



wwPDB EM Validation Summary Report ⓘ

Aug 5, 2026 – 01:57 AM EDT

PDB ID : 8FDT / pdb_00008fdt
EMDB ID : EMD-29012
Title : Engineered human dynein motor domain in the microtubule-unbound state
with LIS1 complex in the buffer containing ATP-Vi
Authors : Ton, W.; Wang, Y.; Chai, P.
Deposited on : 2022-12-04
Resolution : 3.20 Å(reported)

This is a wwPDB EM Validation Summary 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.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

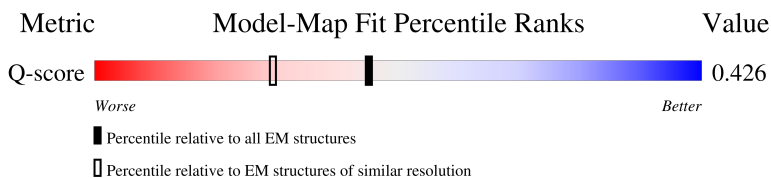
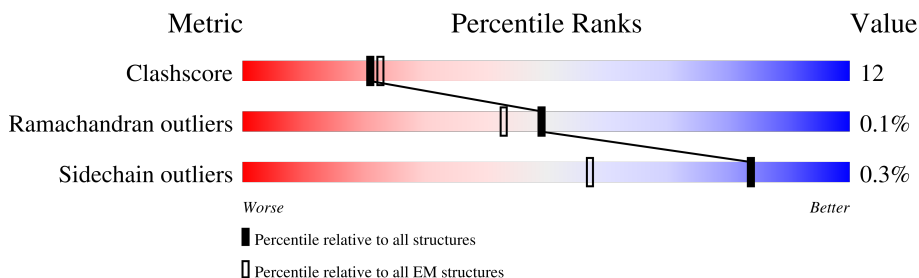
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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

Mol	Chain	Length	Quality of chain
1	A	3126	
2	B	598	
2	C	598	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 27096 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, Serine-tRNA ligase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2736	Total	C	N	O	S	0	0
			21981	14013	3800	4058	110		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q14204
A	2	SER	-	expression tag	UNP Q14204
A	3125	GLU	-	expression tag	UNP Q14204
A	3126	PHE	-	expression tag	UNP Q14204

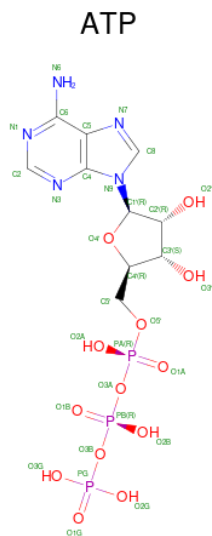
- Molecule 2 is a protein called Platelet-activating factor acetylhydrolase IB subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	316	Total	C	N	O	S	0	0
			2499	1571	441	467	20		
2	C	316	Total	C	N	O	S	0	0
			2499	1571	441	467	20		

There are 4 discrepancies between the modelled and reference sequences:

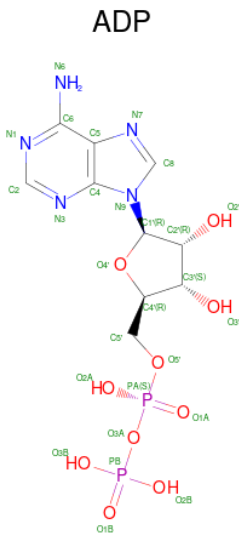
Chain	Residue	Modelled	Actual	Comment	Reference
B	1	GLY	-	expression tag	UNP P43034
B	2	SER	-	expression tag	UNP P43034
C	1	GLY	-	expression tag	UNP P43034
C	2	SER	-	expression tag	UNP P43034

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (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 ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).



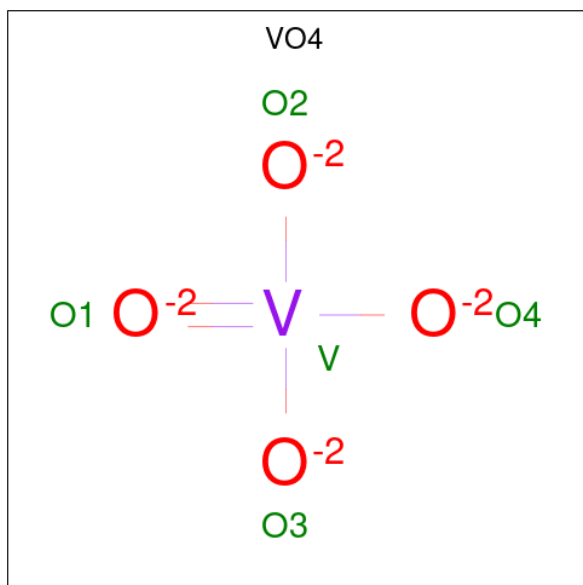
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total 27	C 10	N 5	O 10	P 2	0
4	A	1	Total 27	C 10	N 5	O 10	P 2	0

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

- Molecule 5 is VANADATE ION (CCD ID: VO4) (formula: O_4V) (labeled as "Ligand of Interest" by depositor).

