



wwPDB EM Validation Summary Report ⓘ

Aug 5, 2025 – 01:45 pm BST

PDB ID : 9GCG / pdb_00009gcg
EMDB ID : EMD-51229
Title : CryoEM structure of the human INO80 core- H2A.Z nucleosome complex
Authors : Aggarwal, P.; Sharma, M.; Hopfner, K.P.
Deposited on : 2024-08-01
Resolution : 3.43 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

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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.dev126
Mogul : 1.8.4, CSD as541be (2020)
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) : 2.45.1

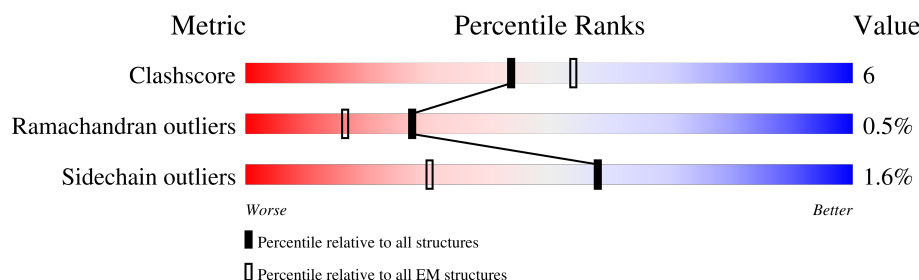
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.43 Å.

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







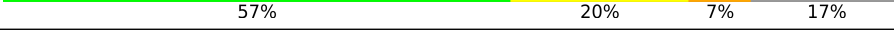

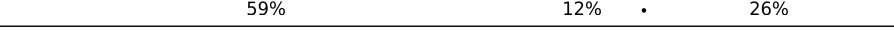

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	456	89% 6% 5%
1	B	456	91% 7% .
1	C	456	93% . .
2	D	463	81% 10% . 8%
2	E	463	89% 5% 5%
2	F	463	83% 10% . 6%
3	I	192	45% 10% . 44%
4	G	1556	40% . 56%

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Mol	Chain	Length	Quality of chain
5	H	356	
6	J	607	
7	K	152	
8	L	152	
9	M	136	
9	Q	136	
10	N	102	
10	R	102	
11	O	127	
12	P	125	
12	T	125	
13	S	127	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 43167 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 RuvB-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	443	Total	C	N	O	S	0	0
			3412	2148	585	662	17		
1	A	434	Total	C	N	O	S	0	0
			3344	2107	575	646	16		
1	B	447	Total	C	N	O	S	0	0
			3453	2173	592	672	16		

- Molecule 2 is a protein called RuvB-like 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	439	Total	C	N	O	S	0	0
			3403	2125	597	665	16		
2	D	426	Total	C	N	O	S	0	0
			3317	2074	583	645	15		
2	F	434	Total	C	N	O	S	0	0
			3376	2110	592	658	16		

- Molecule 3 is a protein called INO80 complex subunit C.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	I	107	Total	C	N	O	0	0
			850	545	150	155		

- Molecule 4 is a protein called Chromatin-remodeling ATPase INO80.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	682	Total	C	N	O	S	0	0
			5608	3599	1004	975	30		

- Molecule 5 is a protein called INO80 complex subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	101	Total	C	N	O	S	0	0
			785	478	161	137	9		

- Molecule 6 is a protein called Actin-related protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	412	Total	C	N	O	S	0	0
			3277	2088	572	596	21		

- Molecule 7 is a DNA chain called Nucleosomal DNA Strand 1 (152-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	152	Total	C	N	O	P	0	0
			3132	1483	590	907	152		

- Molecule 8 is a DNA chain called Nucleosomal DNA Strand 2 (152-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	152	Total	C	N	O	P	0	0
			3100	1474	557	917	152		

- Molecule 9 is a protein called Histone H3.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	91	Total	C	N	O	S	0	0
			739	467	138	130	4		
9	Q	97	Total	C	N	O	S	0	0
			800	503	155	138	4		

- Molecule 10 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	81	Total	C	N	O	S	0	0
			646	407	126	112	1		
10	R	79	Total	C	N	O	S	0	0
			627	395	121	110	1		

- Molecule 11 is a protein called Histone H2A.Z.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	O	106	Total	C	N	O	0	0
			803	504	157	142		

- | Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|--------|---------|-------|
| 12 | P | 94 | Total
735 | C
462 | N
132 | O
139 | S
2 | 0 | 0 |
| 12 | T | 92 | Total
720 | C
453 | N
129 | O
136 | S
2 | 0 | 0 |

- | Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|---------|-------|
| 13 | S | 108 | Total
819 | C
514 | N
160 | O
145 | 0 | 0 |

Chain	Residue	Modelled	Actual	Comment	Reference
S	108	LEU	ILE	conflict	UNP P0C0S5

- # ADP

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

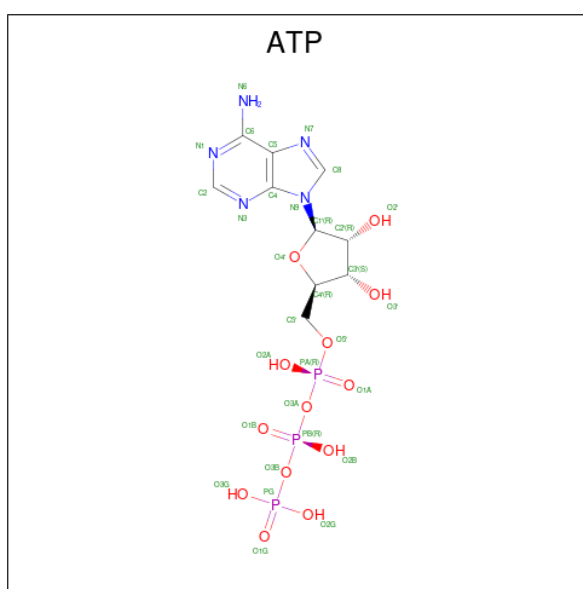


WORLD WIDE
PDB
PROTEIN DATA BANK

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Mol	Chain	Residues	Atoms					AltConf
14	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
14	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
14	G	1	Total	C	N	O	P	0
			27	10	5	10	2	
14	J	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 15 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
16	H	1	Total	Zn	0
			1	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.

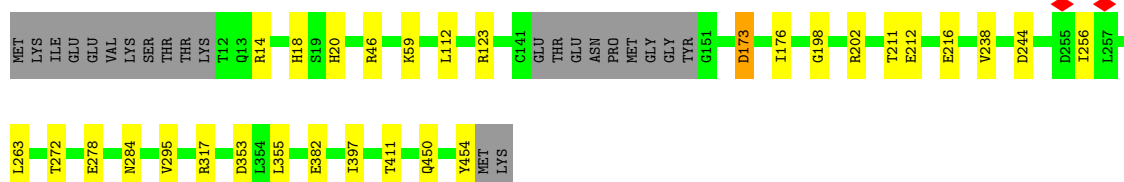
• Molecule 1: RuvB-like 1

Chain C:  93%



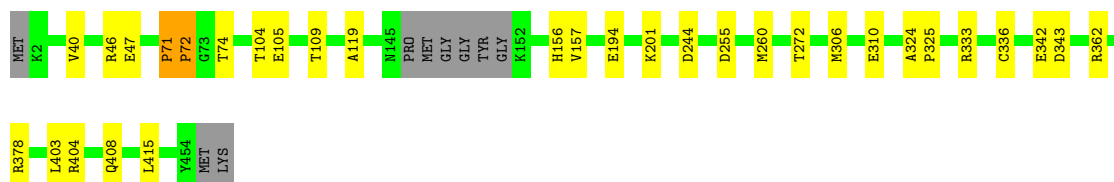
• Molecule 1: RuvB-like 1

Chain A:  89% 6% 5%




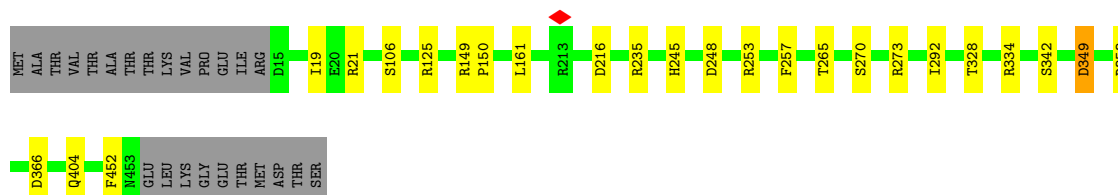
• Molecule 1: RuvB-like 1

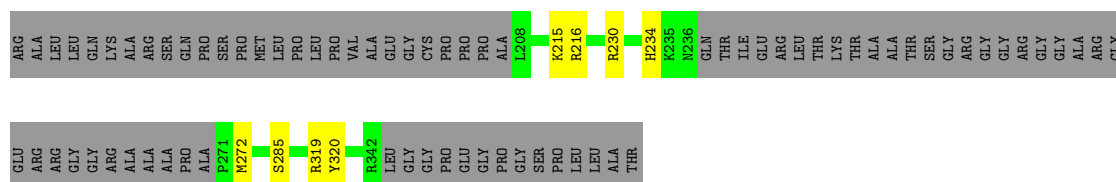
Chain B:  91% 7%



• Molecule 2: RuvB-like 2

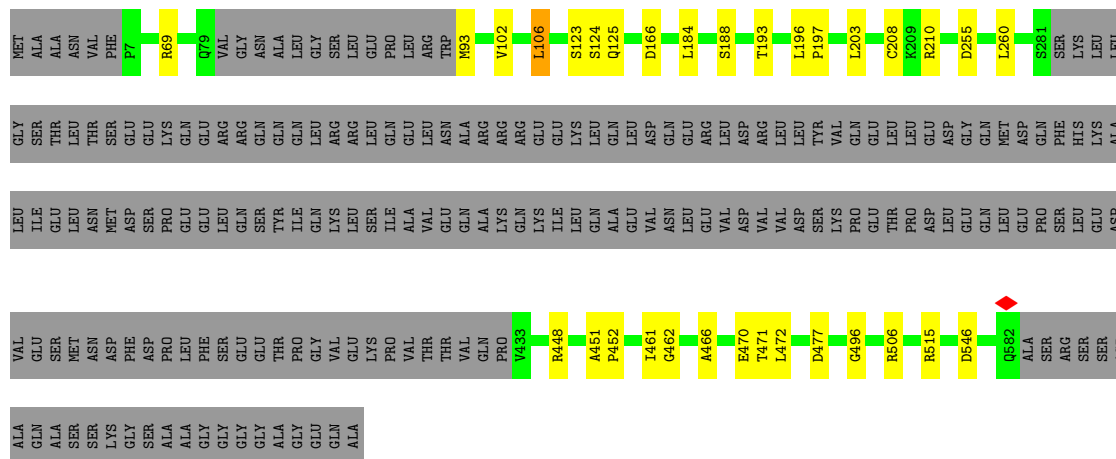
Chain E:  89% 5% 5%





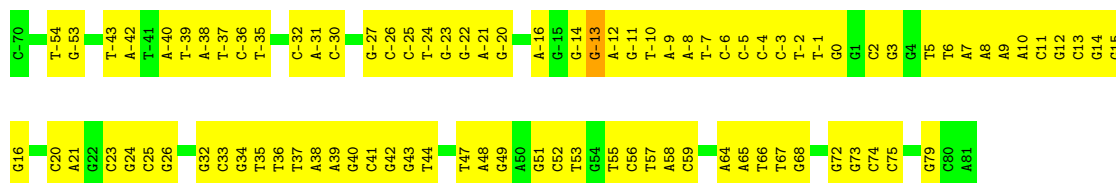
• Molecule 6: Actin-related protein 5

Chain J: 63% 5% 32%



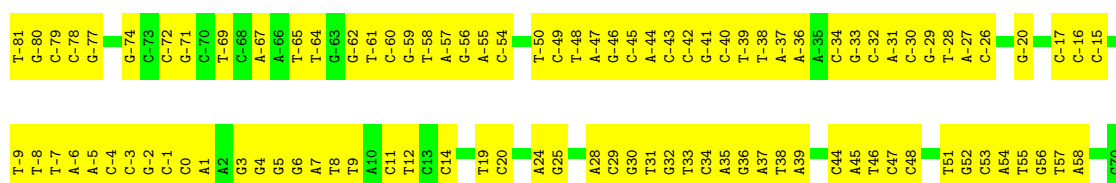
• Molecule 7: Nucleosomal DNA Strand 1 (152-MER)

