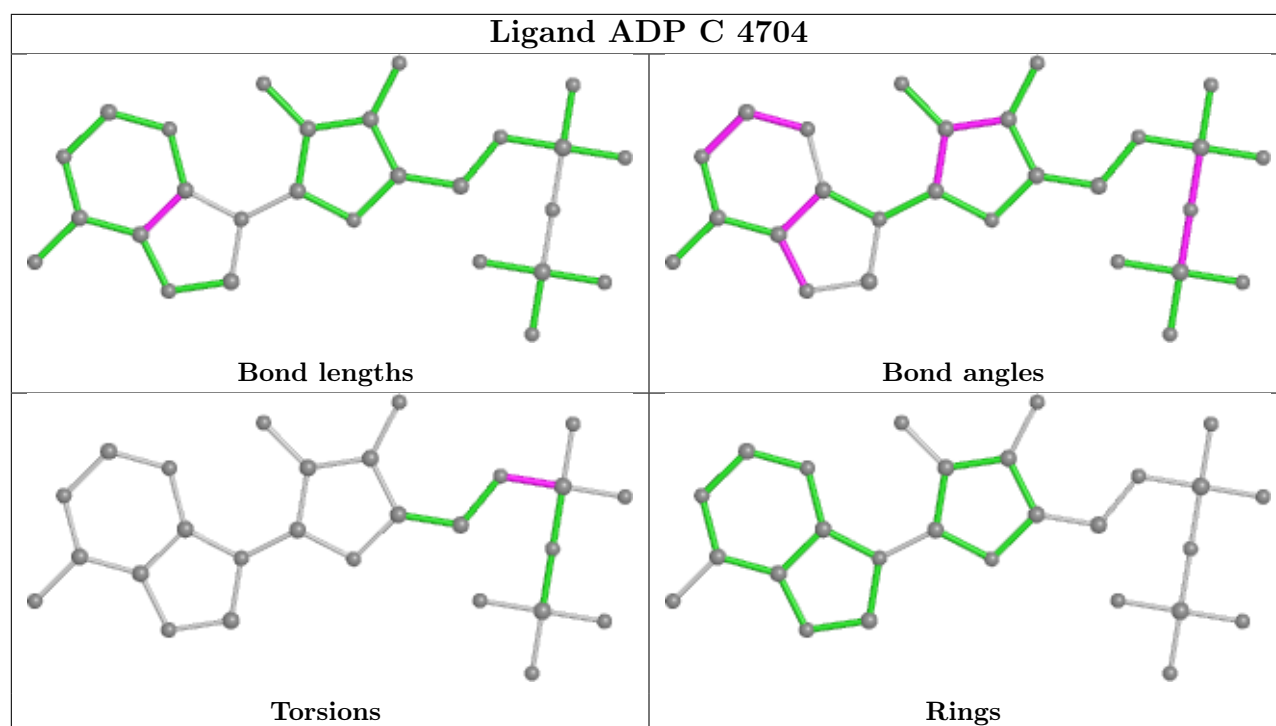
No monomer is involved in short contacts.

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.

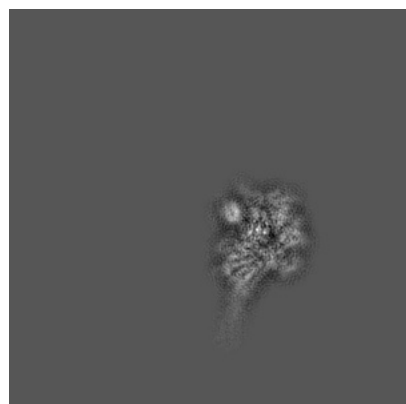
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11581. These allow visual inspection of the internal detail of the map and identification of artifacts.

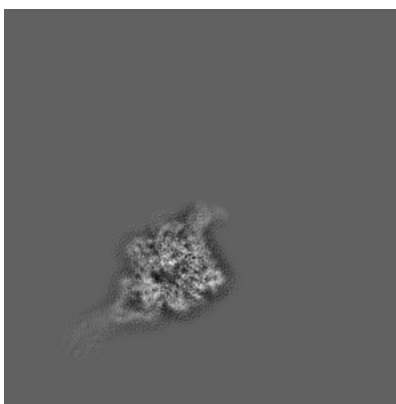
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