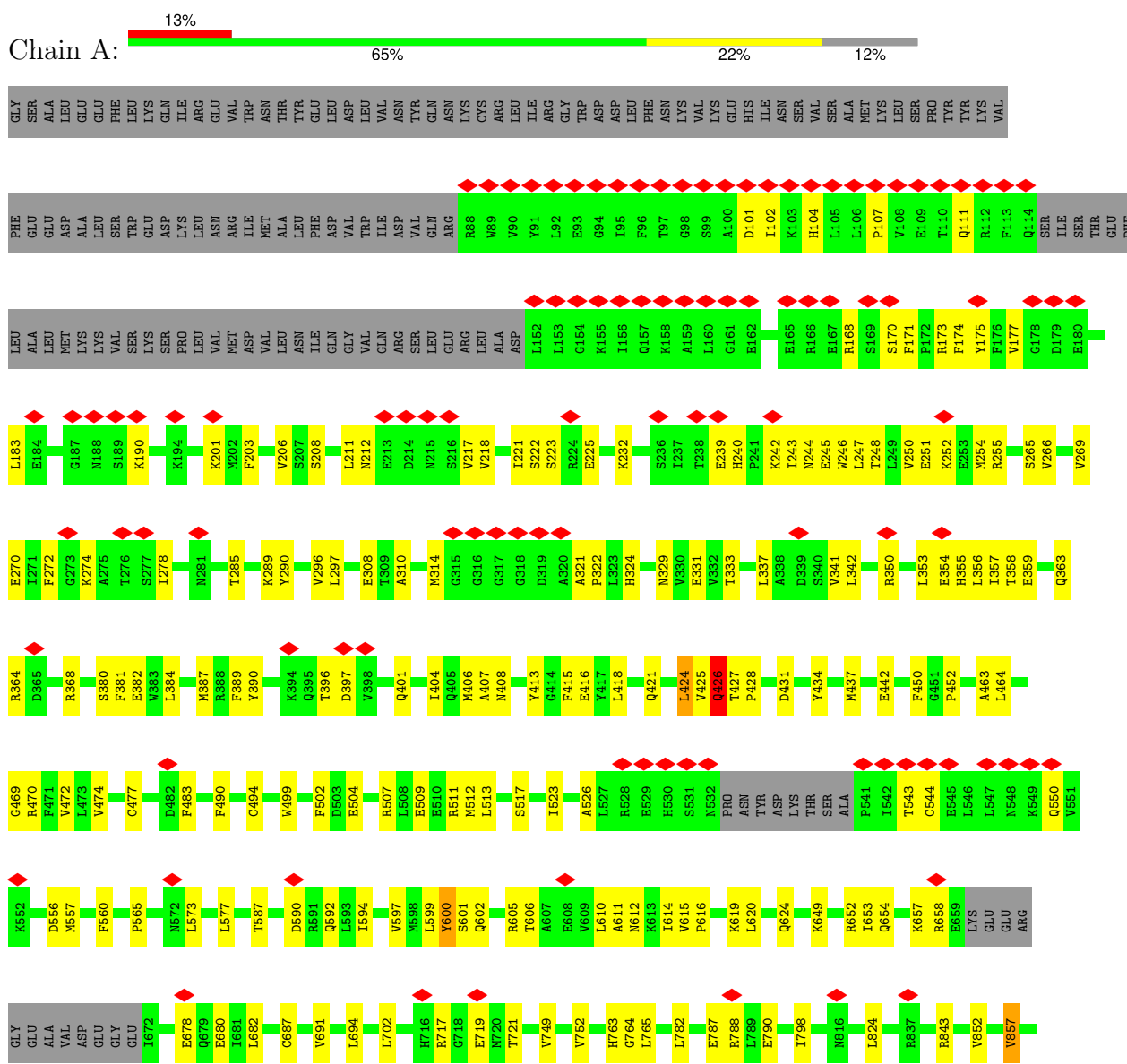


Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	O	V	0
			5	4	1	

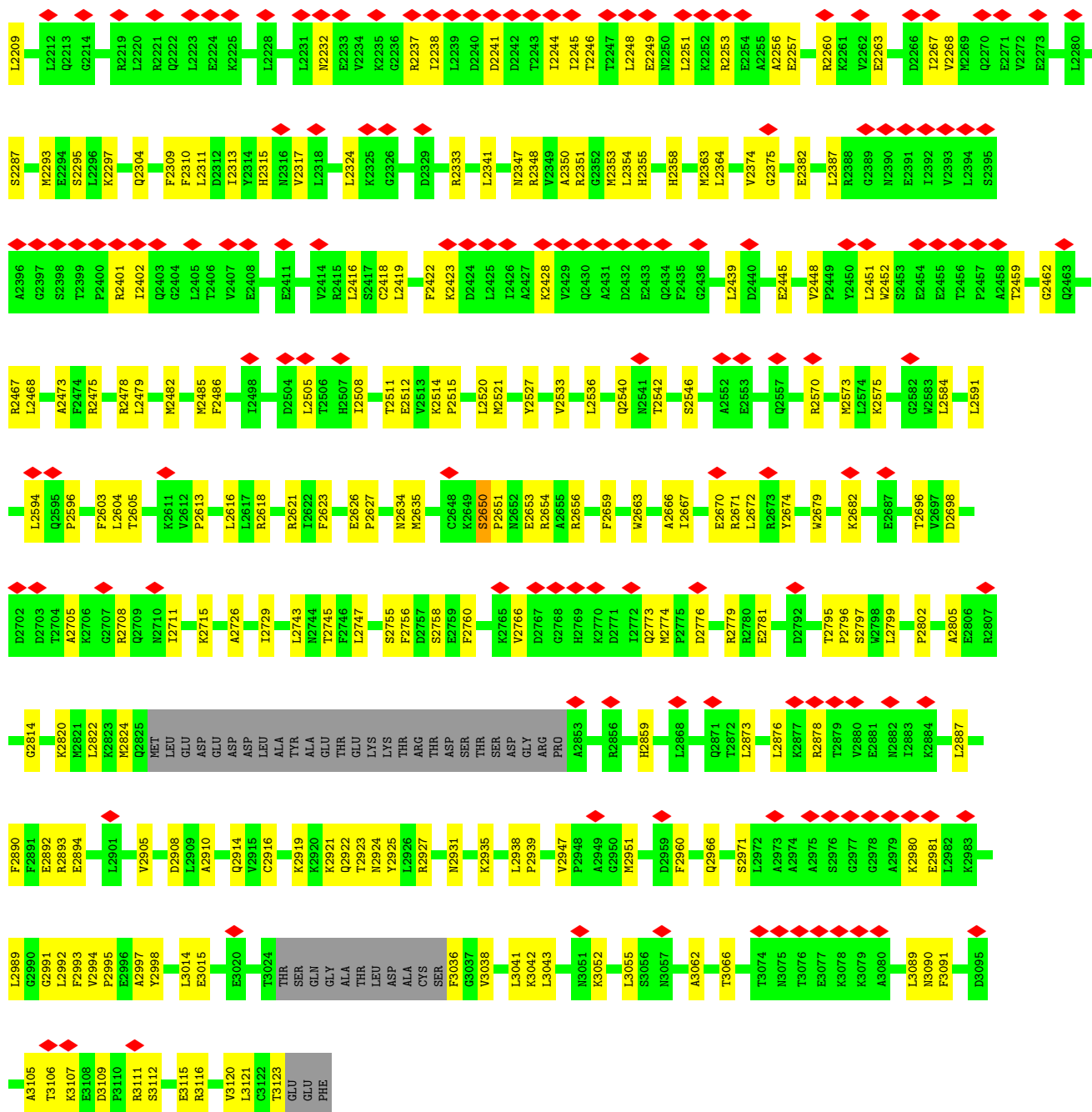
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

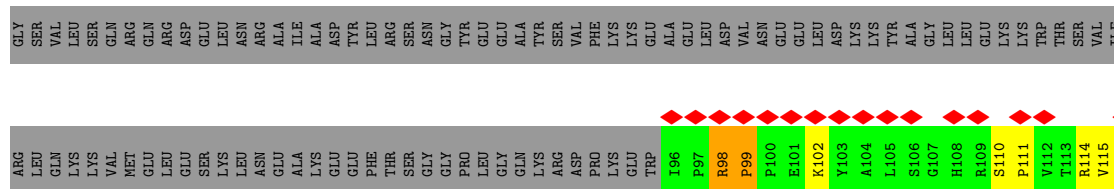
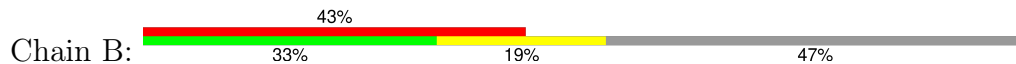
- Molecule 1: Cytoplasmic dynein 1 heavy chain 1, Serine-tRNA ligase



A2096	L1866	ALA	GLN	E1740	E1645	L1566	H1463	L1358	F1253	T1128	P993	M861
F2097	L1887	ARG	ILE	H1745	M1658	E1561	I1467	E1359	V1254	W1129	R996	S862
R2098	S1888	GLY	ARG	L1746	D1659	E1660	I1470	T1360	G1255	E1132	V863	V863
R2106	Y1994	ALA	ALA	M1747	N1664	E1567	L1478	L1366	C1257	K1134	L1000	L869
F2107	F1998	LEU	LEU	V1748	Y1665	D1569	L1479	L1367	M1258	P1135	G1001	R877
D2115	D1999	VAL	GLY	G1749	I1666	E1570	L1480	R1368	T1261	L1138	F1003	M887
V2116	Q2000	LEU	GLN	L1750	I1666	E1571	I1481	R1369	D1262	C1139	S1005	R903
E2117	Q2001	ILE	ALA	K1751	D1669	T1576	G1485	W1370	G1264	P1142	M1006	C904
S2118	M2002	SER	GLN	K1752	V1670	Q1577	K1488	A1371	R1265	G1143	Q1009	G905
Y2119	L2006	GLU	VAL	I1753	M1671	C1578	K1579	A1374	K1266	S1144	G1145	M906
N2124	L2014	ALA	ILE	K1754	P1672	E1579	M1498	Q1379	P1277	T1148	F1024	F920
P2125	L2014	GLU	ASP	T1755	P1672	E1579	M1498	Q1379	V1278	T1149	P1025	S929
V2126	L2014	ALA	GLN	V1757	Y1673	E1580	M1498	Q1379	P1284	L1150	M1026	I930
Q2020	Q2020	LEU	GLN	D1758	Y1675	E1581	L1501	D1380	P1284	P1158	E1029	P931
F2021	R2021	ASP	MET	Q1759	D1676	G1581	S1502	R1385	S1288	L1176	Q1030	L932
R2022	R2022	GLY	SER	Q1759	K1677	Q1583	Y1504	E1386	L1289	GLY	L1031	ASP
T2023	T2023	LEU	LEU	E1761	L1678	Q1584	Q1505	E1387	L1289	GLY	E1032	GLY
D2024	D2024	ALA	ALA	E1761	L1678	E1584	Q1505	R1388	L1289	GLY	E1032	GLY
I2025	I2025	VAL	LEU	E1762	P1679	E1585	I1506	R1388	L1289	GLY	E1032	GLY
L2031	L2031	GLU	ASP	L1763	Q1680	E1585	K1507	R1389	L1289	GLY	E1032	GLY
G2135	G2135	GLN	GLN	R1764	P1681	G1586	V1508	R1389	L1289	GLY	E1032	GLY
G2136	G2136	ALA	GLU	R1765	P1682	L1587	V1508	R1389	L1289	GLY	E1032	GLY
R2137	R2137	ASP	VAL	R1765	S1683	L1587	H1509	R1389	L1289	GLY	E1032	GLY
V2138	V2138	LEU	GLN	ASP	E1686	E1588	R1510	R1389	L1289	GLY	E1032	GLY
L2139	L2139	LEU	GLN	LEU	E1686	E1588	R1510	R1389	L1289	GLY	E1032	GLY
I2140	I2140	LEU	LEU	LEU	E1686	E1588	R1510	R1389	L1289	GLY	E1032	GLY
T2141	T2141	GLN	LYS	ILE	V1693	H1591	D1590	A1399	L1308	V1193	D1050	LYS
L2050	L2050	LYS	LYS	LYS	F1694	H1592	T1512	L1400	T1309	V1198	D1050	LYS
E2053	E2053	ARG	ARG	SER	V1695	E1593	E1515	D1407	A1311	Q1199	G1060	ASP
K2059	K2059	LEU	LEU	GLN	H1696	E1593	E1515	R1408	E1312	Y1062	E1061	GLU
R2060	R2060	GLU	GLU	GLU	H1696	E1593	E1515	E1409	P1313	C1208	T1066	GLU
F2061	F2061	ASP	GLU	LEU	Q1697	L1594	D1516	E1409	F1329	E1210	P1070	ALA
L2062	L2062	VAL	VAL	GLU	T1698	E1596	R1526	E1409	F1329	T1211	P1072	ALA
R2063	R2063	GLU	VAL	GLU	L1699	E1596	R1526	E1409	F1329	N1212	P1072	S955
L2066	L2066	ALA	GLN	VAL	L1699	E1596	R1526	E1409	F1329	D1215	P1072	P956
I2067	I2067	ALA	GLN	VAL	L1699	E1596	R1526	E1409	F1329	D1215	P1072	P956
D2069	D2069	ALA	GLN	VAL	L1699	E1596	R1526	E1409	F1329	D1215	P1072	P956
Q2073	Q2073	ALA	VAL	VAL	L1699	E1596	R1526	E1409	F1329	D1215	P1072	P956
E2076	E2076	ALA	VAL	VAL	L1699	E1596	R1526	E1409	F1329	D1215	P1072	P956
M2079	M2079	ALA	VAL	VAL	L1699	E1596	R1526	E1409	F1329	D1215	P1072	P956
D2084	D2084	ALA	VAL	VAL	L1699	E1596	R1526	E1409	F1329	D1215	P1072	P956
R2085	R2085	ALA	VAL	VAL	L1699	E1596	R1526	E1409	F1329	D1215	P1072	P956
K2086	K2086	ALA	VAL	VAL	L1699	E1596	R1526	E1409	F1329	D1215	P1072	P956
R2089	R2089	ALA	VAL	VAL	L1699	E1596	R1526	E1409	F1329	D1215	P1072	P956
D2095	D2095	ALA	VAL	VAL	L1699	E1596	R1526	E1409	F1329	D1215	P1072	P956
D2103	D2103	ALA	VAL	VAL	L1699	E1596	R1526	E1409	F1329	D1215	P1072	P956
E2204	E2204	ALA	VAL	VAL	L1699	E1596	R1526	E1409	F1329	D1215	P1072	P956
D2208	D2208	ALA	VAL	VAL	L1699	E1596	R1526	E1409	F1329	D1215	P1072	P956



• Molecule 2: Platelet-activating factor acetylhydrolase IB subunit beta



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	53572	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	1.563	Depositor
Minimum map value	-0.893	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.045	Depositor
Recommended contour level	0.3	Depositor
Map size ($\text{\AA}$)	413.64, 413.64, 413.64	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.149, 1.149, 1.149	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: VO4, ADP, ATP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.35	0/22453	0.50	2/30431 (0.0%)
2	B	0.25	1/2563 (0.0%)	0.46	1/3472 (0.0%)
2	C	0.25	0/2563	0.44	1/3472 (0.0%)
All	All	0.34	1/27579 (0.0%)	0.49	4/37375 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	98	ARG	N-CA	5.06	1.49	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	99	PRO	N-CA-C	6.33	118.42	110.70
2	B	99	PRO	N-CA-C	5.62	117.56	110.70
1	A	1674	VAL	N-CA-C	-5.60	106.75	111.56
1	A	763	HIS	N-CA-C	-5.07	107.48	113.97

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	21981	0	22048	497	0
2	B	2499	0	2434	86	0
2	C	2499	0	2434	68	0
3	A	31	0	12	0	0
4	A	81	0	36	2	0
5	A	5	0	0	0	0
All	All	27096	0	26964	642	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 12.