Chain K: 40% 59%



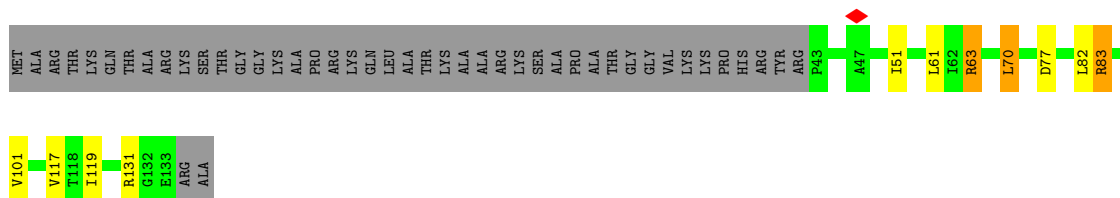
• Molecule 8: Nucleosomal DNA Strand 2 (152-MER)

Chain L: 35% 65%

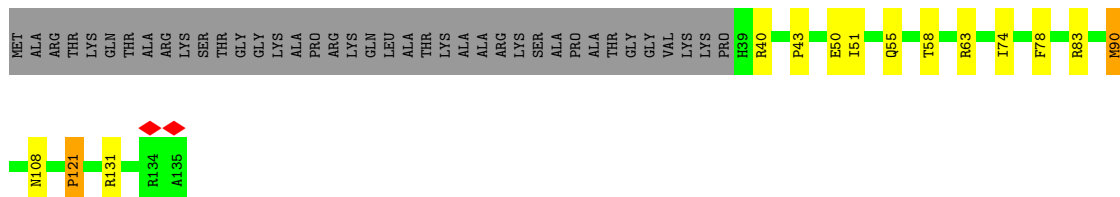


• Molecule 9: Histone H3.1

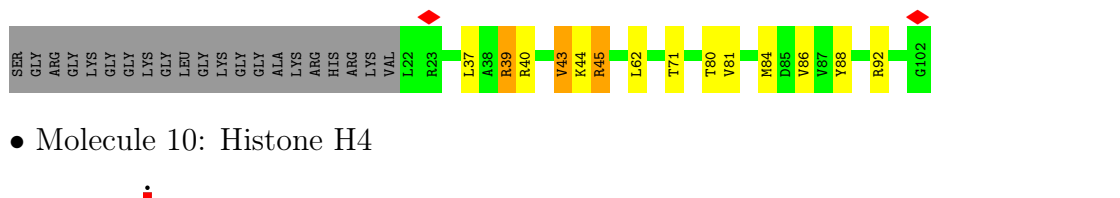
Chain M: 59% 6% 33%



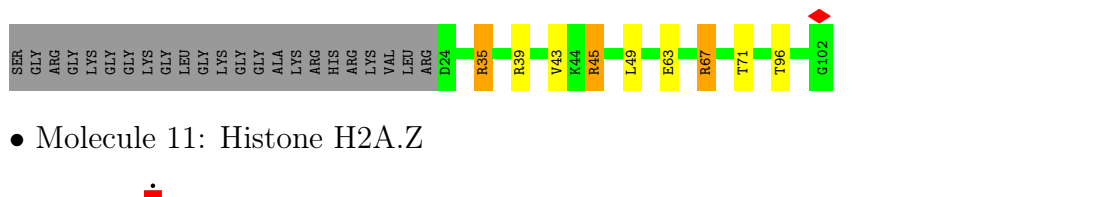
• Molecule 9: Histone H3.1



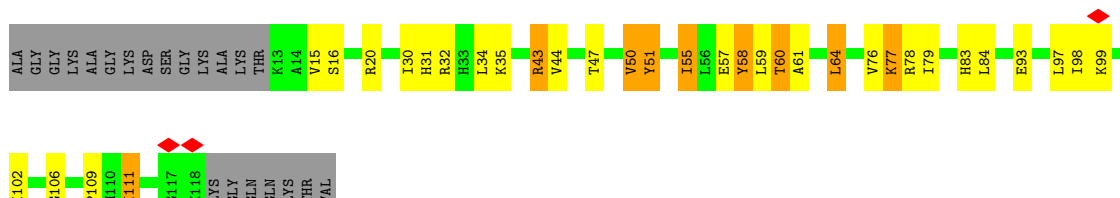
• Molecule 10: Histone H4



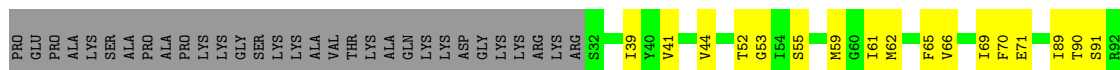
• Molecule 10: Histone H4

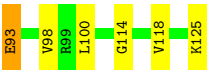


• Molecule 11: Histone H2A.Z

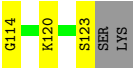
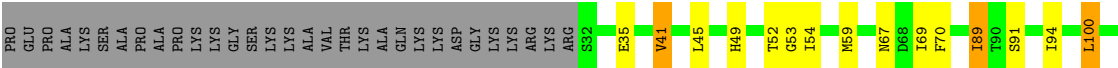


• Molecule 12: Histone H2B type 2-E

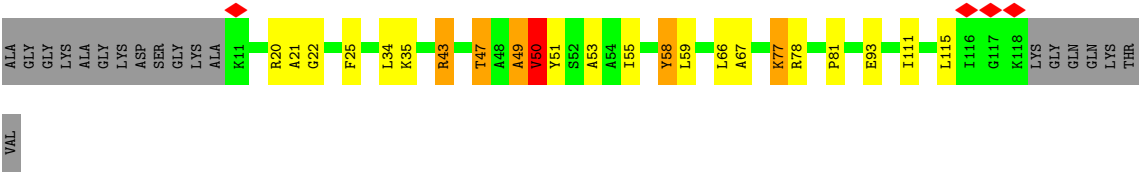




- Molecule 12: Histone H2B type 2-E



- Molecule 13: Histone H2A.Z



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	94892	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 ($e^-/\text{\AA}^2$)	1.0	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2900	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.592	Depositor
Minimum map value	-0.268	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	414.92, 414.92, 414.92	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.943, 0.943, 0.943	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.76	2/3387 (0.1%)	1.23	6/4564 (0.1%)
1	B	0.71	0/3496	1.17	15/4710 (0.3%)
1	C	0.71	0/3458	1.16	2/4662 (0.0%)
2	D	0.75	2/3353 (0.1%)	1.25	12/4510 (0.3%)
2	E	0.69	0/3443	1.21	12/4636 (0.3%)
2	F	0.74	1/3415 (0.0%)	1.28	22/4596 (0.5%)
3	I	0.67	0/873	1.15	2/1183 (0.2%)
4	G	0.63	0/5744	1.11	15/7759 (0.2%)
5	H	0.66	0/802	1.06	0/1080
6	J	0.69	0/3362	1.13	5/4558 (0.1%)
7	K	0.58	0/3518	0.95	2/5431 (0.0%)
8	L	0.59	0/3472	0.96	0/5353
9	M	0.75	0/748	1.31	3/1003 (0.3%)
9	Q	0.74	0/811	1.30	0/1086
10	N	0.76	0/653	1.28	0/873
10	R	0.76	0/634	1.36	2/848 (0.2%)
11	O	0.90	1/814 (0.1%)	1.68	12/1095 (1.1%)
12	P	0.74	0/746	1.28	2/1001 (0.2%)
12	T	0.72	0/731	1.23	0/983
13	S	0.88	0/830	1.49	8/1116 (0.7%)
All	All	0.70	6/44290 (0.0%)	1.17	120/61047 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	1
2	D	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	E	0	2
2	F	0	4
3	I	0	1
4	G	0	5
5	H	0	1
6	J	0	2
9	M	0	2
9	Q	0	3
10	N	0	3
10	R	0	1
11	O	0	3
12	P	0	1
13	S	0	1
All	All	0	37

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	O	83	HIS	CG-CD2	-6.70	1.28	1.35
2	D	86	ILE	CB-CG1	-6.16	1.41	1.53
1	A	454	TYR	CA-C	5.65	1.64	1.52
2	D	335	ILE	CB-CG1	-5.27	1.43	1.53
1	A	46	ARG	NE-CZ	-5.09	1.27	1.33

The worst 5 of 120 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	O	64	LEU	N-CA-CB	8.80	125.37	110.49
10	R	45	ARG	NE-CZ-NH2	8.61	126.95	119.20
2	D	273	ARG	NE-CZ-NH1	-8.54	112.96	121.50
2	F	214	ASP	CA-CB-CG	7.81	120.41	112.60
11	O	50	VAL	N-CA-CB	7.39	123.42	111.23

There are no chirality outliers.

5 of 37 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	123	ARG	Sidechain
1	C	64	ARG	Sidechain
2	E	125	ARG	Sidechain
2	E	253	ARG	Sidechain

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Mol	Chain	Res	Type	Group
3	I	138	ASN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3344	0	3451	17	0
1	B	3453	0	3563	17	0
1	C	3412	0	3508	16	0
2	D	3317	0	3395	29	0
2	E	3403	0	3472	9	0
2	F	3376	0	3446	20	0
3	I	850	0	852	31	0
4	G	5608	0	5651	50	0
5	H	785	0	794	19	0
6	J	3277	0	3215	31	0
7	K	3132	0	1705	119	0
8	L	3100	0	1710	137	0
9	M	739	0	777	11	0
9	Q	800	0	836	20	0
10	N	646	0	687	16	0
10	R	627	0	663	18	0
11	O	803	0	853	46	0
12	P	735	0	755	31	0
12	T	720	0	740	17	0
13	S	819	0	873	31	0
14	B	27	0	12	0	0
14	C	27	0	12	0	0
14	D	27	0	12	0	0
14	E	27	0	12	0	0
14	F	27	0	12	1	0
14	G	27	0	12	0	0
14	J	27	0	12	0	0
15	A	31	0	12	3	0
16	H	1	0	0	0	0
All	All	43167	0	41042	458	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 6.