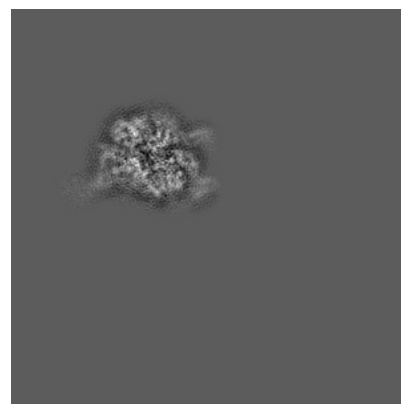
6.1.1 Primary map



X

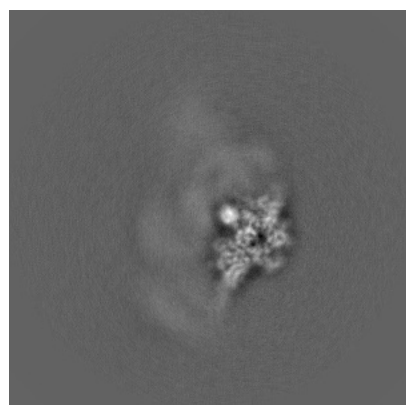


Y

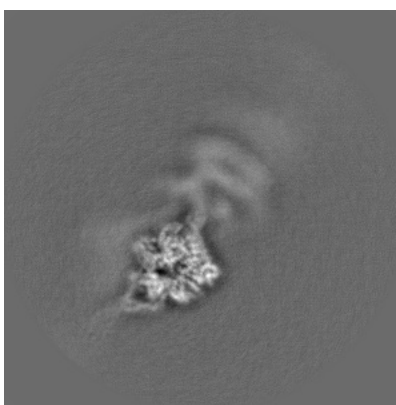


Z

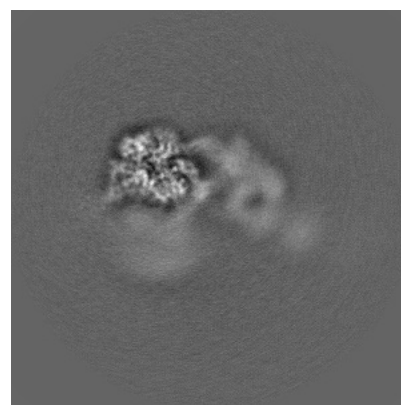
6.1.2 Raw map



X



Y

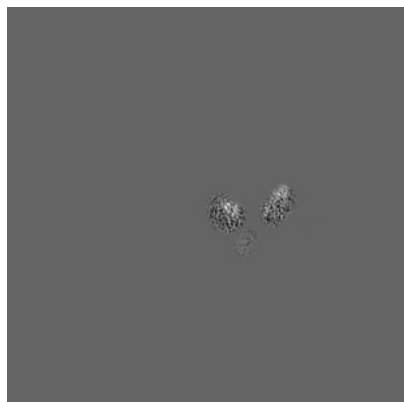


Z

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

6.2 Central slices [i](#)

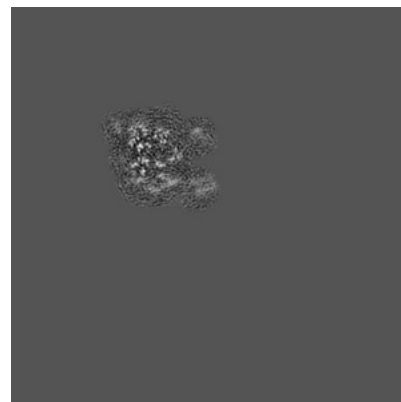
6.2.1 Primary map



X Index: 225

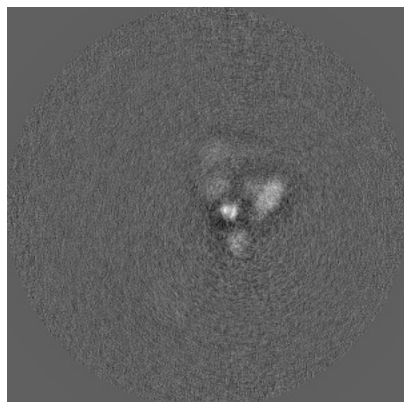


Y Index: 225

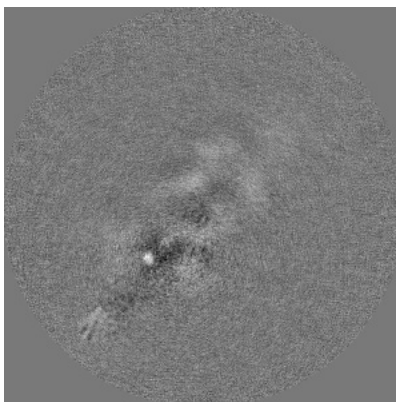


Z Index: 225

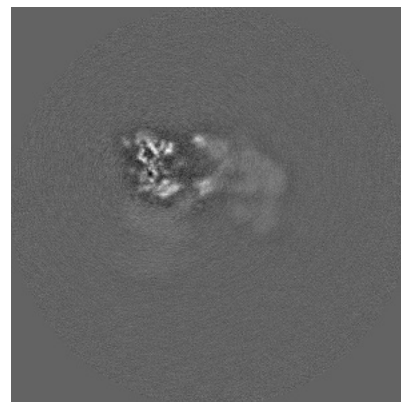
6.2.2 Raw map



X Index: 256



Y Index: 256

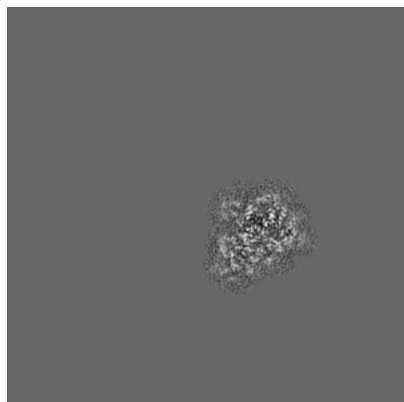


Z Index: 256

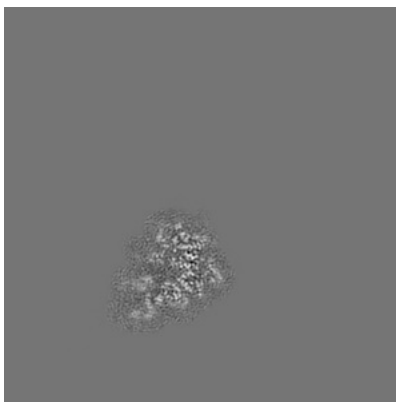
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