The worst 5 of 642 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:426:GLN:OE1	1:A:426:GLN:N	1.59	1.34
1:A:1261:THR:HG22	1:A:2923:THR:HG23	1.21	1.16
1:A:1261:THR:CG2	1:A:2923:THR:HG23	1.86	1.05
1:A:991:ILE:HD12	1:A:1139:CYS:SG	2.05	0.97
1:A:1263:PRO:HD3	1:A:2927:ARG:HH22	1.31	0.95

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2720/3126 (87%)	2611 (96%)	104 (4%)	5 (0%)	43	73
2	B	314/598 (52%)	298 (95%)	16 (5%)	0	100	100
2	C	314/598 (52%)	301 (96%)	13 (4%)	0	100	100
All	All	3348/4322 (78%)	3210 (96%)	133 (4%)	5 (0%)	49	79

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2650	SER
1	A	426	GLN
1	A	905	GLY
1	A	600	TYR
1	A	2402	ILE

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	2429/2766 (88%)	2421 (100%)	8 (0%)	86	88
2	B	281/505 (56%)	281 (100%)	0	100	100
2	C	281/505 (56%)	281 (100%)	0	100	100
All	All	2991/3776 (79%)	2983 (100%)	8 (0%)	84	88

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2766	VAL
1	A	1503	VAL
1	A	1091	SER
1	A	863	VAL
1	A	1218	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2124	ASN
1	A	2592	HIS
1	A	2490	ASN
1	A	2813	GLN
1	A	922	ASN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

5 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	$\# Z > 2$
5	VO4	A	3205	-	0,4,4	-	-	-		
4	ADP	A	3203	-	28,29,29	0.49	0	43,45,45	0.49	0
4	ADP	A	3204	-	28,29,29	0.46	0	43,45,45	0.47	0
3	ATP	A	3201	-	32,33,33	0.54	0	48,52,52	0.55	0
4	ADP	A	3202	-	28,29,29	0.46	0	43,45,45	0.51	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	A	3201	-	-	0/22/38/38	0/3/3/3
4	ADP	A	3202	-	-	1/16/32/32	0/3/3/3
4	ADP	A	3203	-	-	0/16/32/32	0/3/3/3
4	ADP	A	3204	-	-	2/16/32/32	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

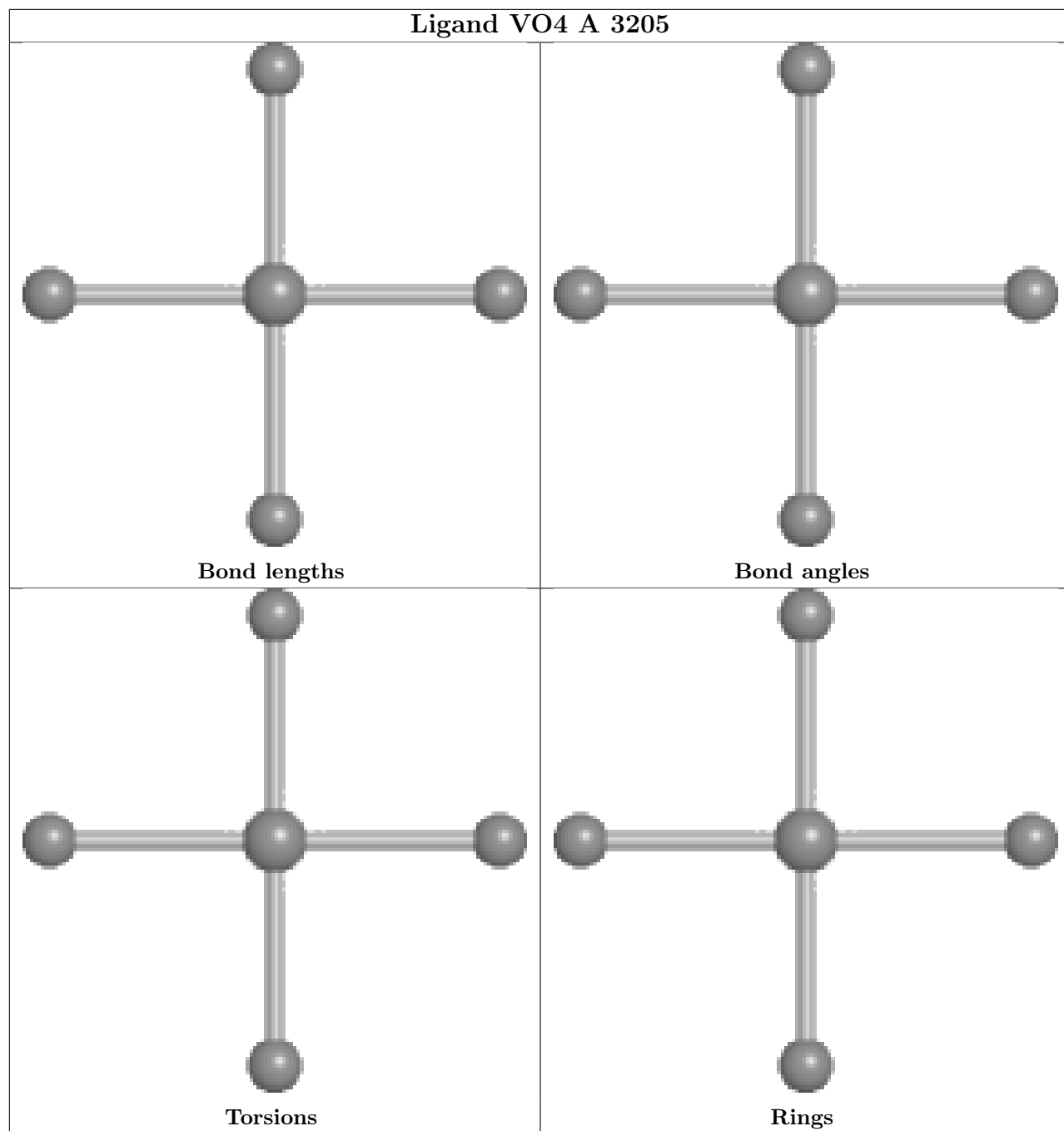
Mol	Chain	Res	Type	Atoms
4	A	3204	ADP	O4'-C4'-C5'-O5'
4	A	3202	ADP	PA-O3A-PB-O1B
4	A	3204	ADP	PA-O3A-PB-O1B

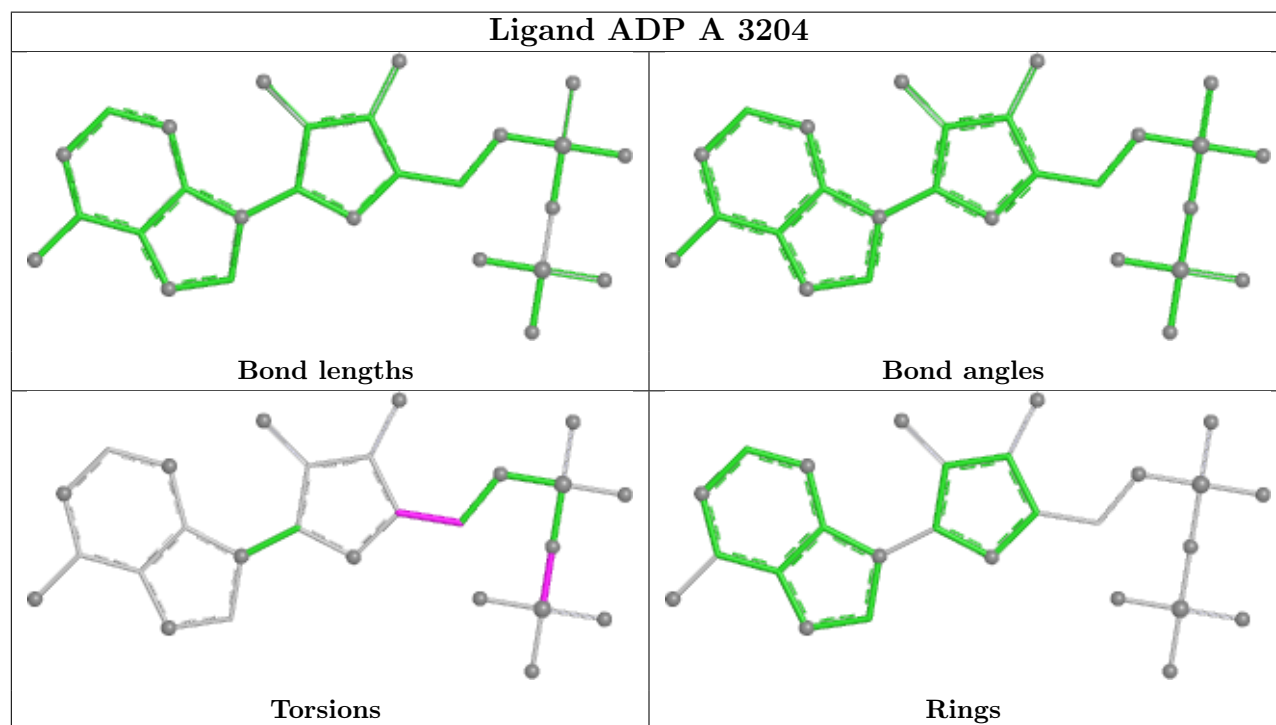
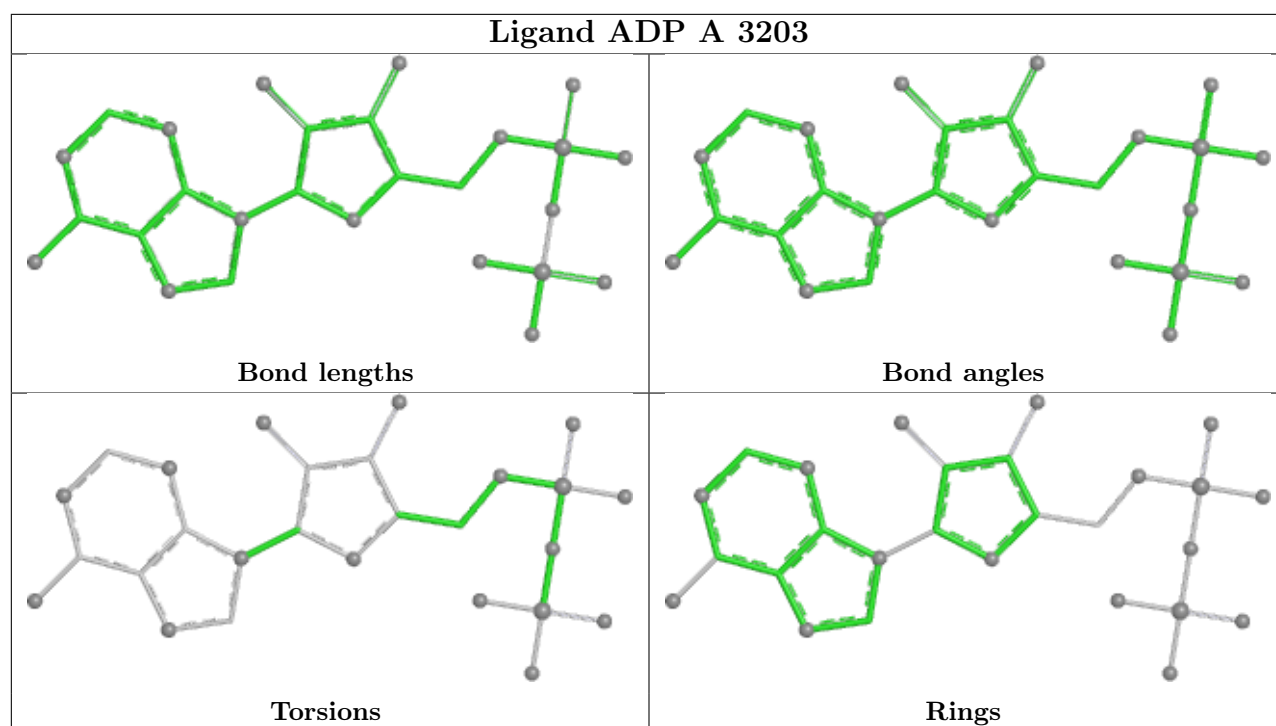
There are no ring outliers.