The worst 5 of 458 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)
4:G:1157:ARG:HH22	5:H:234:HIS:CE1	1.46	1.33
8:L:39:DA:OP1	11:O:35:LYS:HE2	1.40	1.17
5:H:216:ARG:NH1	8:L:14:DC:OP2	1.92	1.01
4:G:1157:ARG:NH2	5:H:234:HIS:CE1	2.29	1.00
6:J:69:ARG:HE	8:L:-30:DC:H1'	1.29	0.97

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	430/456 (94%)	411 (96%)	18 (4%)	1 (0%)	44	74
1	B	443/456 (97%)	430 (97%)	12 (3%)	1 (0%)	44	74
1	C	441/456 (97%)	431 (98%)	10 (2%)	0	100	100
2	D	420/463 (91%)	410 (98%)	9 (2%)	1 (0%)	44	74
2	E	437/463 (94%)	429 (98%)	8 (2%)	0	100	100
2	F	430/463 (93%)	413 (96%)	14 (3%)	3 (1%)	19	52
3	I	105/192 (55%)	96 (91%)	8 (8%)	1 (1%)	13	44
4	G	674/1556 (43%)	633 (94%)	35 (5%)	6 (1%)	14	46
5	H	97/356 (27%)	93 (96%)	4 (4%)	0	100	100
6	J	406/607 (67%)	381 (94%)	20 (5%)	5 (1%)	11	40
9	M	89/136 (65%)	89 (100%)	0	0	100	100
9	Q	95/136 (70%)	92 (97%)	3 (3%)	0	100	100
10	N	79/102 (78%)	73 (92%)	6 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	R	77/102 (76%)	72 (94%)	5 (6%)	0	100	100
11	O	104/127 (82%)	77 (74%)	24 (23%)	3 (3%)	3	24
12	P	92/125 (74%)	89 (97%)	3 (3%)	0	100	100
12	T	90/125 (72%)	86 (96%)	3 (3%)	1 (1%)	12	42
13	S	106/127 (84%)	91 (86%)	14 (13%)	1 (1%)	14	46
All	All	4615/6448 (72%)	4396 (95%)	196 (4%)	23 (0%)	27	58

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	G	743	MET
6	J	123	SER
4	G	747	ILE
4	G	1230	ILE
6	J	124	SER

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	367/387 (95%)	362 (99%)	5 (1%)	62	79
1	B	381/387 (98%)	377 (99%)	4 (1%)	73	84
1	C	374/387 (97%)	370 (99%)	4 (1%)	70	82
2	D	361/390 (93%)	353 (98%)	8 (2%)	47	70
2	E	369/390 (95%)	365 (99%)	4 (1%)	70	82
2	F	367/390 (94%)	358 (98%)	9 (2%)	42	67
3	I	92/158 (58%)	90 (98%)	2 (2%)	47	70
4	G	613/1359 (45%)	608 (99%)	5 (1%)	79	88
5	H	86/288 (30%)	86 (100%)	0	100	100
6	J	351/520 (68%)	349 (99%)	2 (1%)	84	91
9	M	79/111 (71%)	77 (98%)	2 (2%)	42	67

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	Q	84/111 (76%)	82 (98%)	2 (2%)	44	68
10	N	66/78 (85%)	64 (97%)	2 (3%)	36	63
10	R	64/78 (82%)	64 (100%)	0	100	100
11	O	83/96 (86%)	81 (98%)	2 (2%)	44	68
12	P	80/105 (76%)	76 (95%)	4 (5%)	20	48
12	T	79/105 (75%)	73 (92%)	6 (8%)	11	35
13	S	85/96 (88%)	84 (99%)	1 (1%)	67	81
All	All	3981/5436 (73%)	3919 (98%)	62 (2%)	58	76

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	196	ASP
13	S	47	THR
2	F	407	THR
9	Q	121	PRO
12	T	89	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	245	HIS
4	G	583	HIS
6	J	274	HIS
2	F	275	GLN
4	G	552	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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
14	ADP	J	701	-	24,29,29	0.82	0	29,45,45	1.38	4 (13%)
14	ADP	B	501	-	24,29,29	0.90	1 (4%)	29,45,45	0.95	2 (6%)
14	ADP	F	501	-	24,29,29	0.90	1 (4%)	29,45,45	0.81	0
14	ADP	D	501	-	24,29,29	1.03	0	29,45,45	0.99	1 (3%)
15	ATP	A	501	-	26,33,33	0.96	1 (3%)	31,52,52	1.45	4 (12%)
14	ADP	C	501	-	24,29,29	0.95	1 (4%)	29,45,45	0.78	0
14	ADP	G	1601	-	24,29,29	0.68	0	29,45,45	0.89	1 (3%)
14	ADP	E	501	-	24,29,29	0.88	0	29,45,45	0.97	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
14	ADP	J	701	-	-	0/12/32/32	0/3/3/3
14	ADP	B	501	-	-	2/12/32/32	0/3/3/3
14	ADP	F	501	-	-	0/12/32/32	0/3/3/3
14	ADP	D	501	-	-	4/12/32/32	0/3/3/3
15	ATP	A	501	-	-	3/18/38/38	0/3/3/3
14	ADP	C	501	-	-	1/12/32/32	0/3/3/3
14	ADP	G	1601	-	-	3/12/32/32	0/3/3/3
14	ADP	E	501	-	-	4/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	C	501	ADP	PB-O2B	-2.45	1.45	1.54
14	B	501	ADP	C8-N7	-2.20	1.30	1.34
14	F	501	ADP	C8-N7	-2.06	1.31	1.34
15	A	501	ATP	C4-N3	-2.01	1.32	1.35

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	501	ATP	PA-O3A-PB	-4.93	115.92	132.83
14	J	701	ADP	C4-C5-N7	3.09	112.62	109.40
14	B	501	ADP	C4-C5-N7	3.08	112.61	109.40
14	J	701	ADP	C2'-C3'-C4'	2.92	108.33	102.64
14	G	1601	ADP	PA-O3A-PB	-2.81	123.20	132.83

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	D	501	ADP	C5'-O5'-PA-O2A
15	A	501	ATP	C5'-O5'-PA-O3A
15	A	501	ATP	O4'-C4'-C5'-O5'
14	G	1601	ADP	PB-O3A-PA-O1A
14	E	501	ADP	PA-O3A-PB-O2B

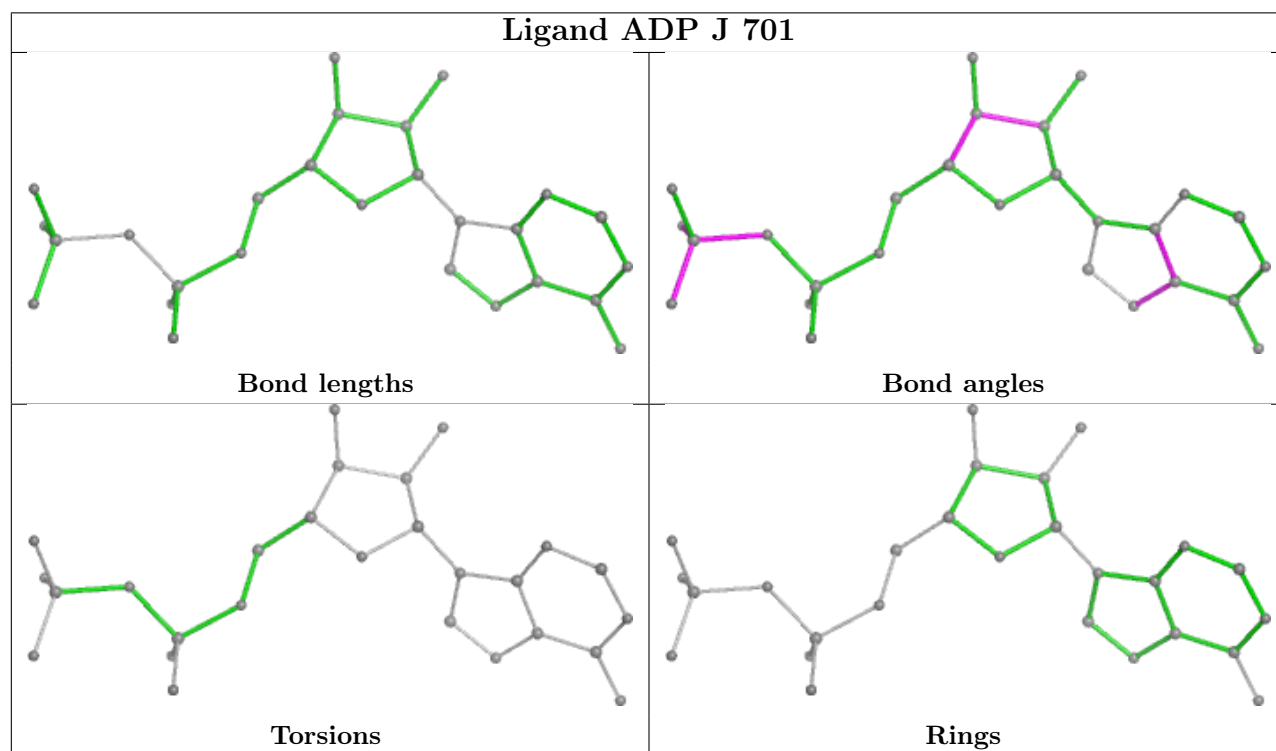
There are no ring outliers.