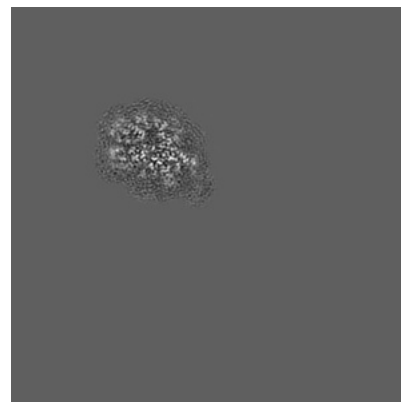
6.3.1 Primary map



X Index: 164

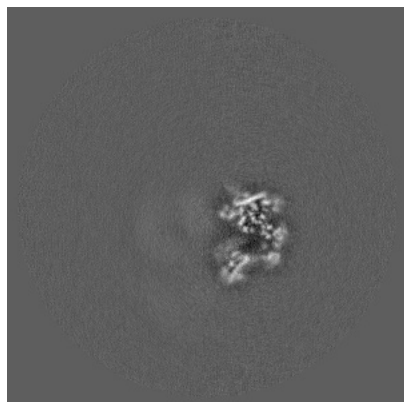


Y Index: 281

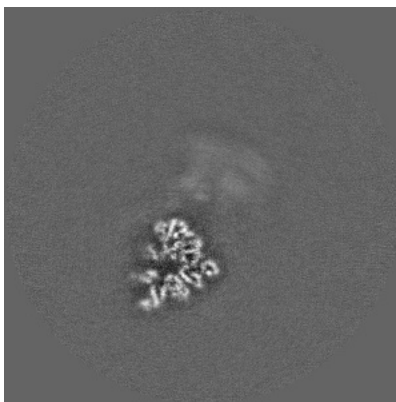


Z Index: 201

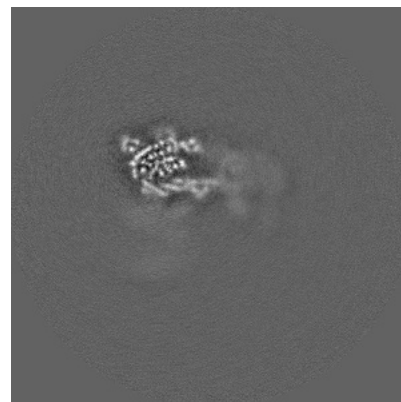
6.3.2 Raw map



X Index: 171



Y Index: 305

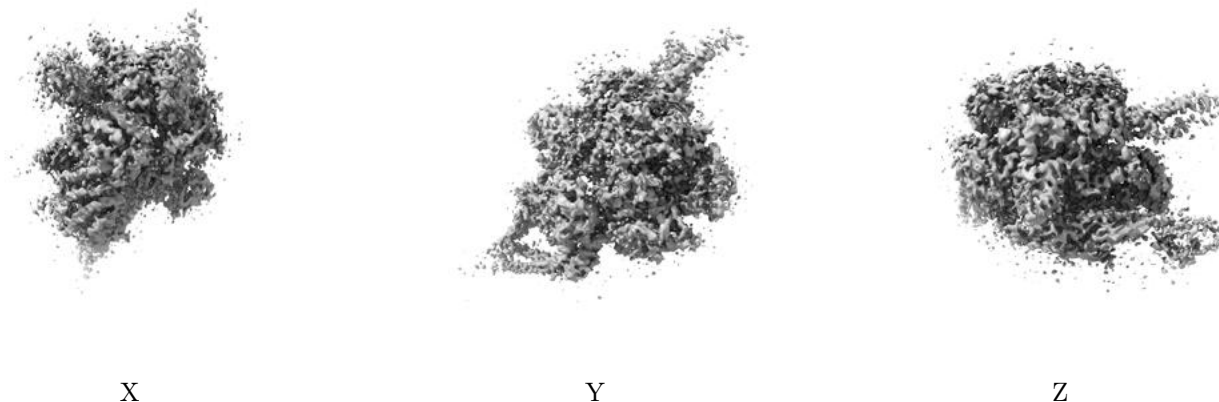


Z Index: 243

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

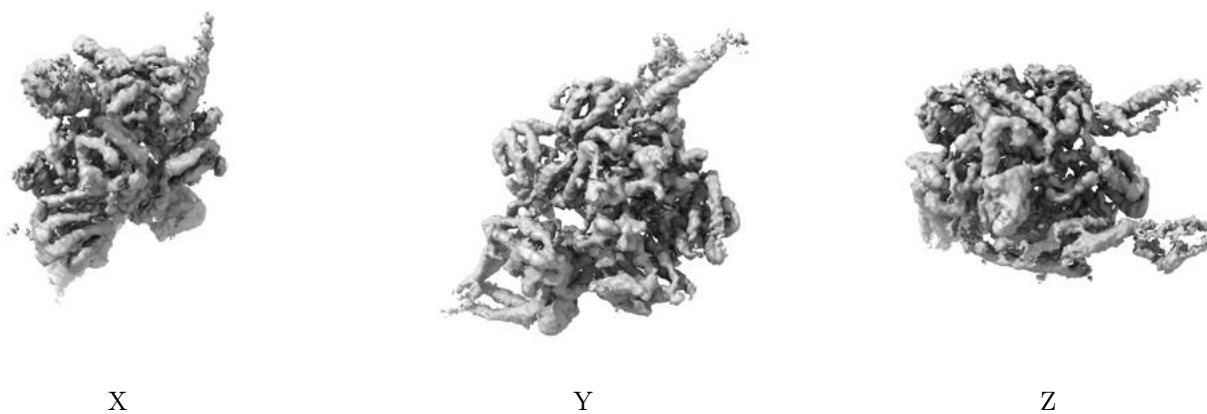
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

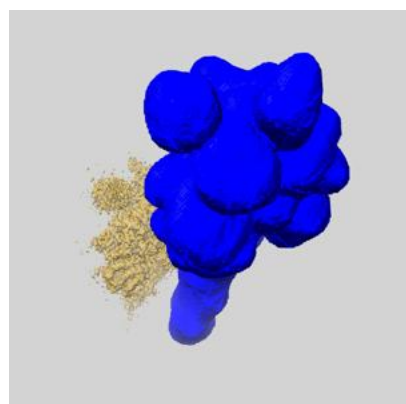
6.5 Mask visualisation [i](#)