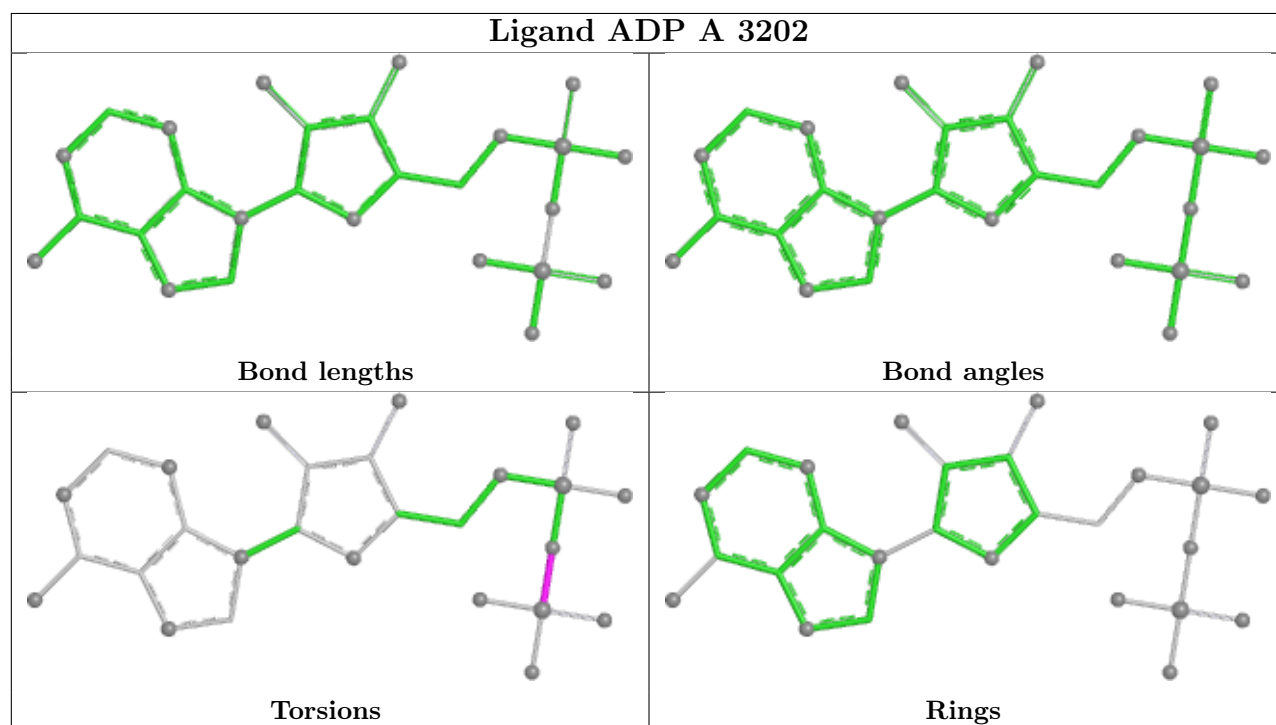
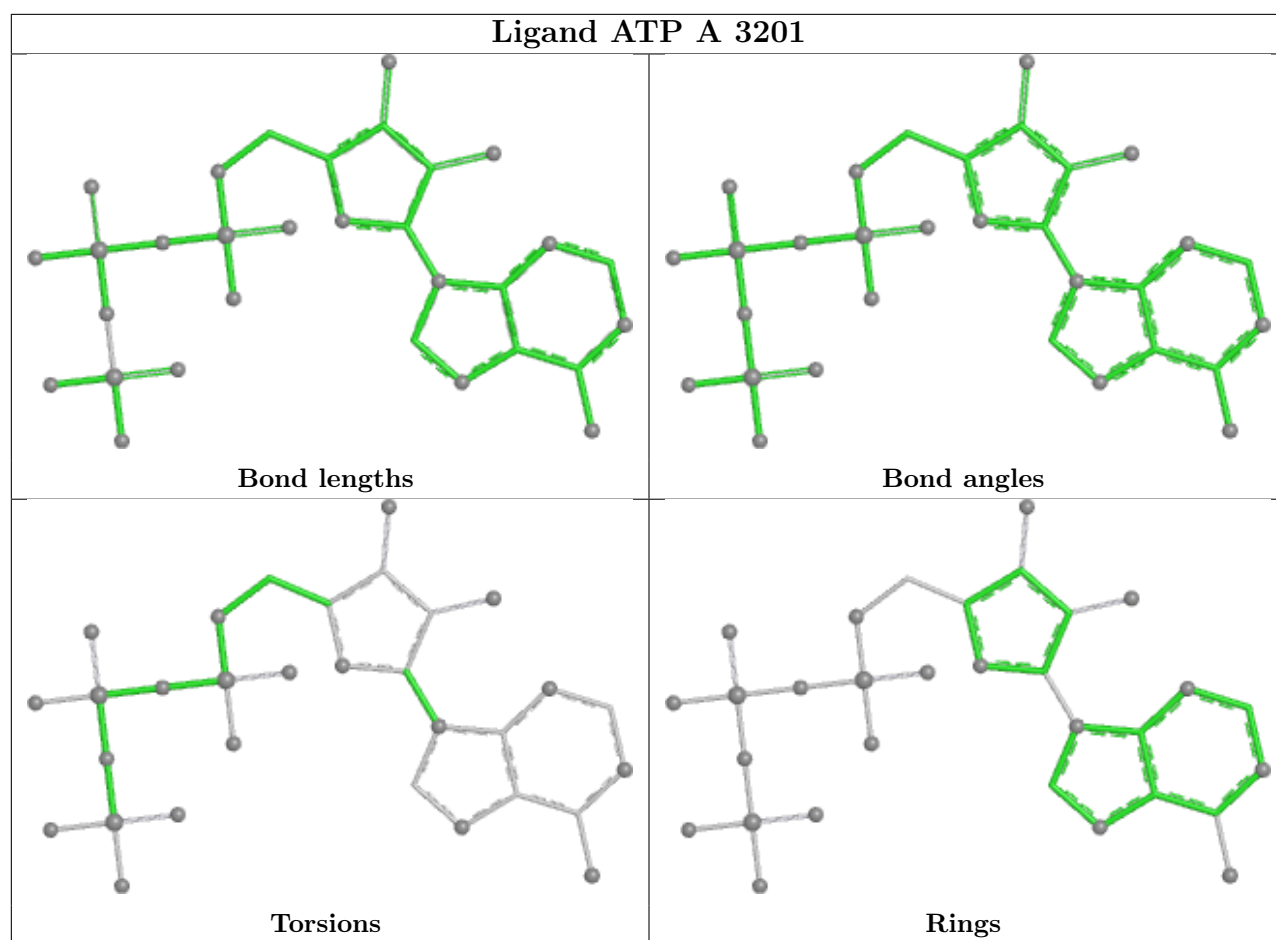
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	3203	ADP	1	0
4	A	3202	ADP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

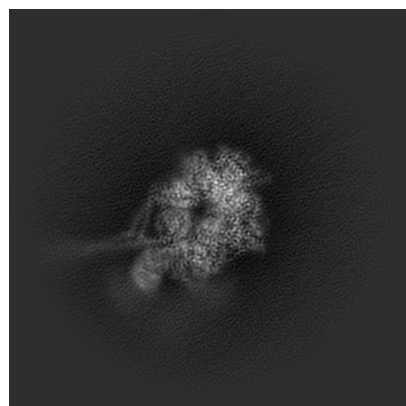
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29012. These allow visual inspection of the internal detail of the map and identification of artifacts.