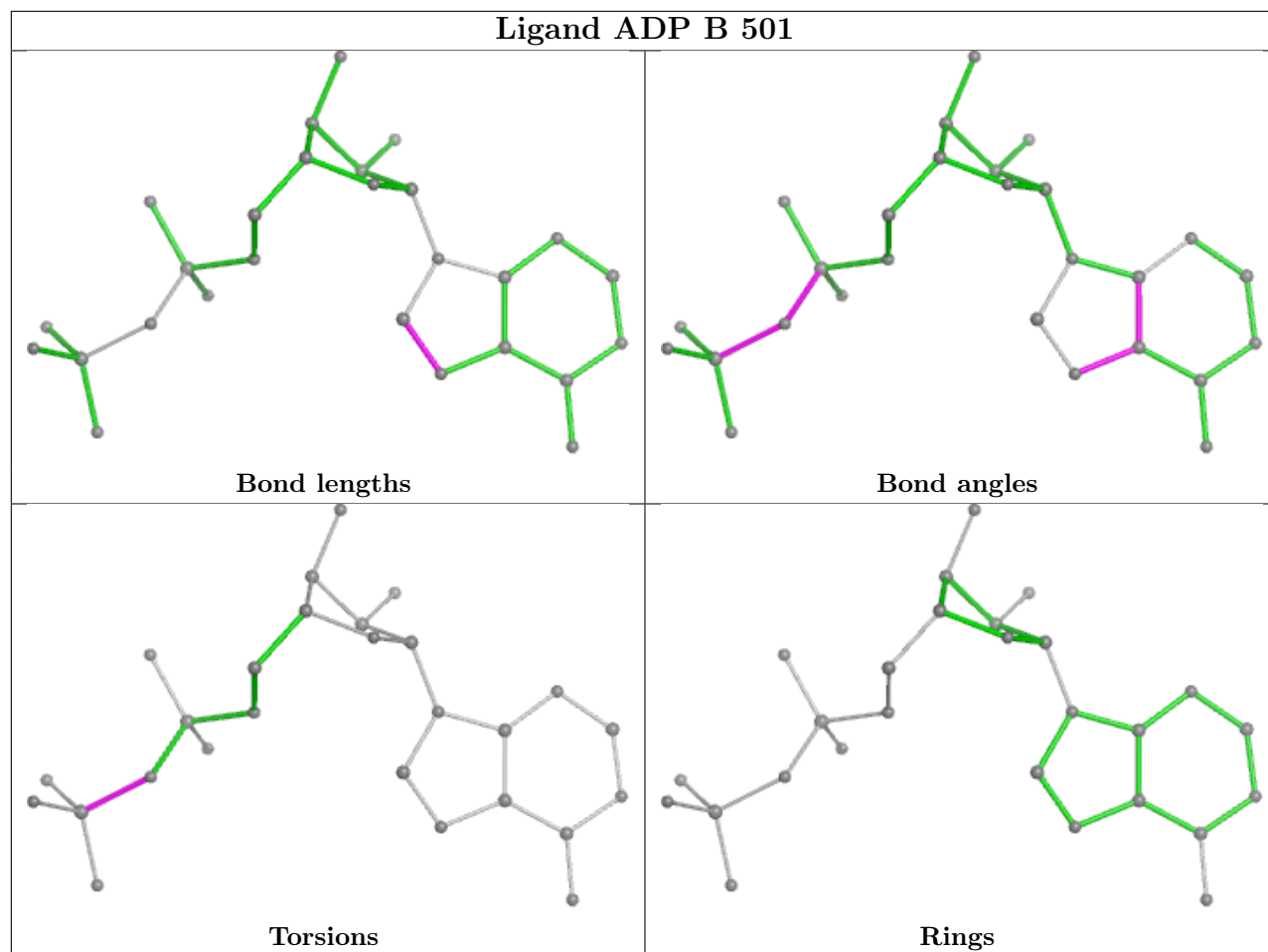
2 monomers are involved in 4 short contacts:

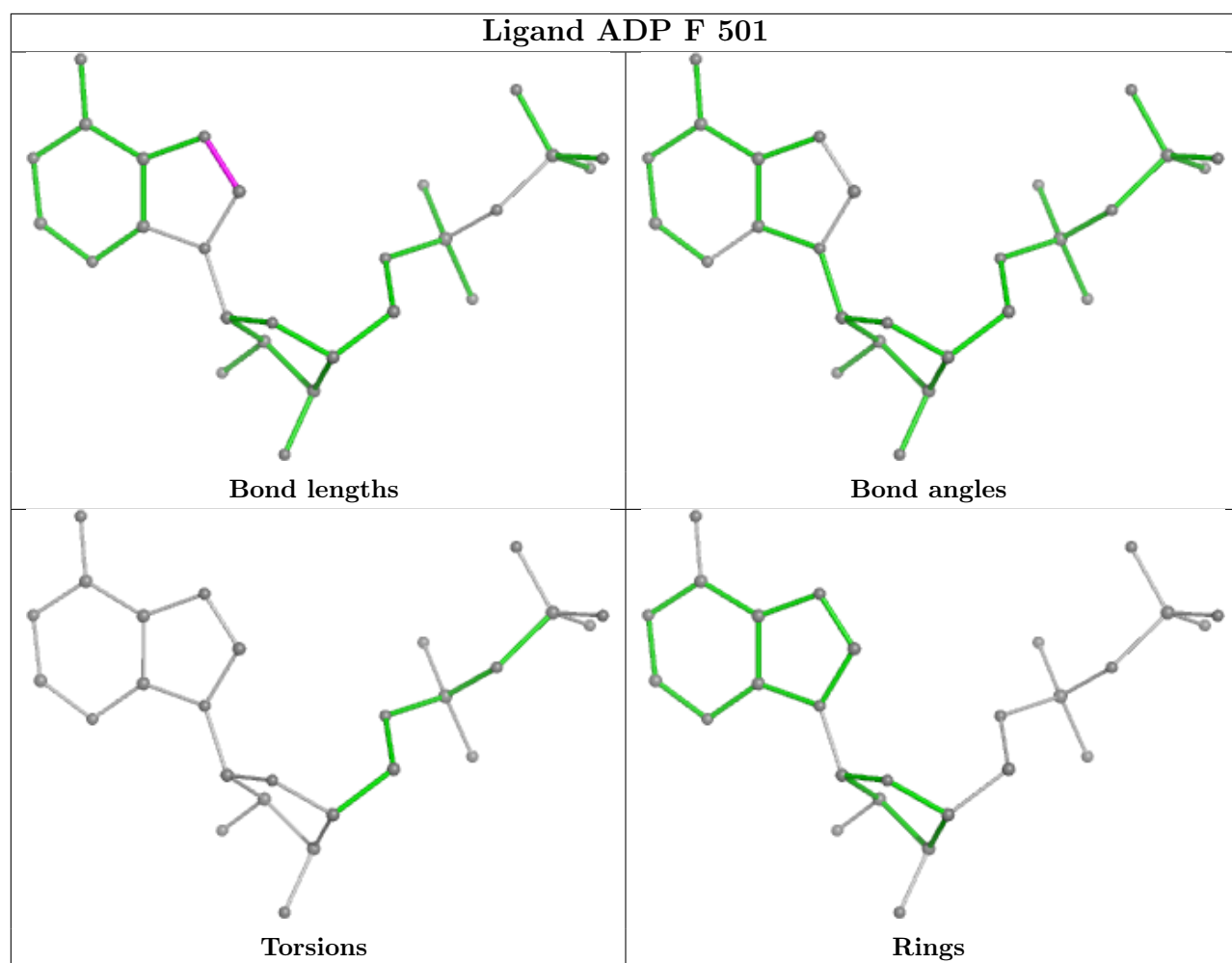
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	F	501	ADP	1	0
15	A	501	ATP	3	0

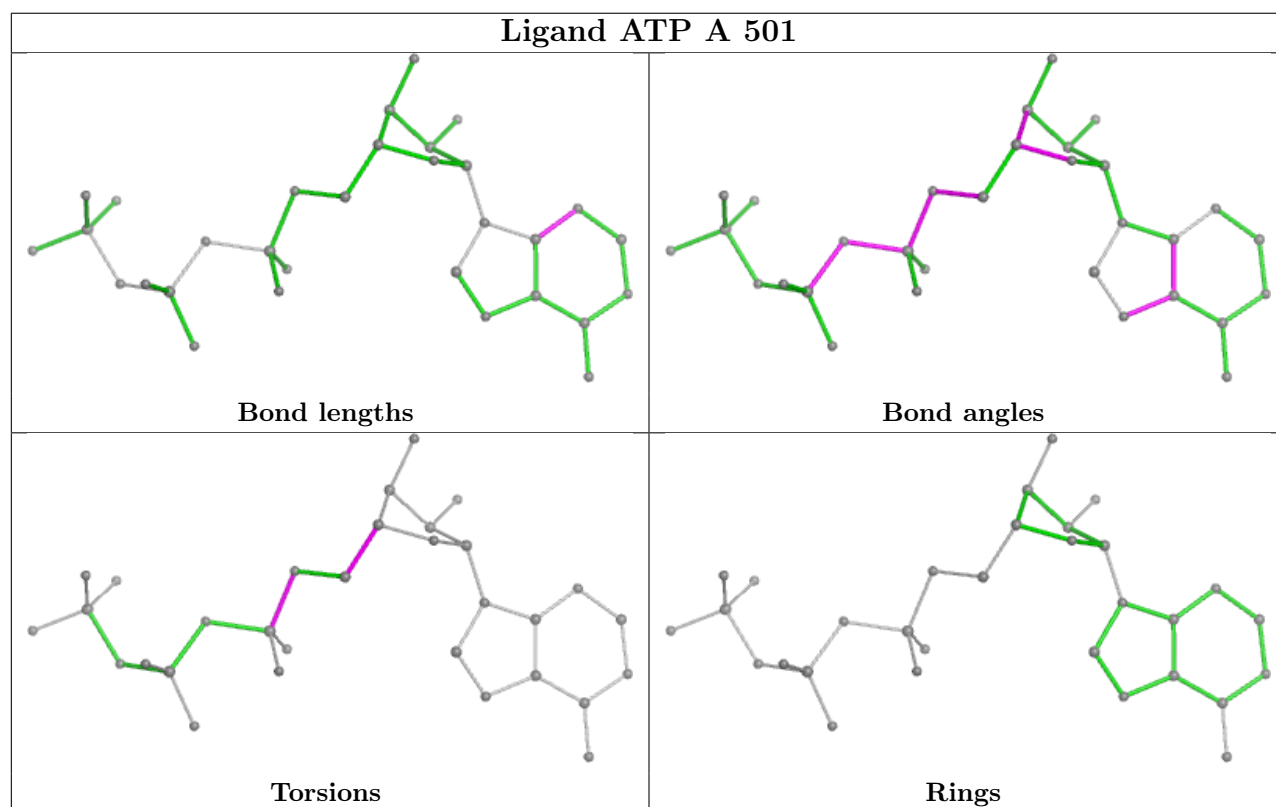
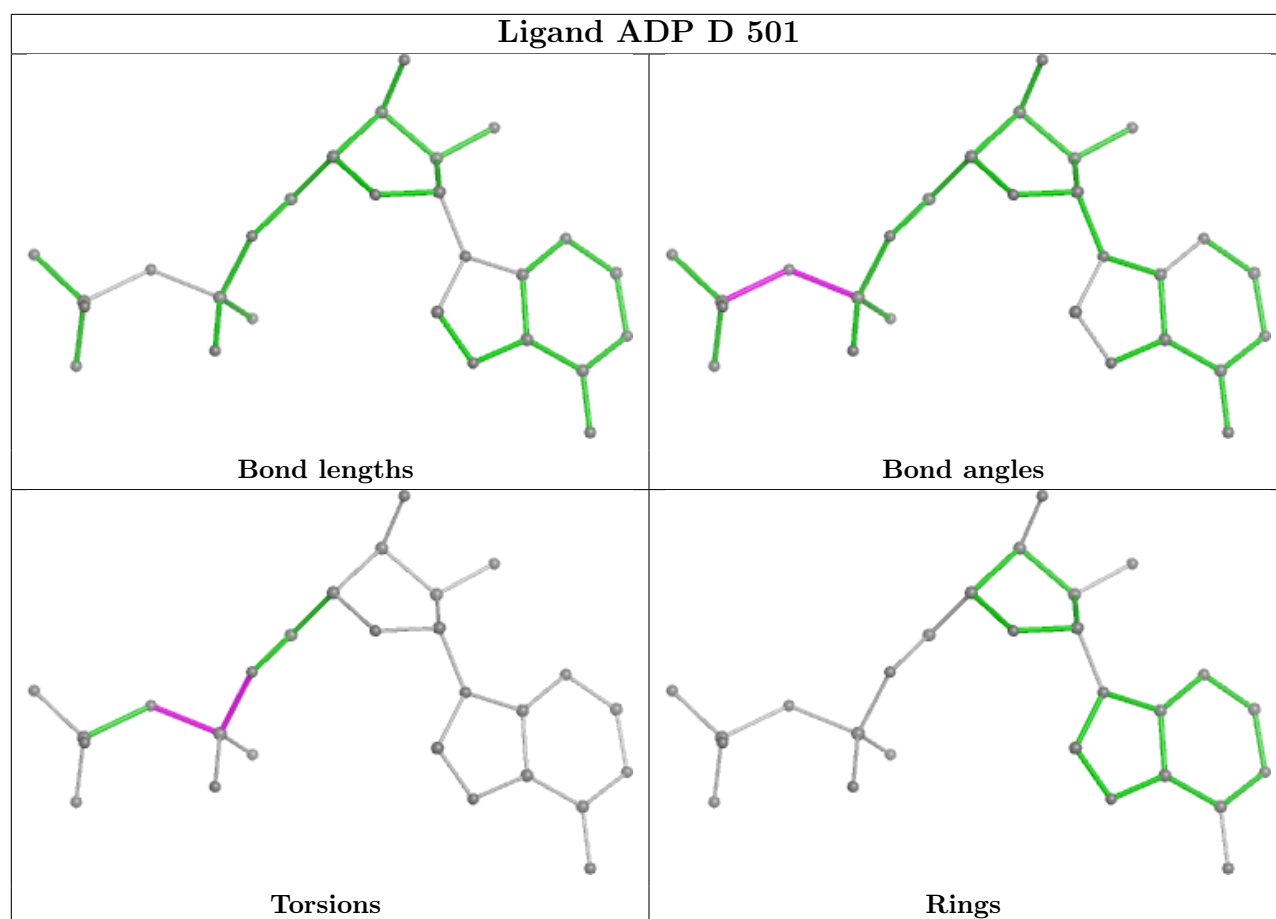
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