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

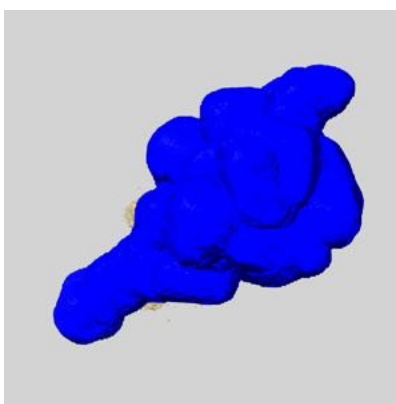
A mask typically either:

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

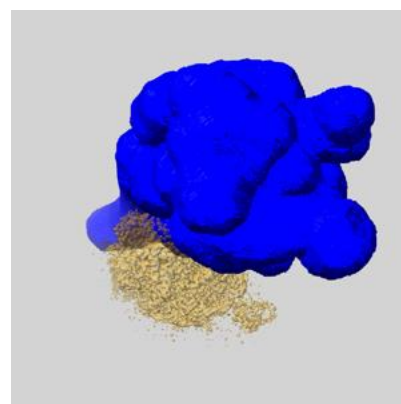
6.5.1 emd_11581_msk_2.map [i](#)



X

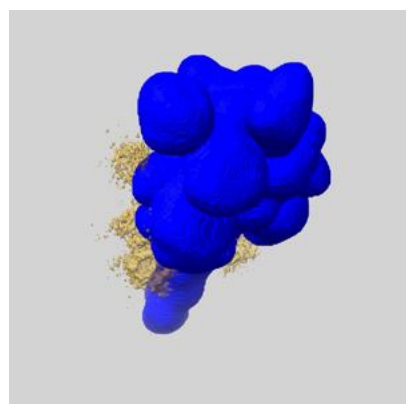


Y

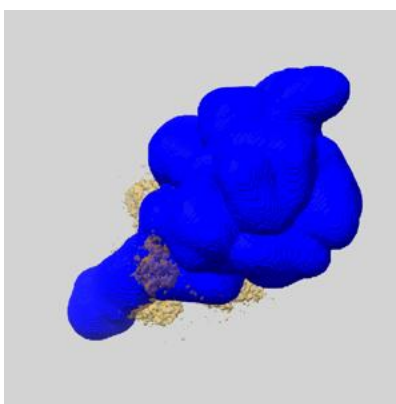


Z

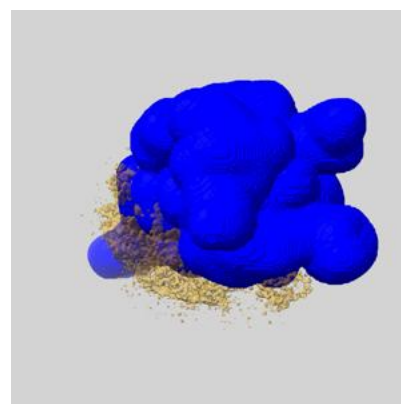
6.5.2 emd_11581_msk_1.map [i](#)