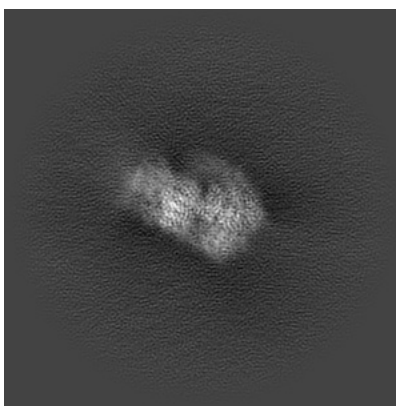
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

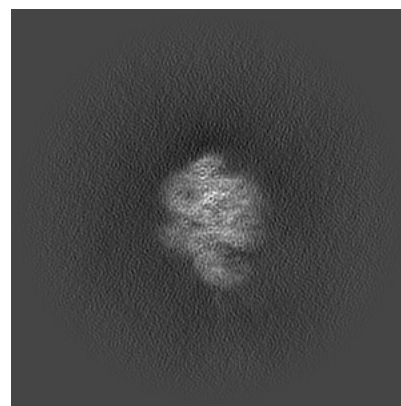
6.1.1 Primary map



X

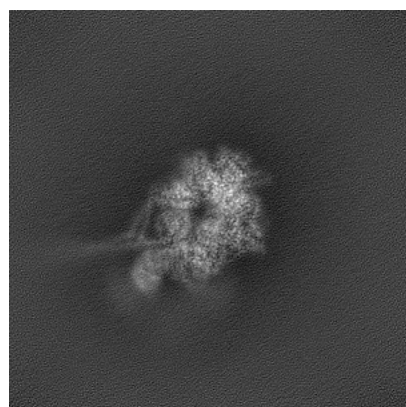


Y

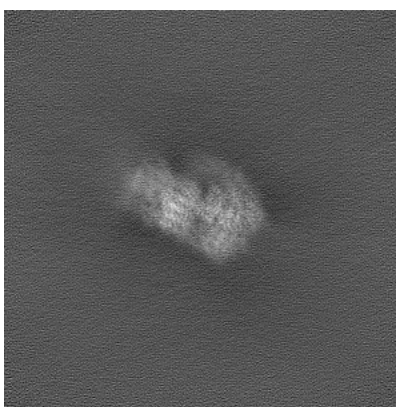


Z

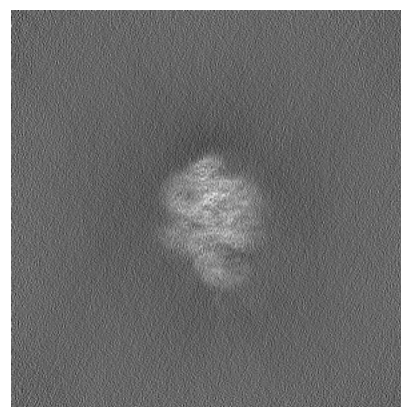
6.1.2 Raw map



X



Y

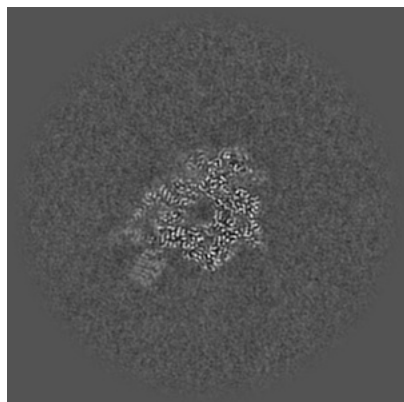


Z

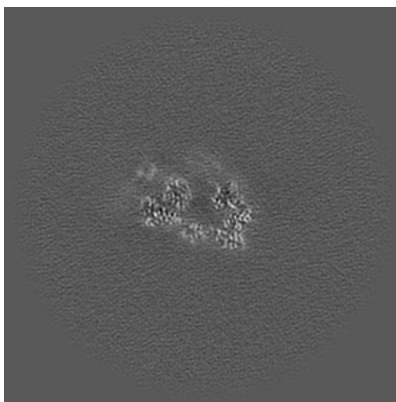
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

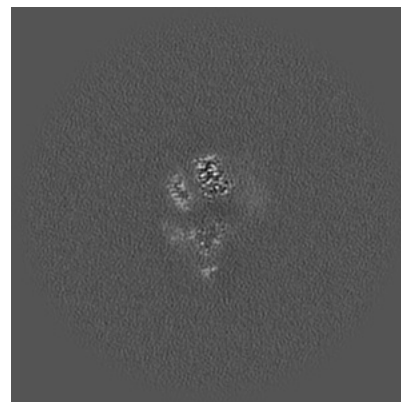
6.2.1 Primary map



X Index: 180

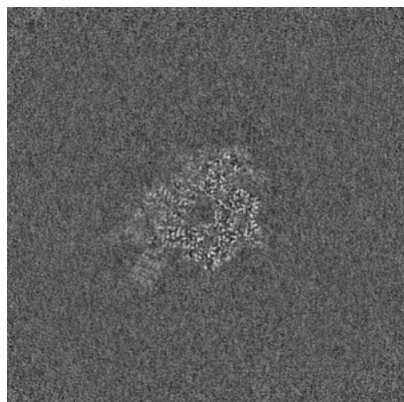


Y Index: 180

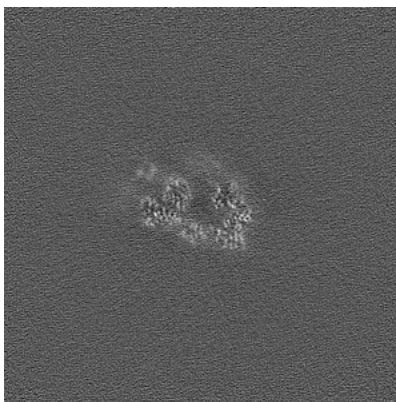


Z Index: 180

6.2.2 Raw map



X Index: 180



Y Index: 180

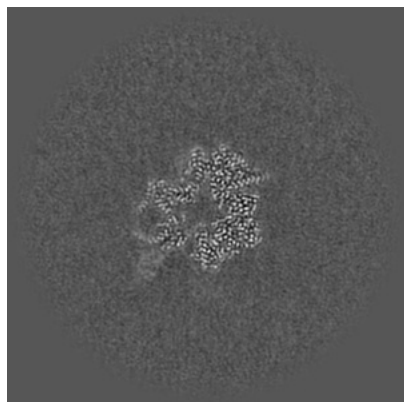


Z Index: 180

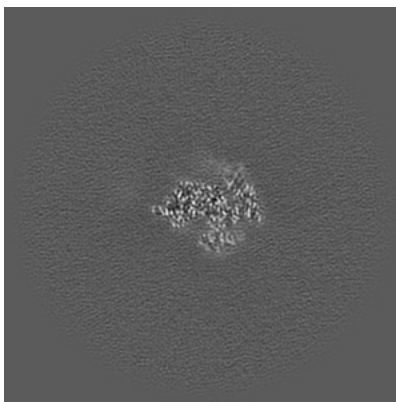
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

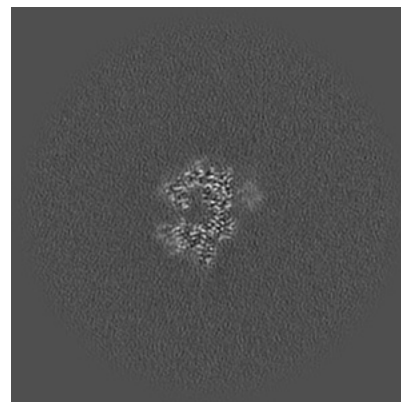
6.3.1 Primary map



X Index: 175

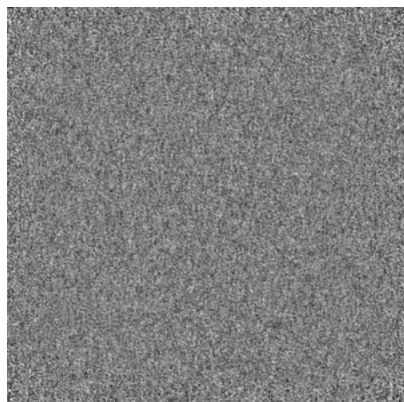


Y Index: 200

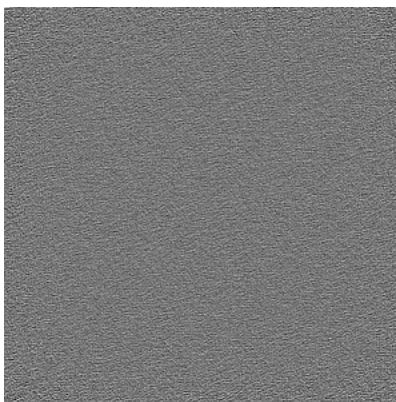


Z Index: 193

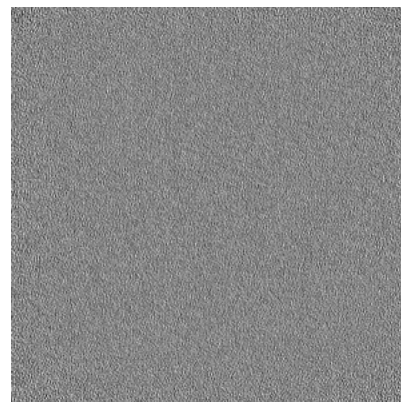
6.3.2 Raw map



X Index: 0



Y Index: 0

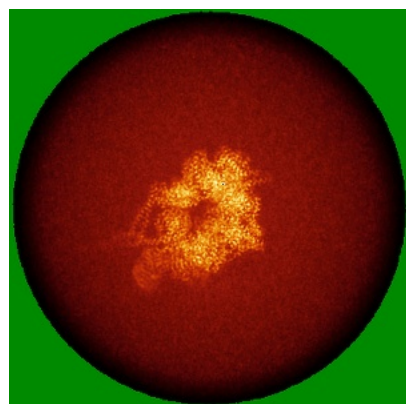


Z Index: 0

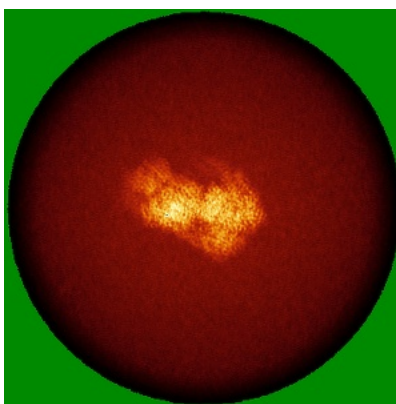
The images above show the largest variance slices of the map in three orthogonal directions.