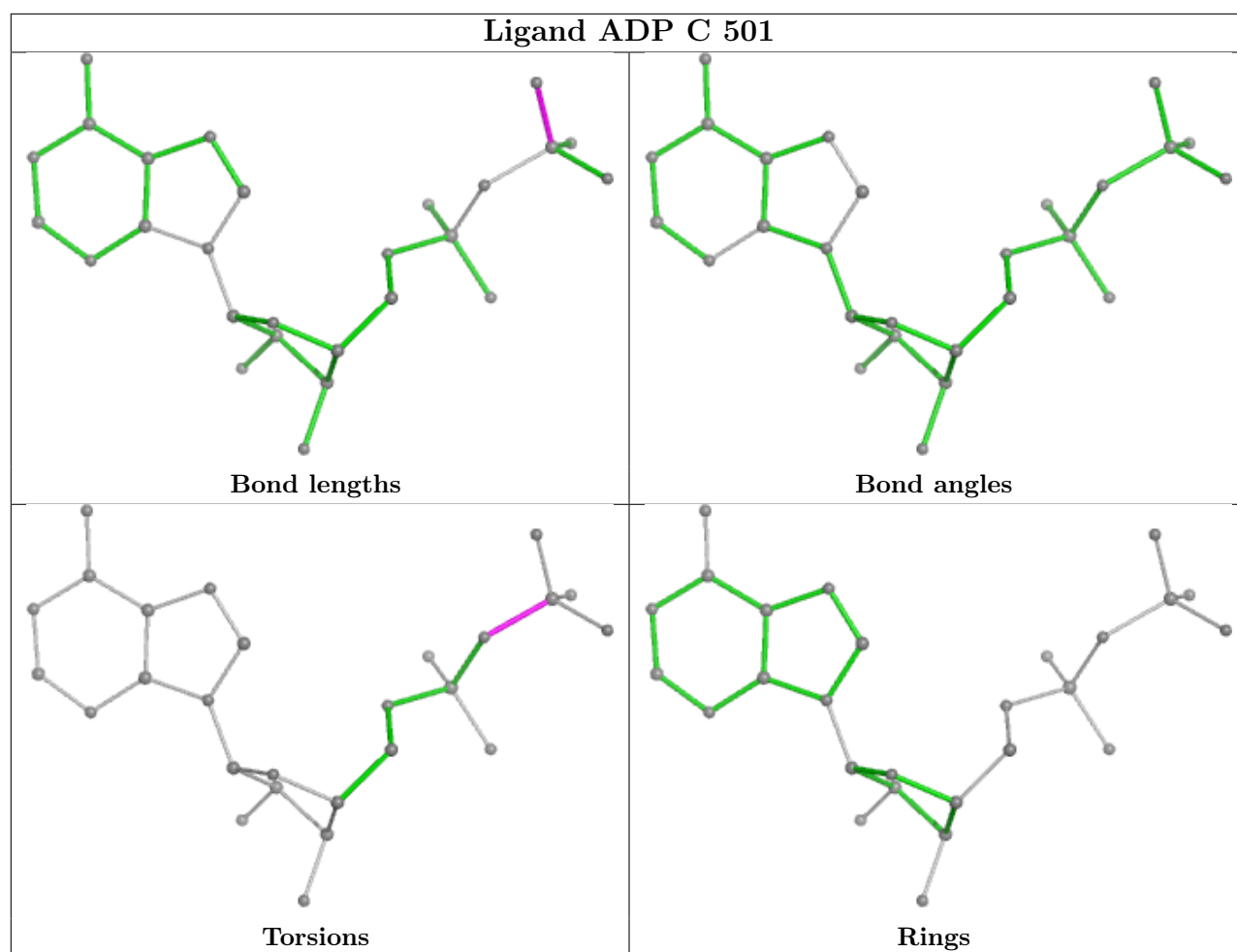
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