X



Y

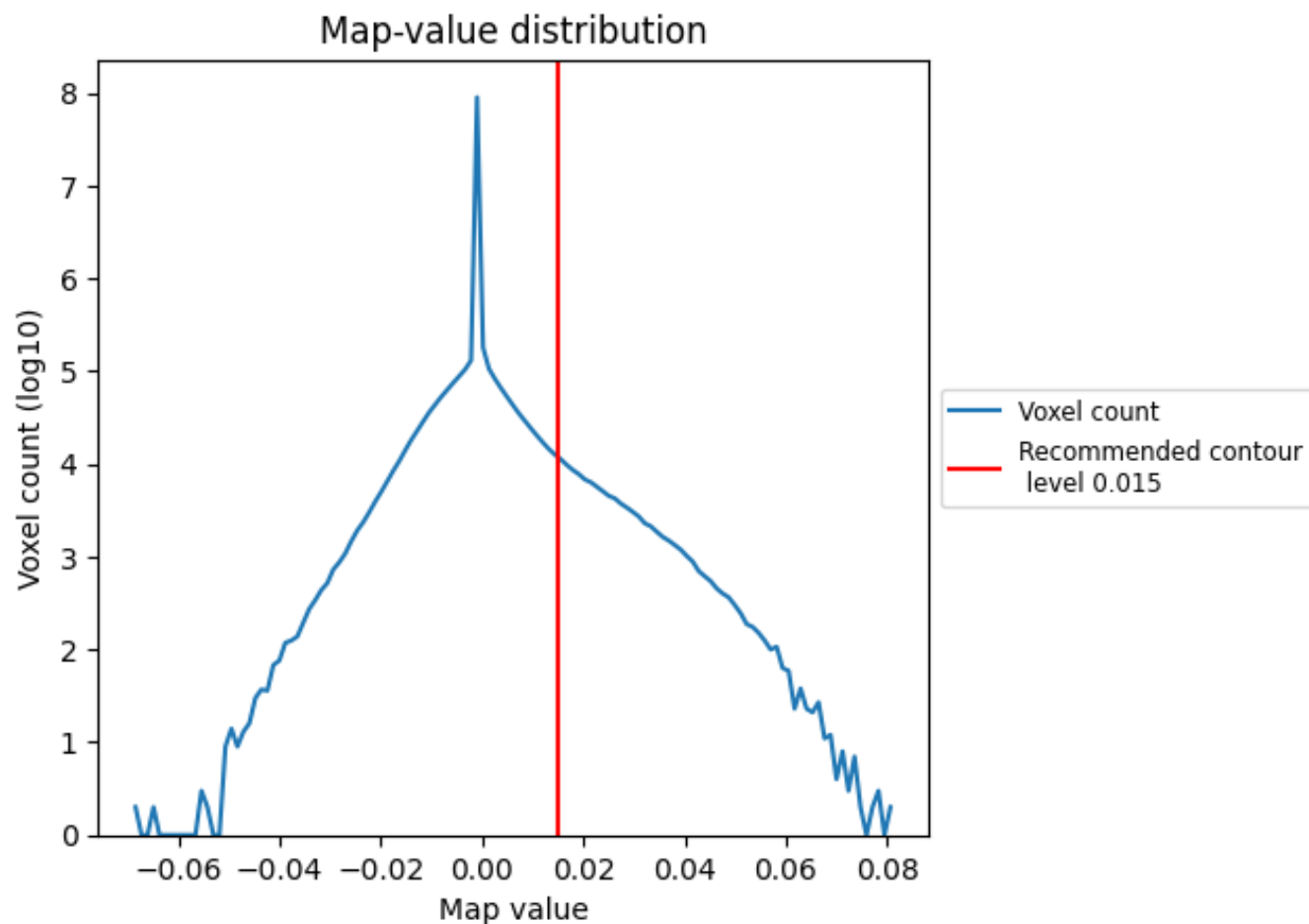


Z

7 Map analysis [i](#)

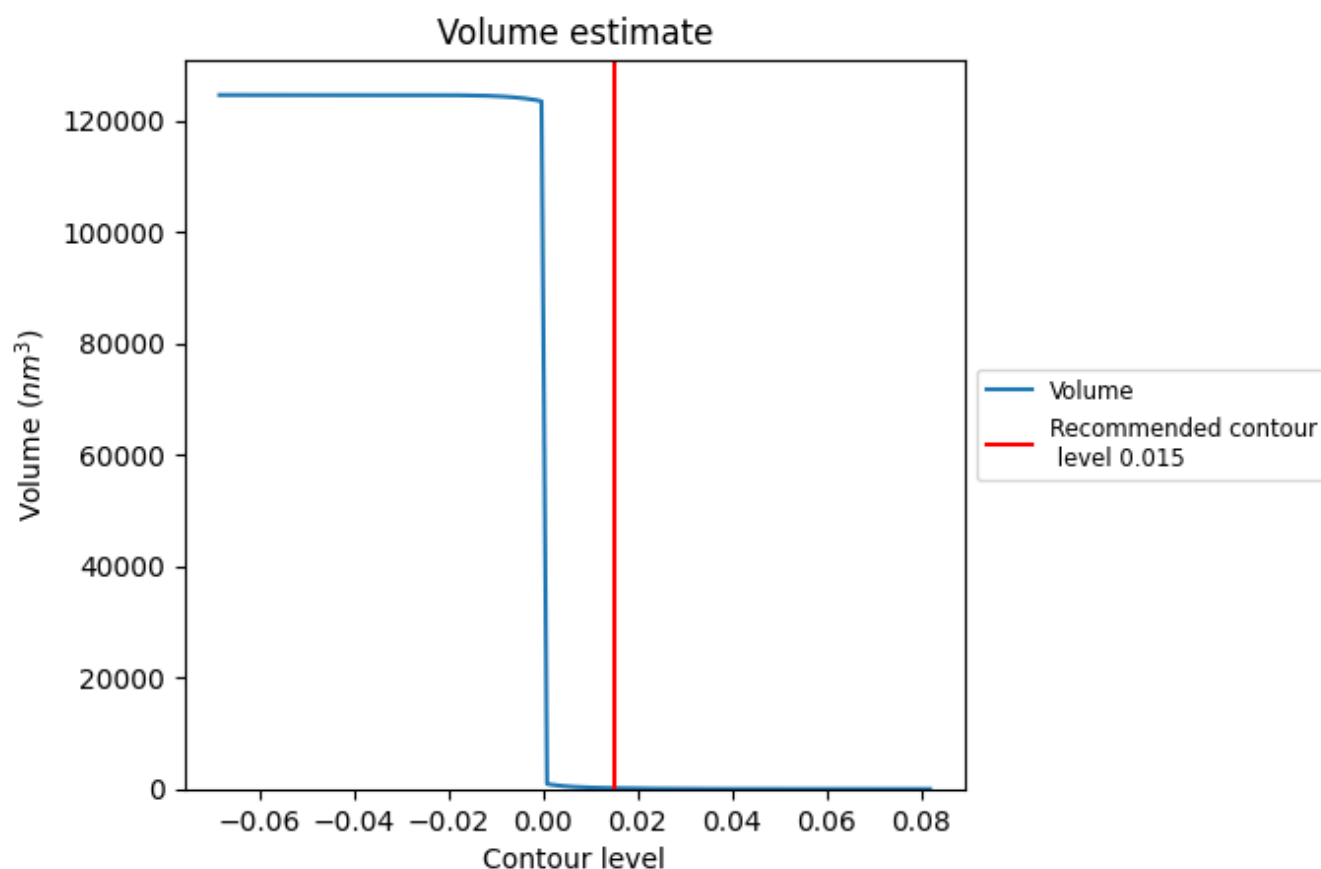
This section contains the results of statistical analysis of the map.

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.