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

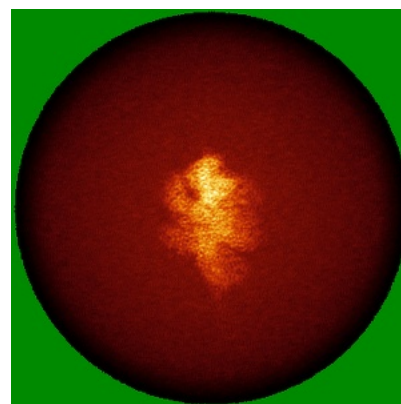
6.4.1 Primary map



X

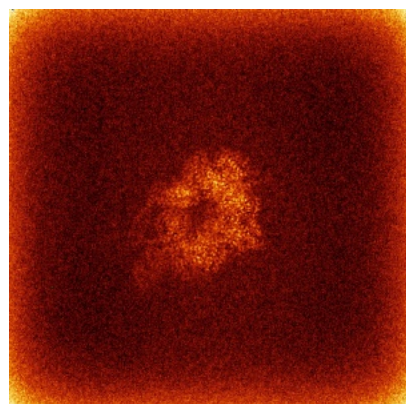


Y

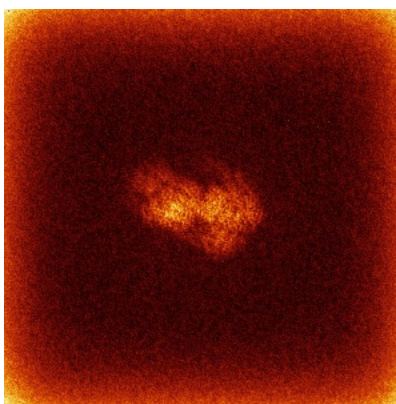


Z

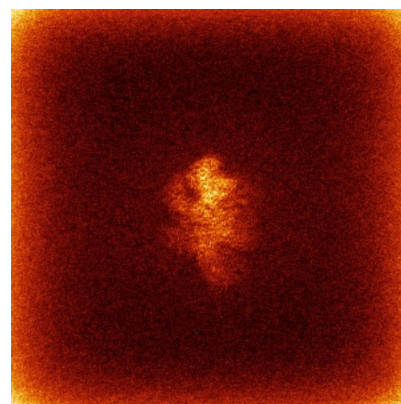
6.4.2 Raw map



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



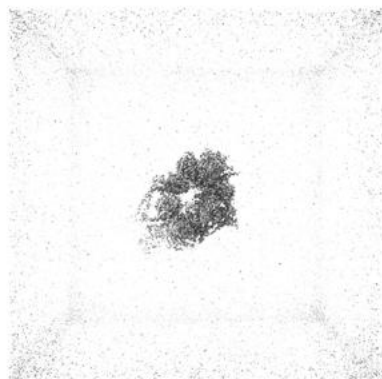
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

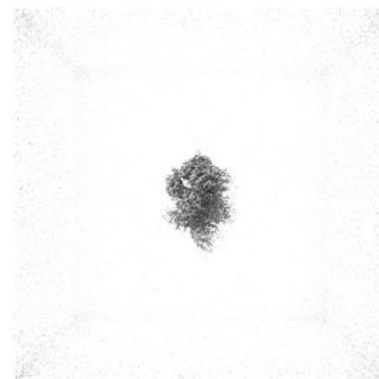
6.5.2 Raw map



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.

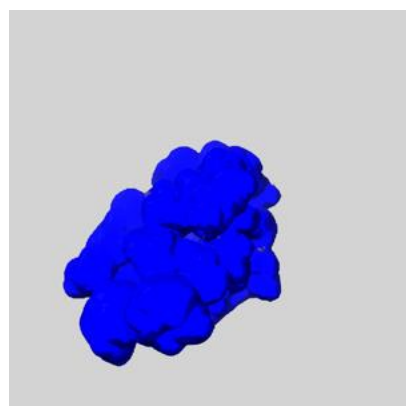
6.6 Mask visualisation [i](#)

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

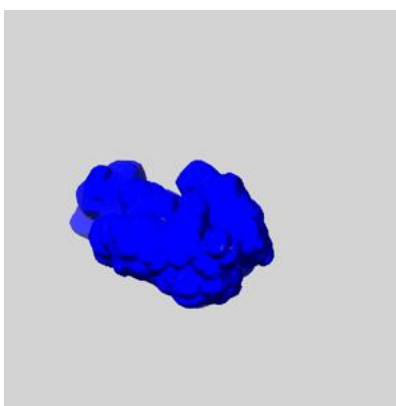
A mask typically either:

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

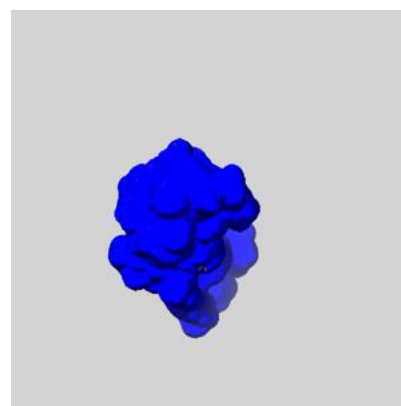
6.6.1 emd_29012_msk_1.map [i](#)