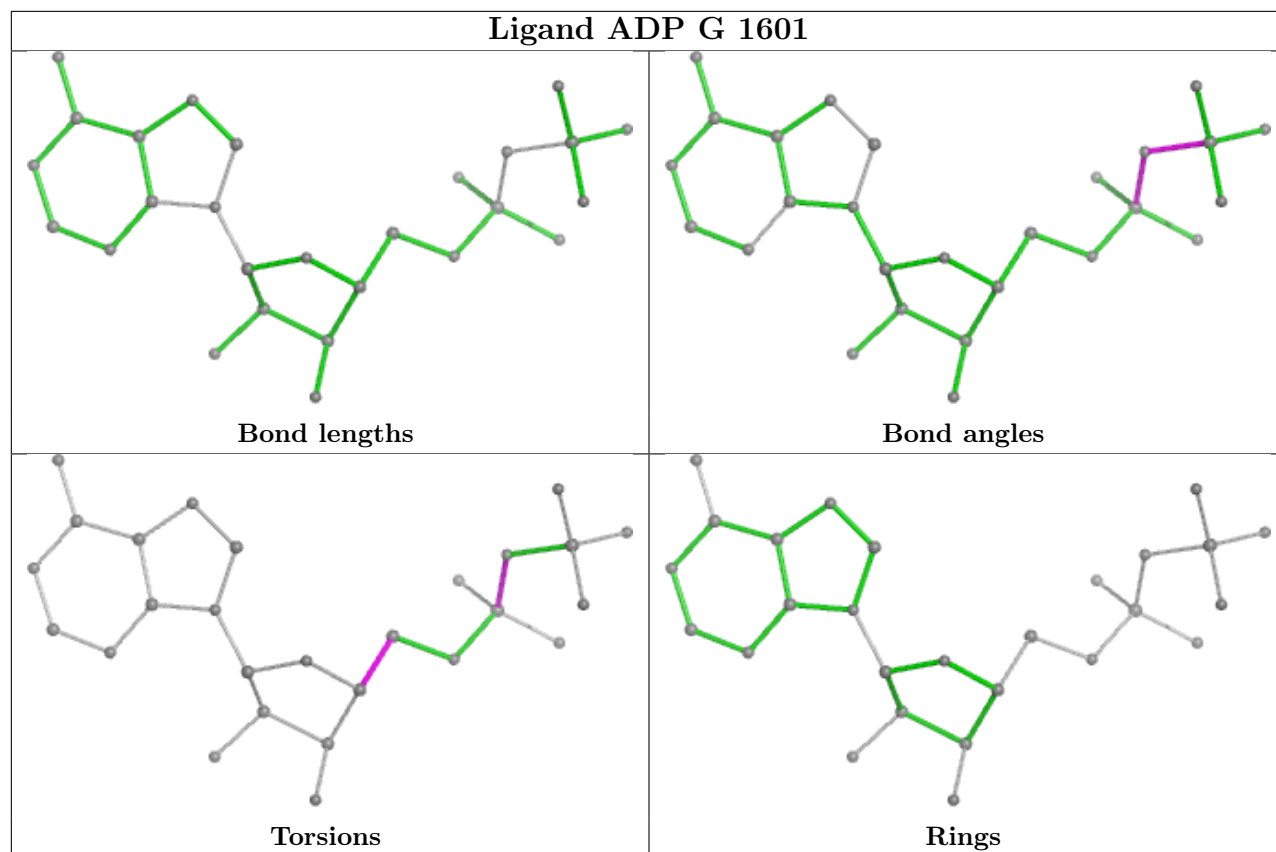


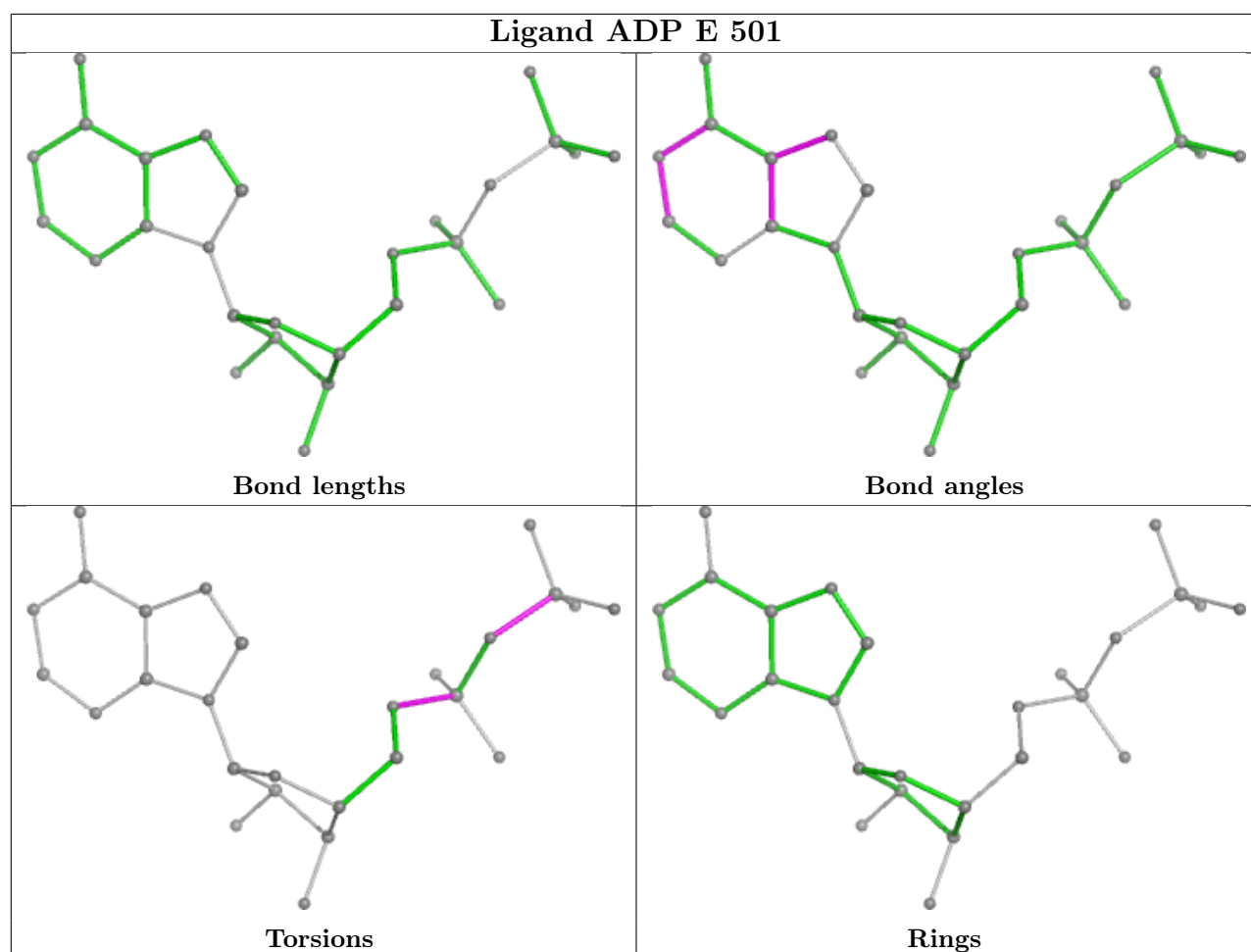












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

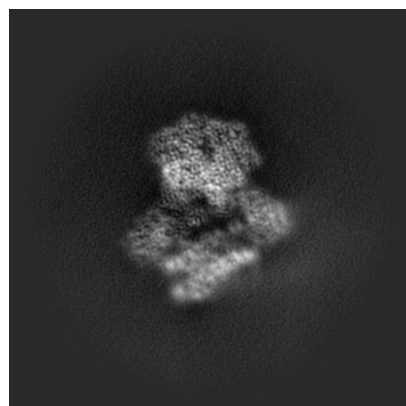
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51229. These allow visual inspection of the internal detail of the map and identification of artifacts.

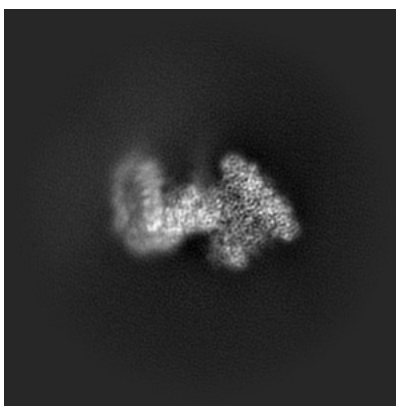
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

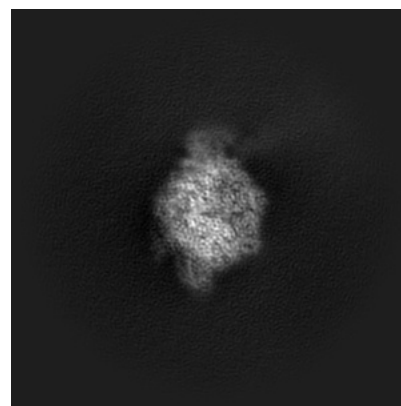
6.1.1 Primary map



X

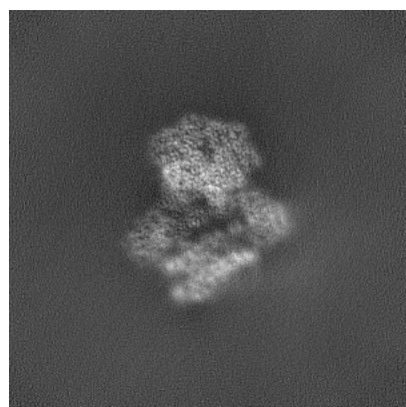


Y

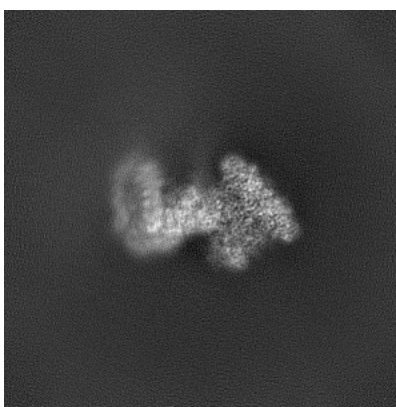


Z

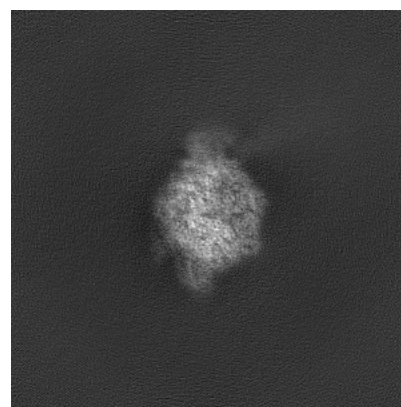
6.1.2 Raw map



X



Y

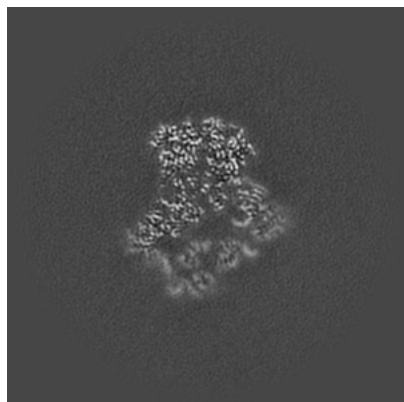


Z

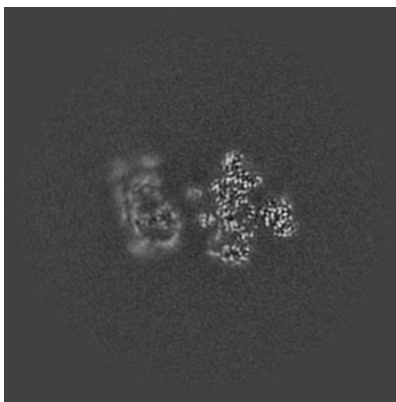
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

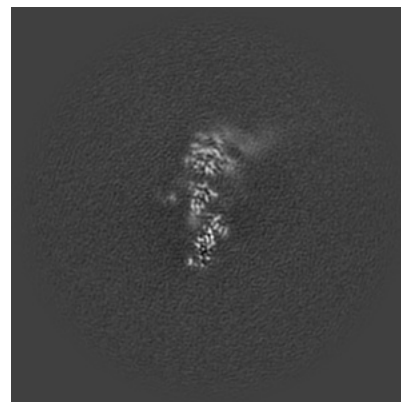
6.2.1 Primary map



X Index: 220

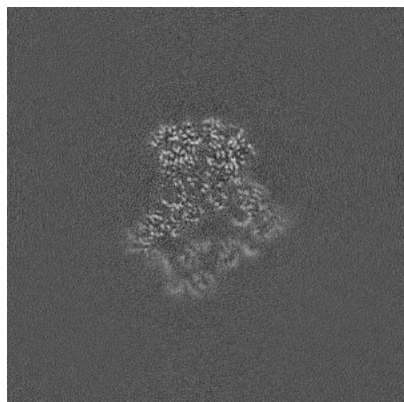


Y Index: 220

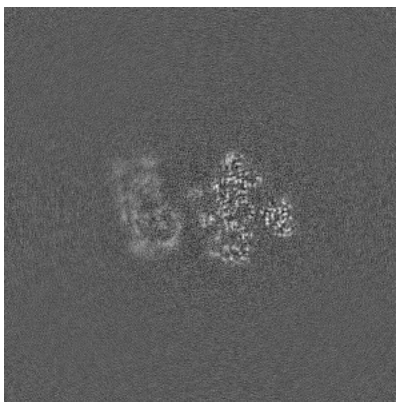


Z Index: 220

6.2.2 Raw map



X Index: 220



Y Index: 220

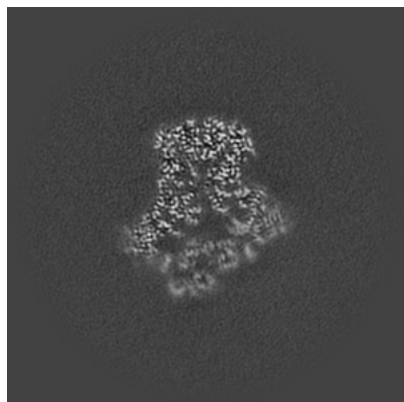


Z Index: 220

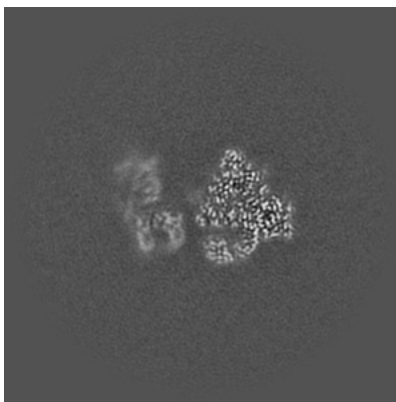
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