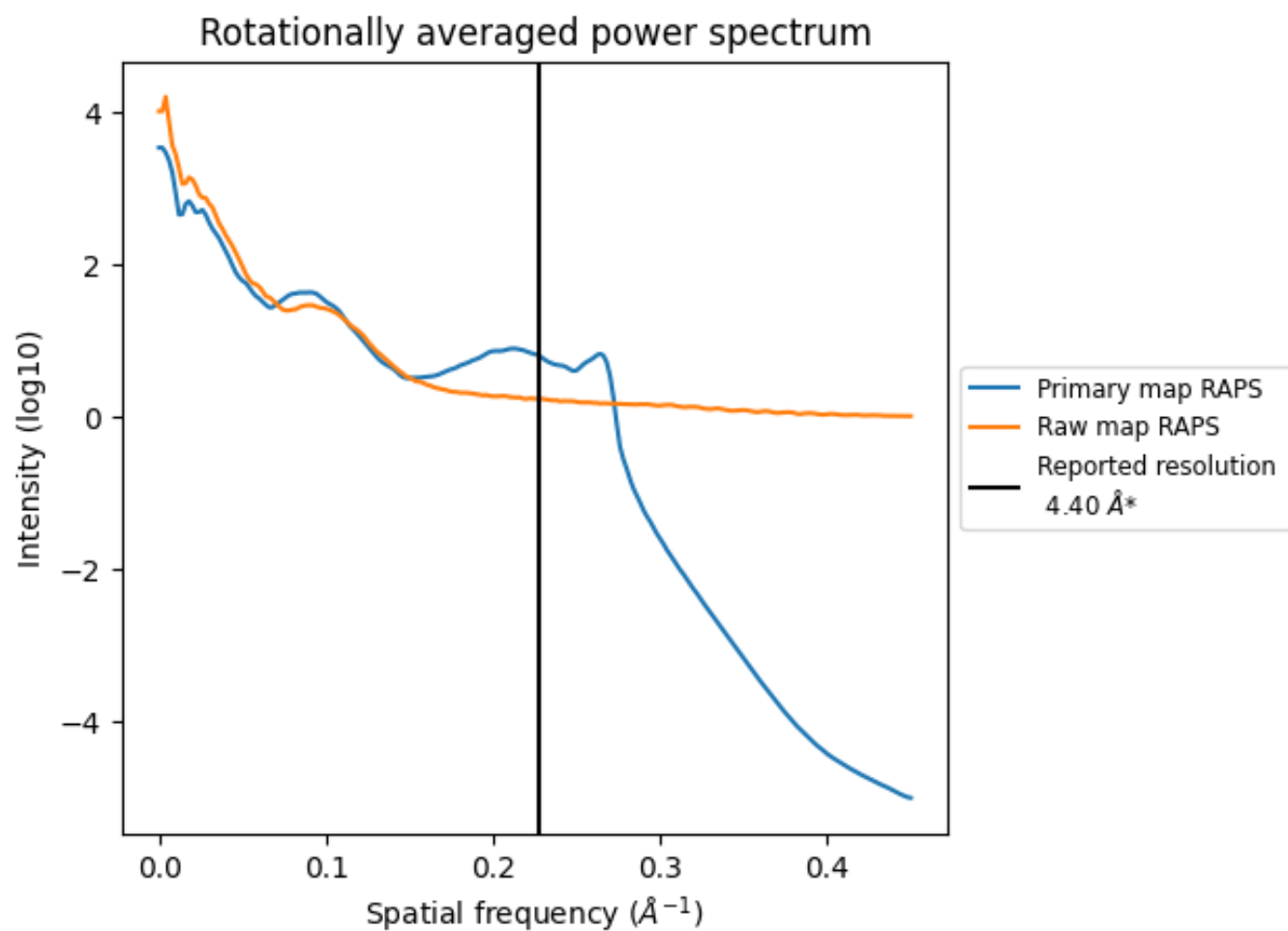
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 147 nm³; this corresponds to an approximate mass of 133 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 ⓘ