X



Y

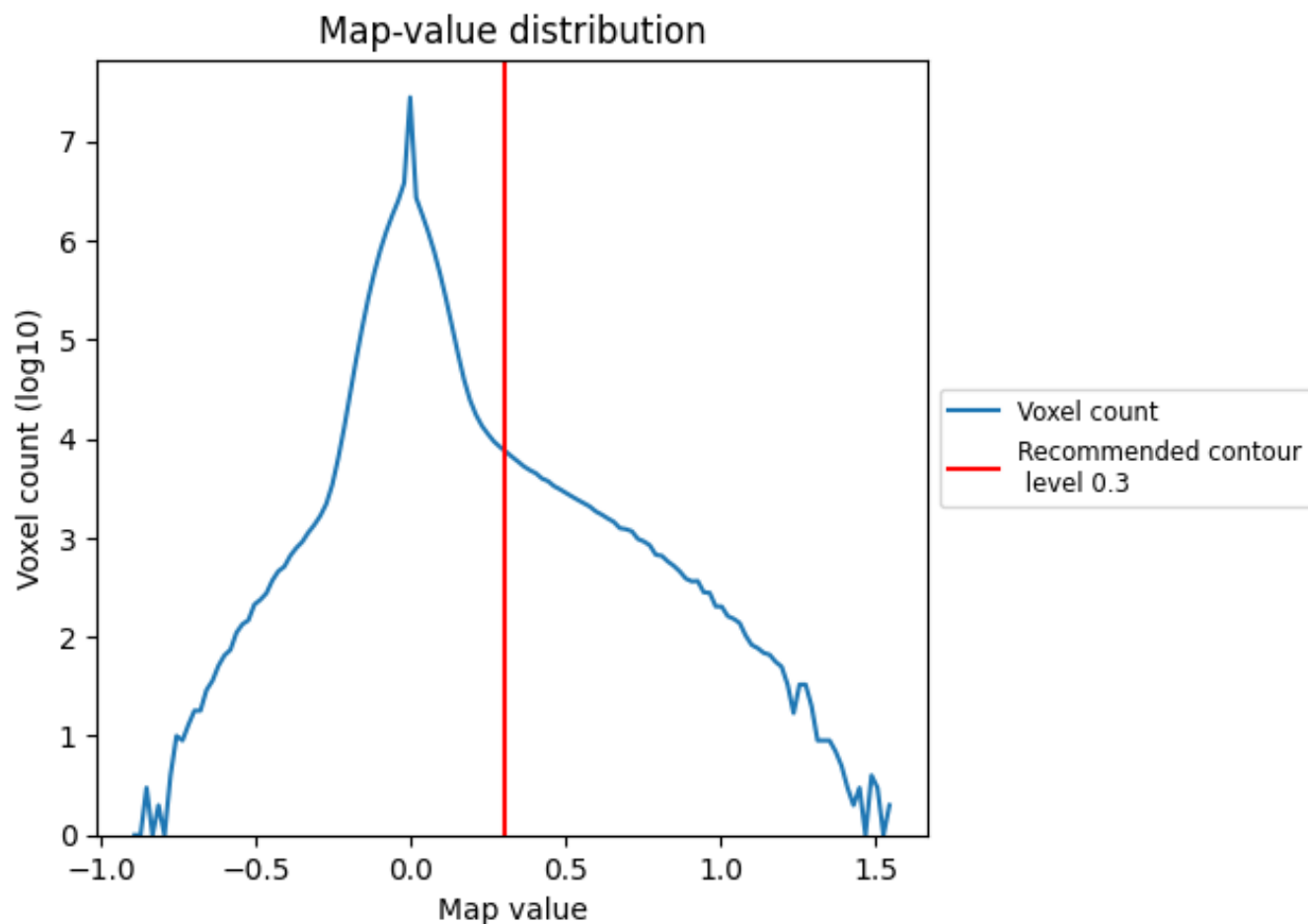


Z

7 Map analysis [i](#)

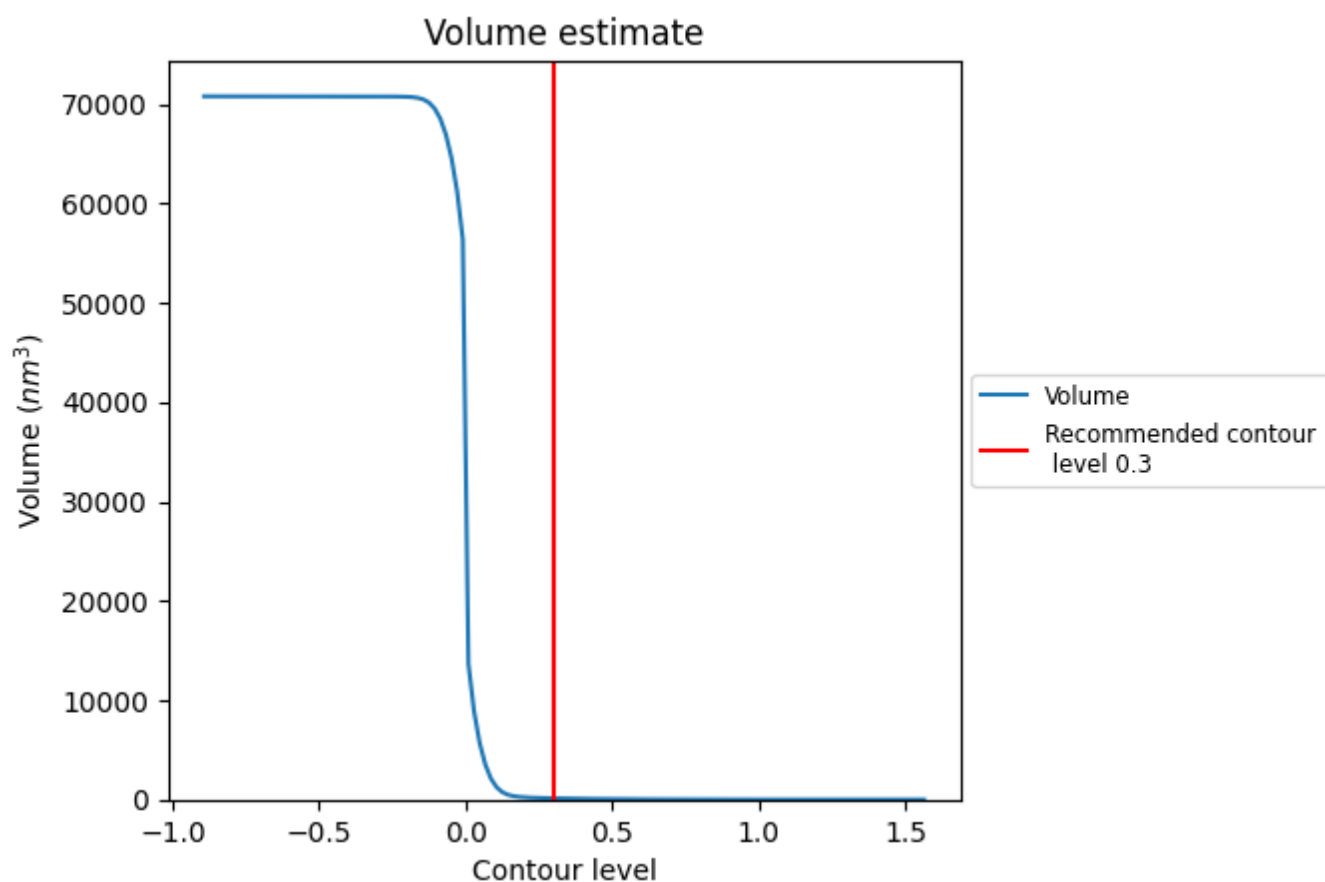
This section contains the results of statistical analysis of the map.

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.

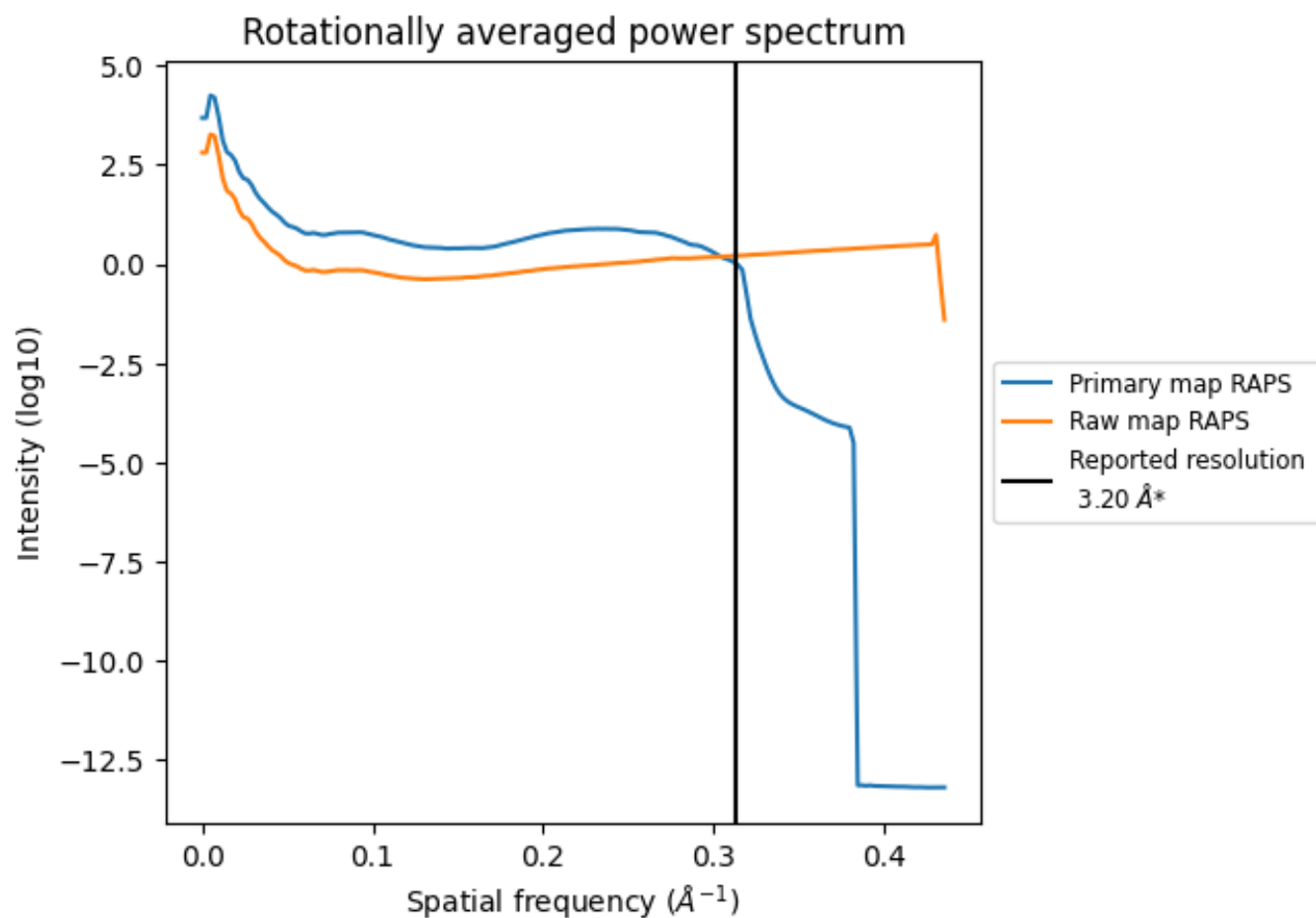
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 125 nm³; this corresponds to an approximate mass of 113 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 ⓘ