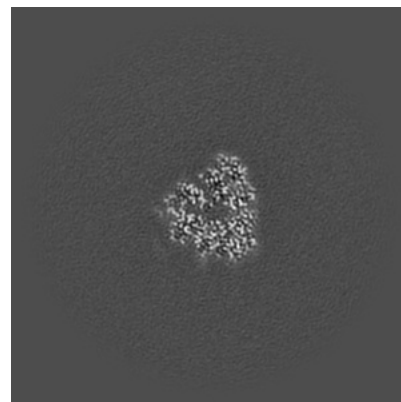
6.3.1 Primary map



X Index: 216

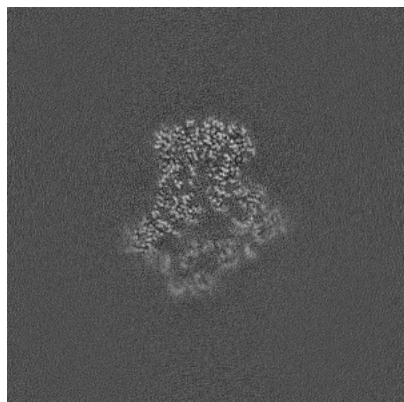


Y Index: 228

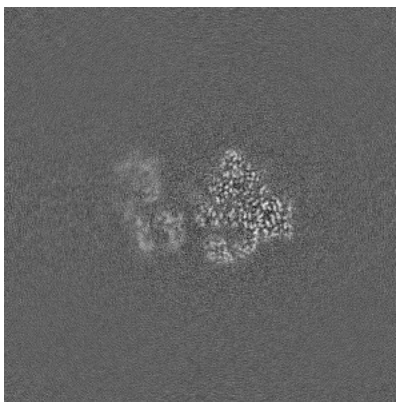


Z Index: 270

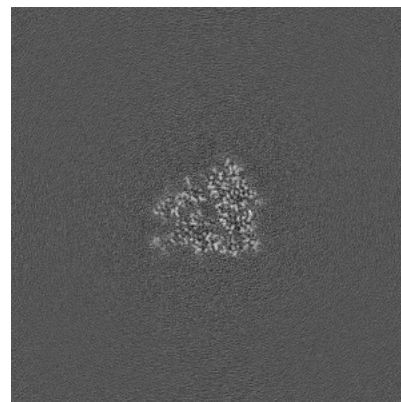
6.3.2 Raw map



X Index: 217



Y Index: 228

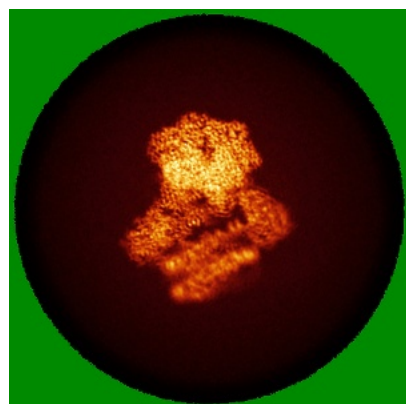


Z Index: 265

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

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

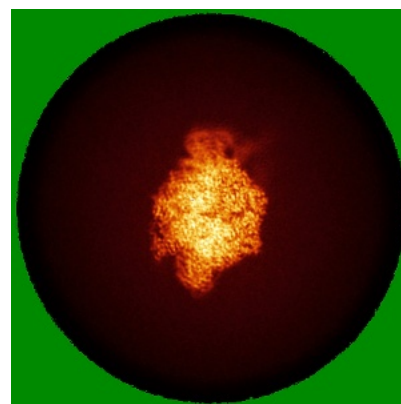
6.4.1 Primary map



X

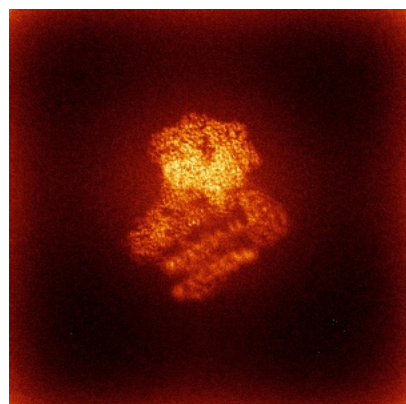


Y

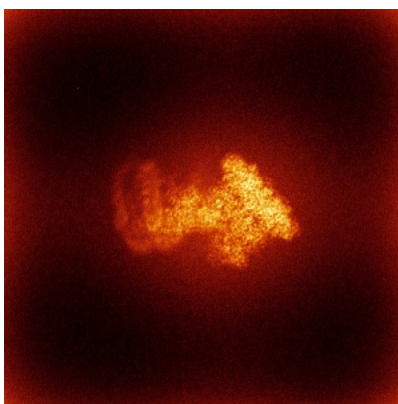


Z

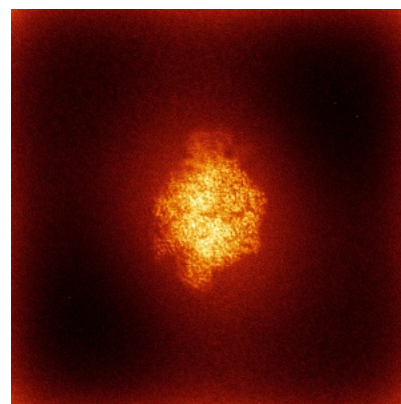
6.4.2 Raw map



X



Y

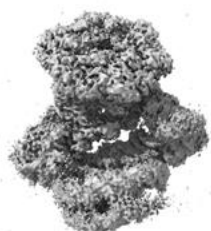


Z

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



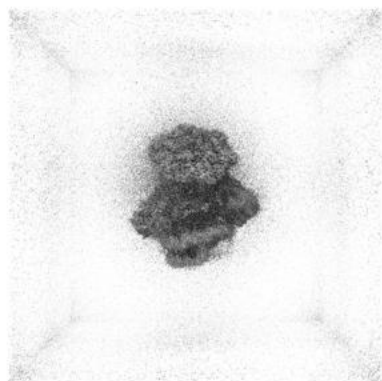
Y



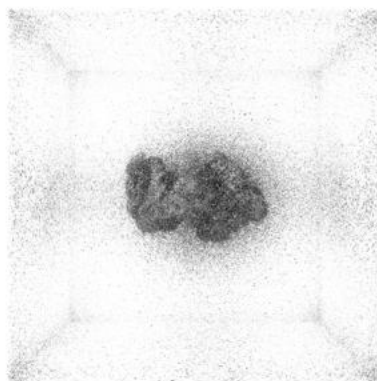
Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

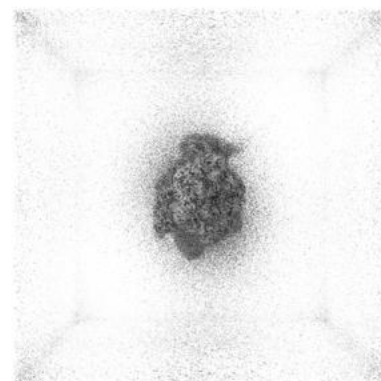
6.5.2 Raw map



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.

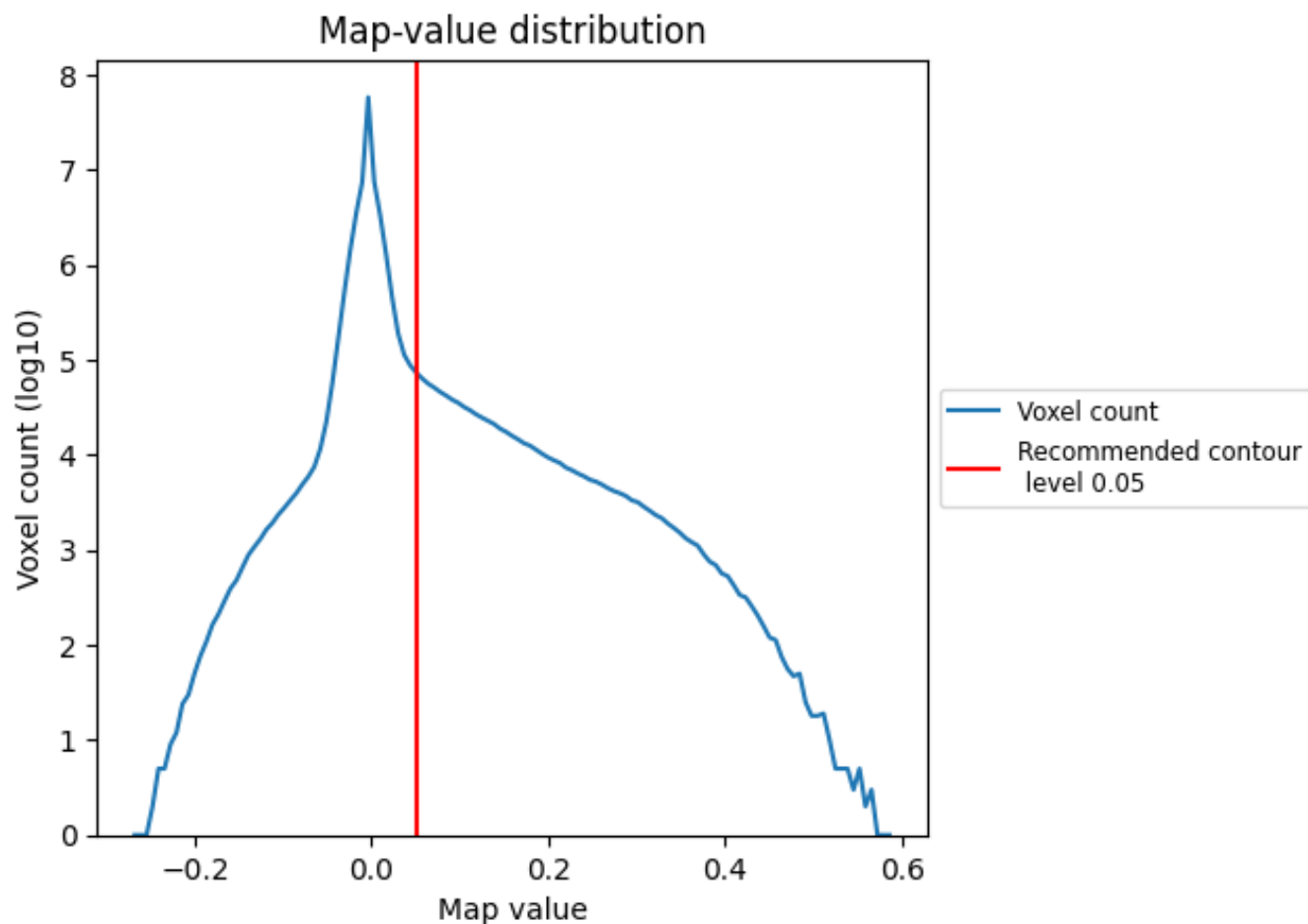
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