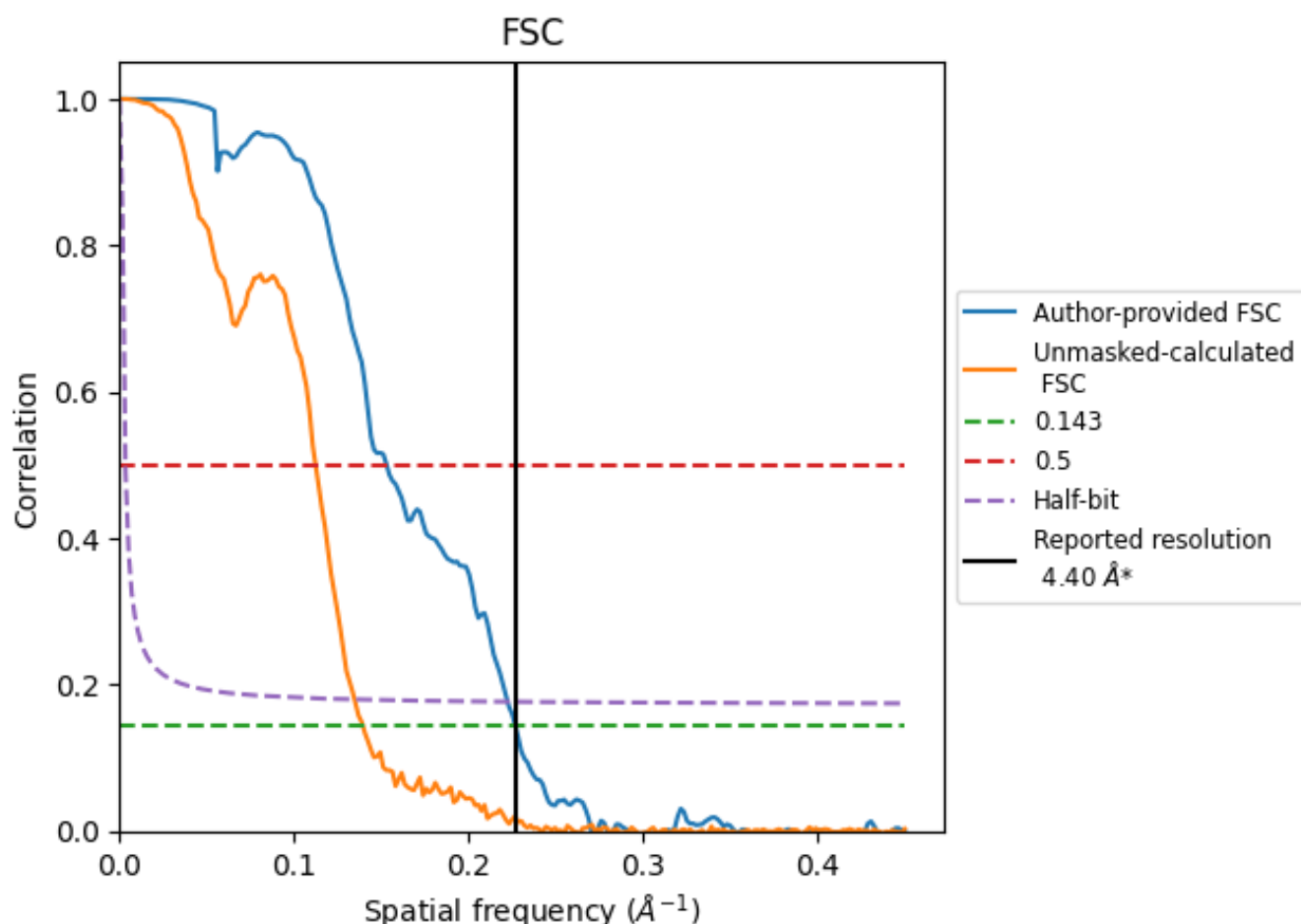


*Reported resolution corresponds to spatial frequency of 0.227 Å⁻¹

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 0.227 Å⁻¹

8.2 Resolution estimates [i](#)

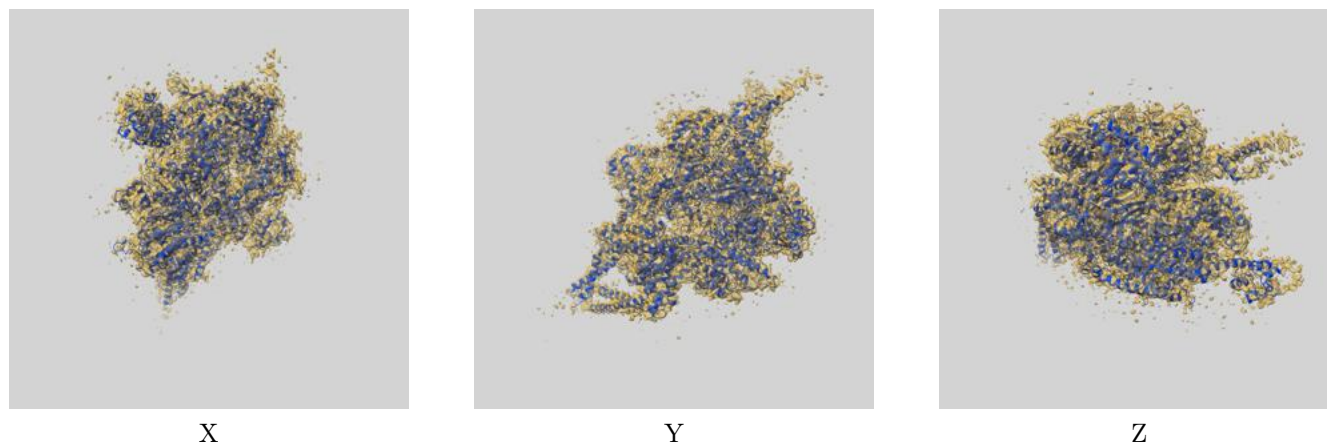
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.40	6.53	4.49
Unmasked-calculated*	7.16	8.88	7.42

*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 7.16 differs from the reported value 4.4 by more than 10 %

9 Map-model fit [i](#)

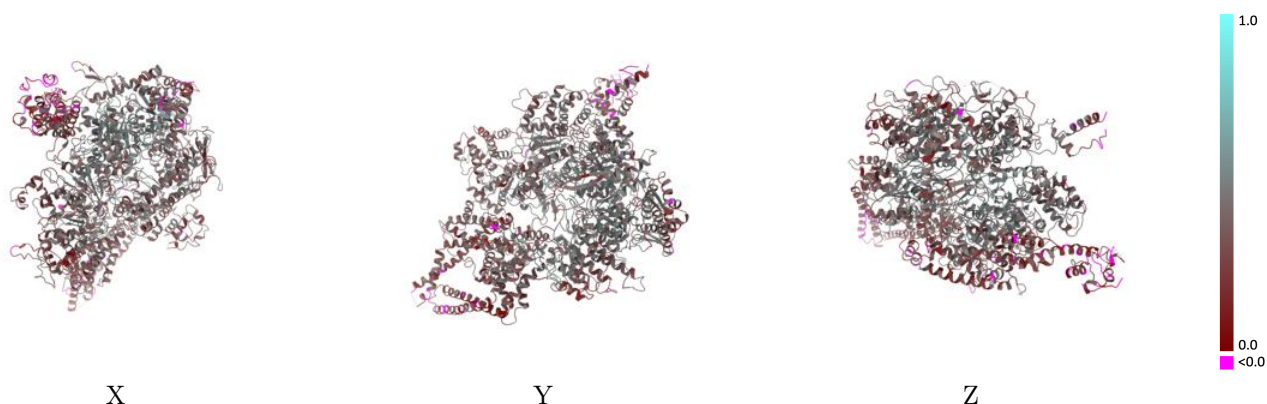
This section contains information regarding the fit between EMDB map EMD-11581 and PDB model 6ZYY. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