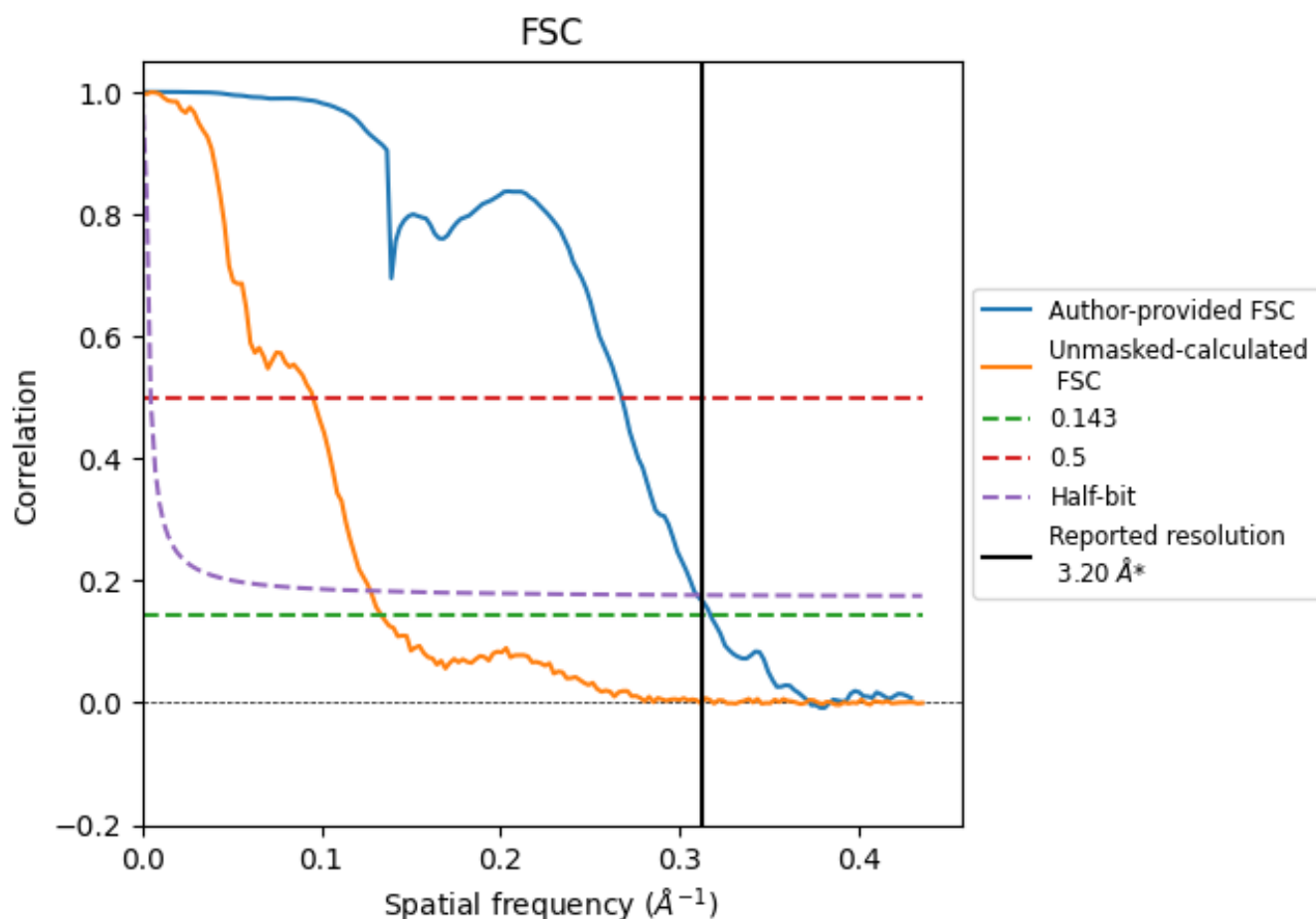


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

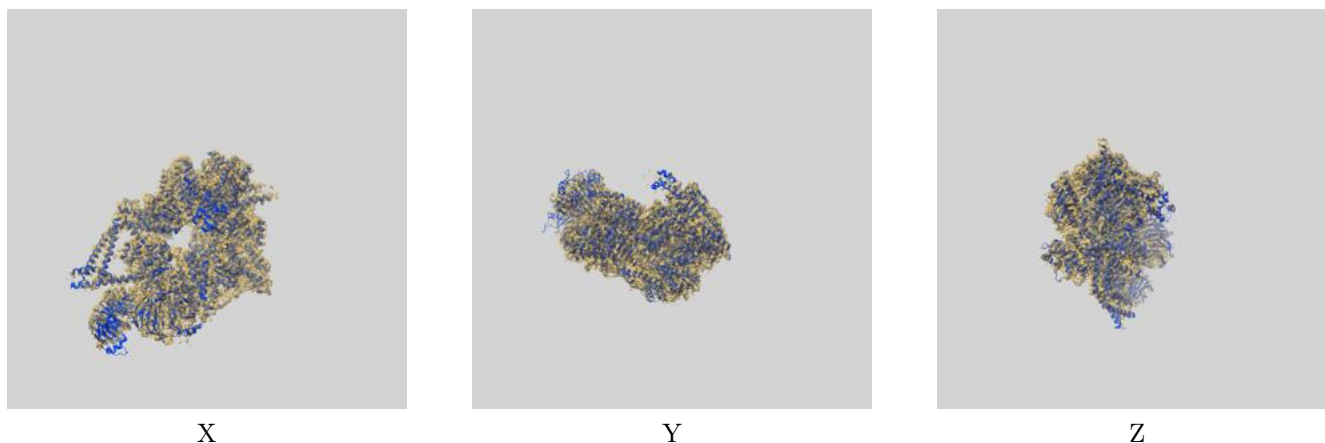
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.15	3.74	3.23
Unmasked-calculated*	7.50	10.50	7.86

*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 7.50 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

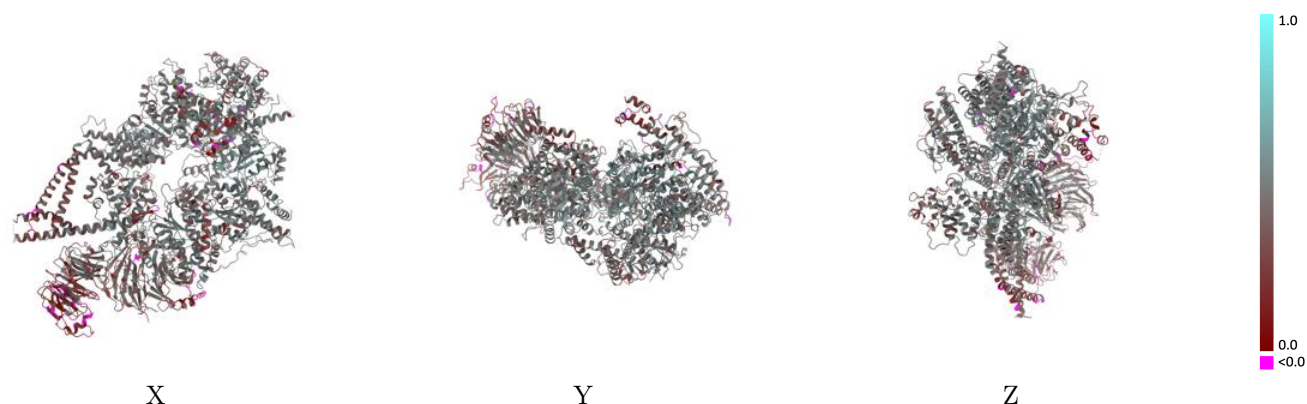
This section contains information regarding the fit between EMDB map EMD-29012 and PDB model 8FDT. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



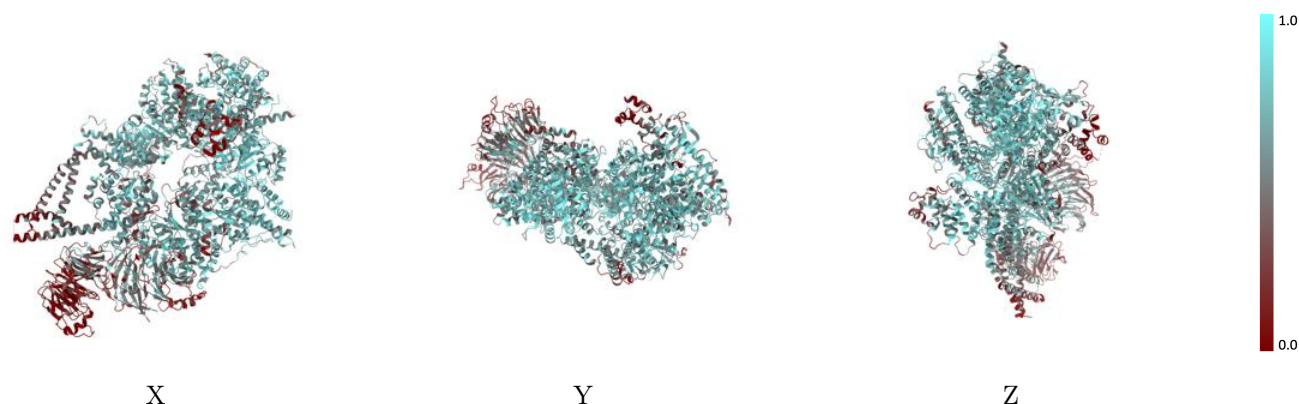
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



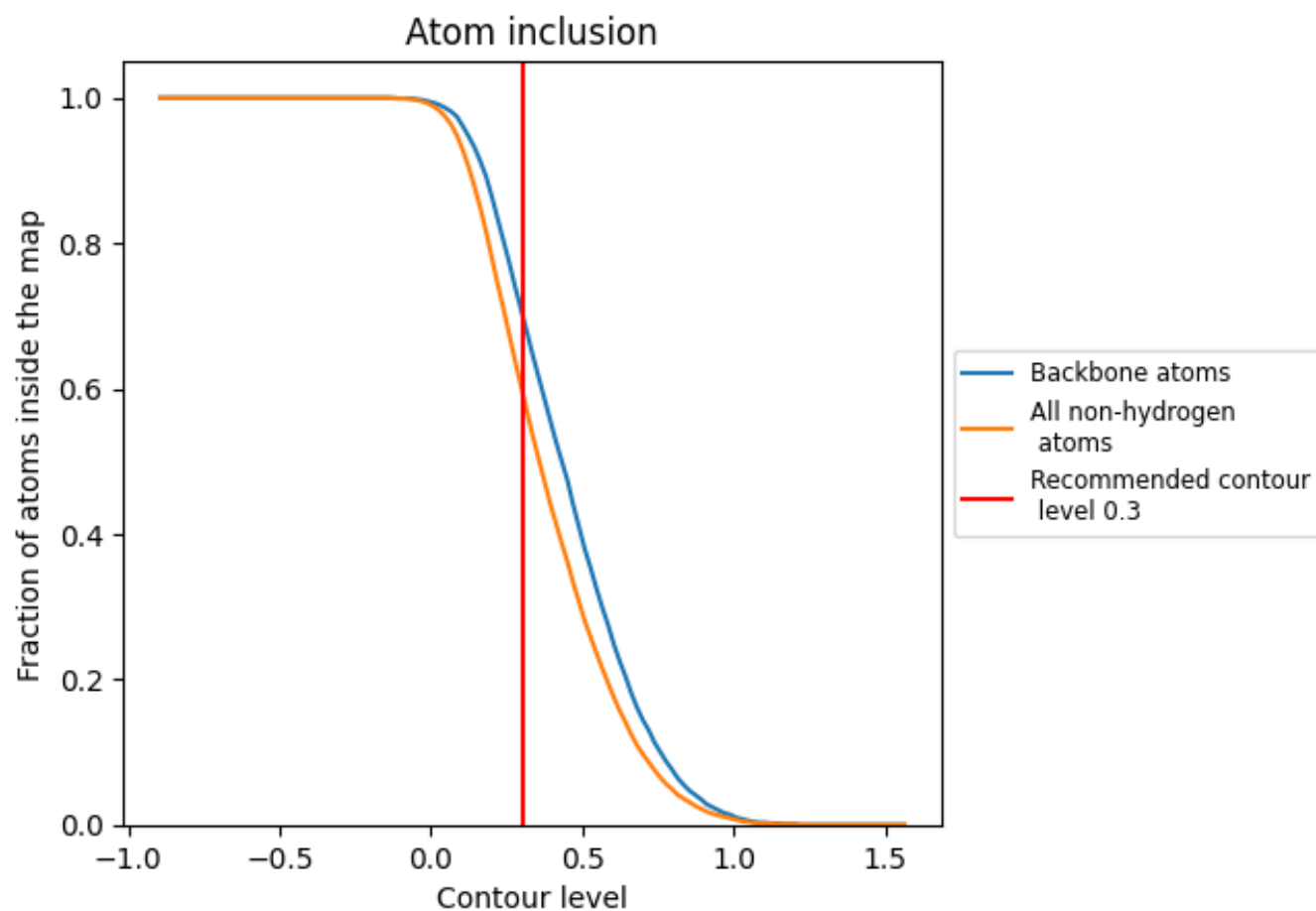
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 60% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5990	0.4260
A	0.6600	0.4510
B	0.1900	0.2530
C	0.4610	0.3750