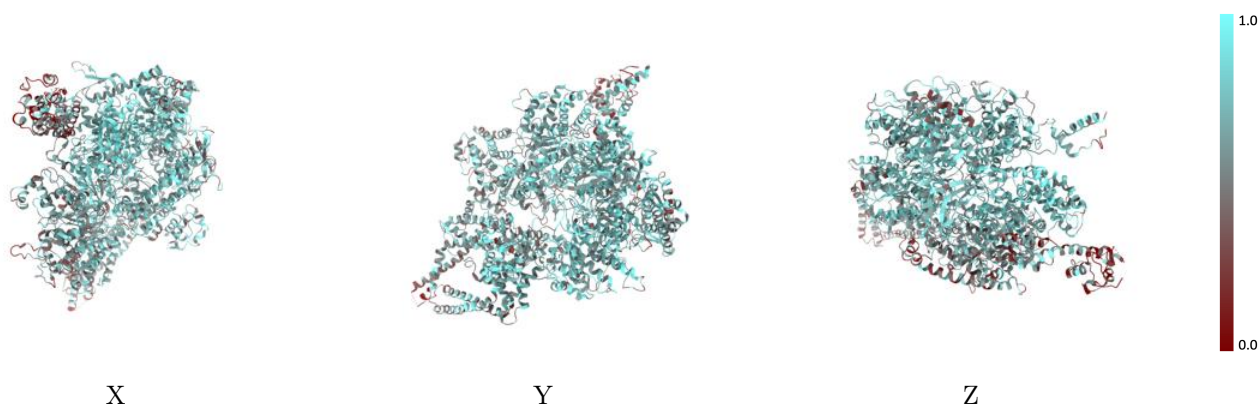
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



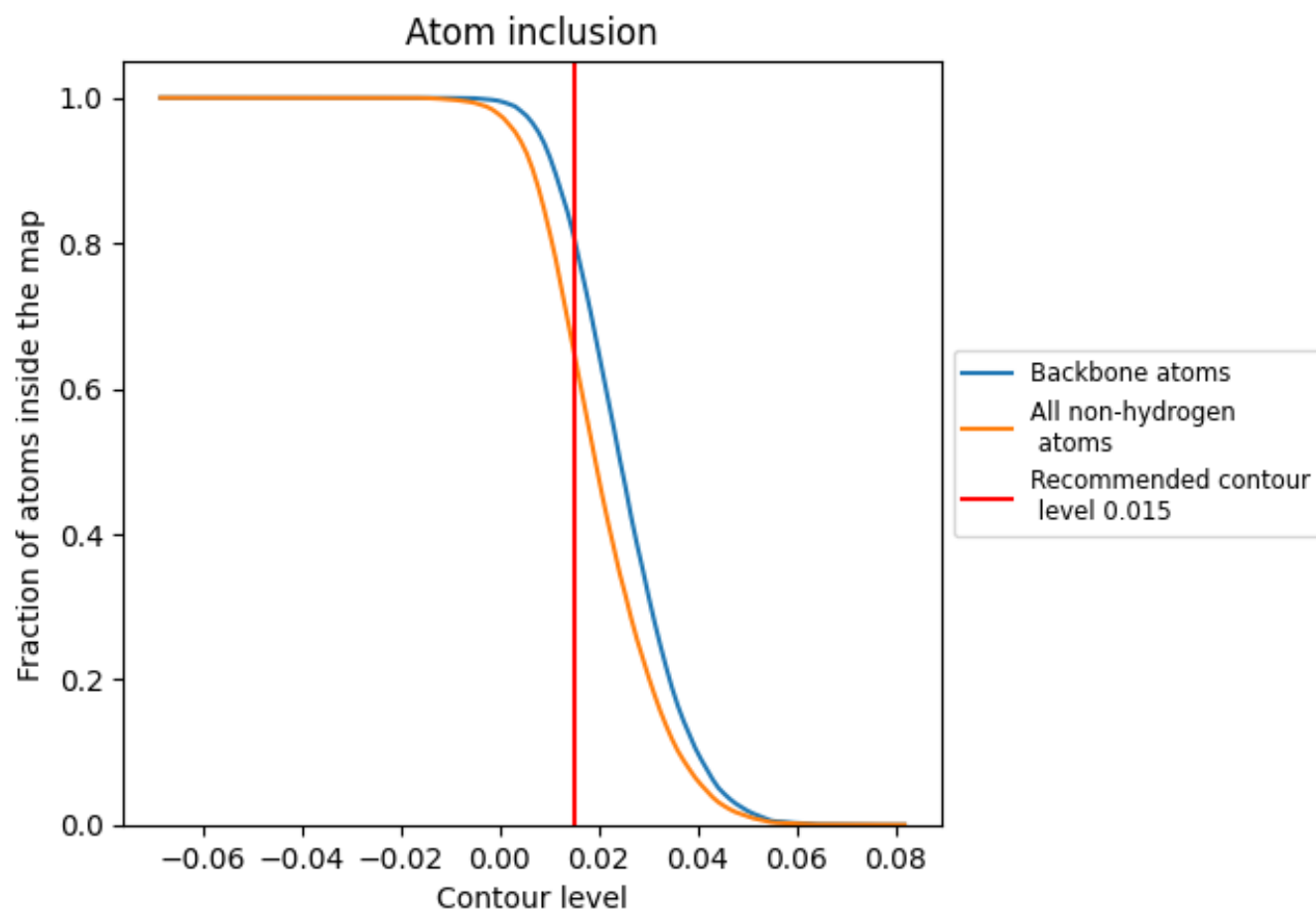
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 65% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6542	<div></div> 0.3880
C	<div></div> 0.6546	<div></div> 0.3890
Y	<div></div> 0.6368	<div></div> 0.3590