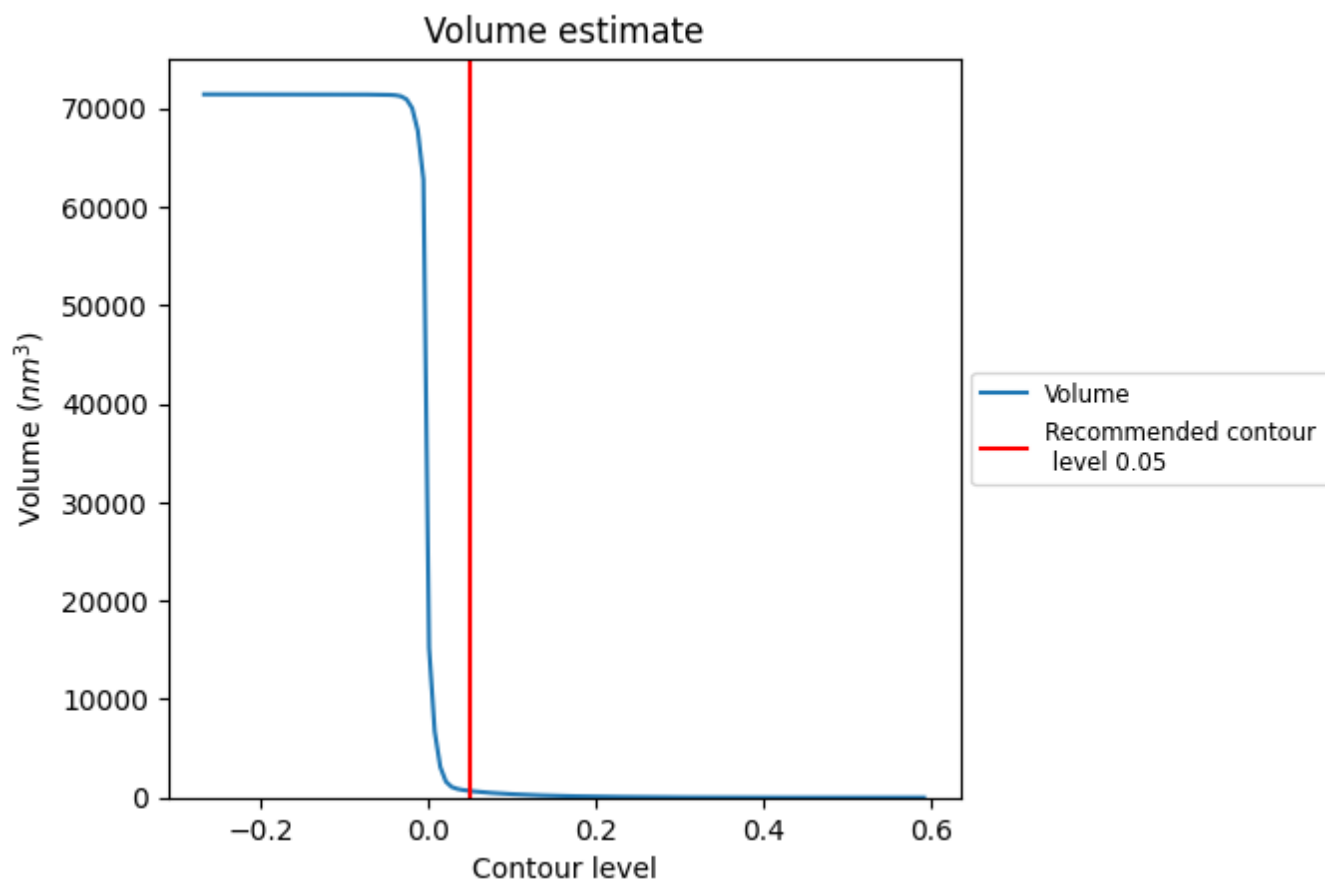
This section contains the results of statistical analysis of the map.

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.

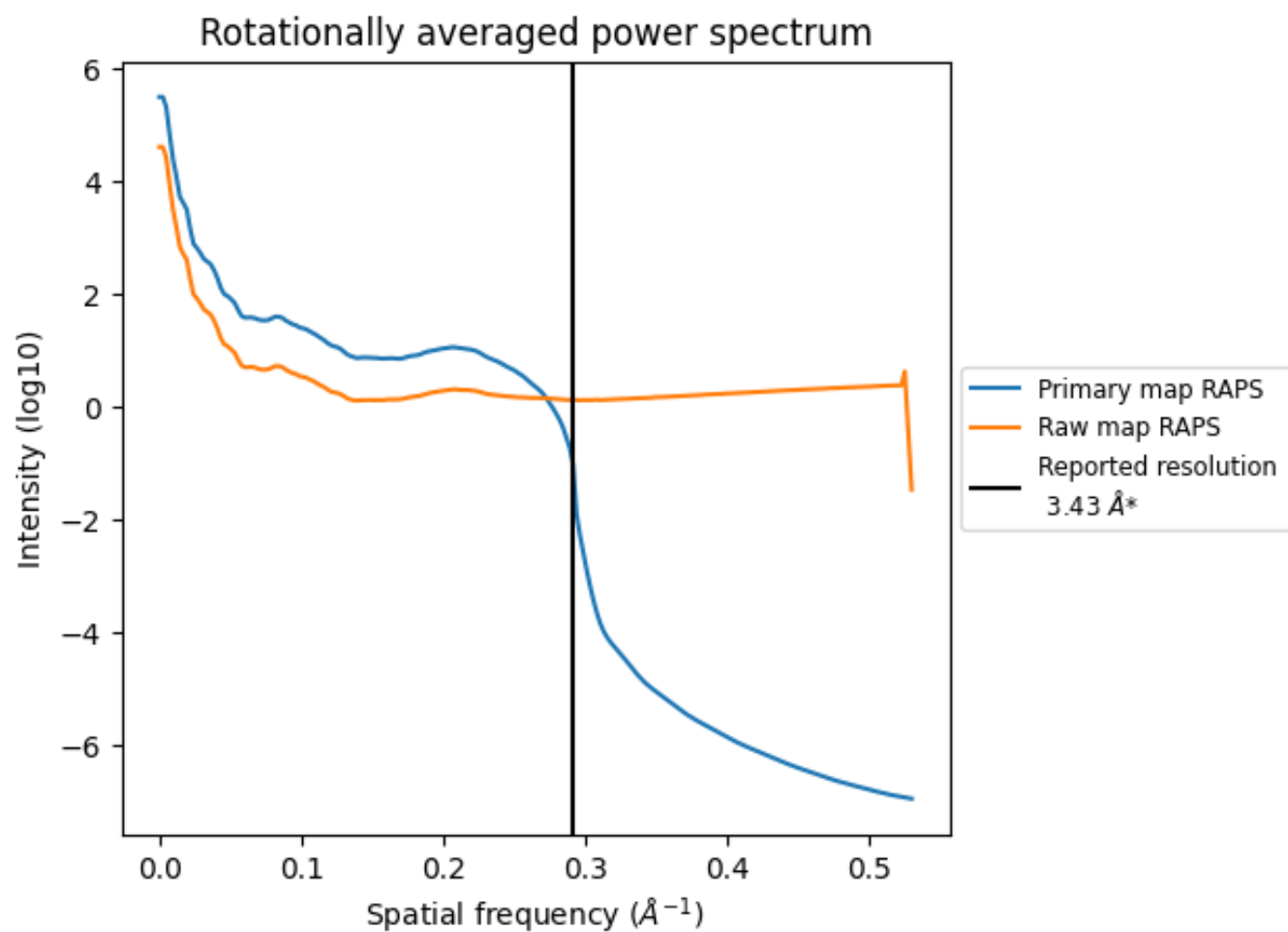
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 672 nm³; this corresponds to an approximate mass of 607 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 [i](#)

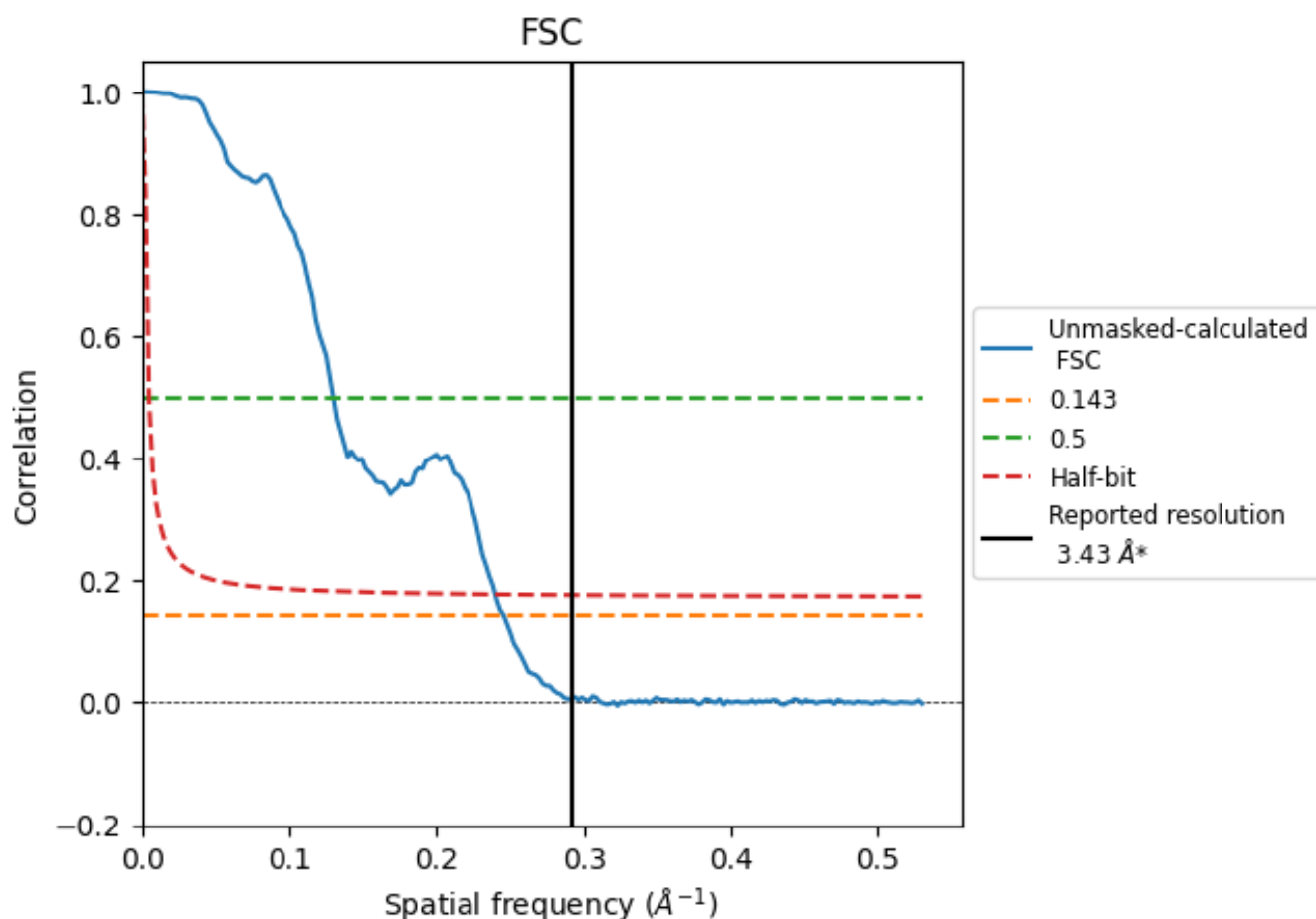


*Reported resolution corresponds to spatial frequency of 0.292 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.292 Å⁻¹

8.2 Resolution estimates [i](#)

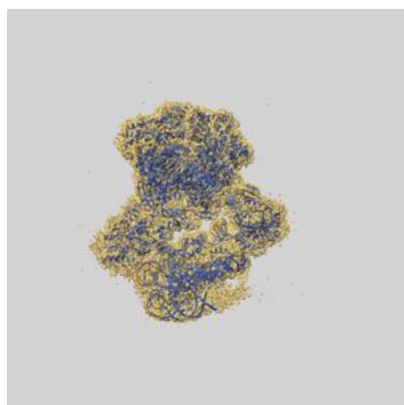
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.43	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.07	7.69	4.16

*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 4.07 differs from the reported value 3.43 by more than 10 %

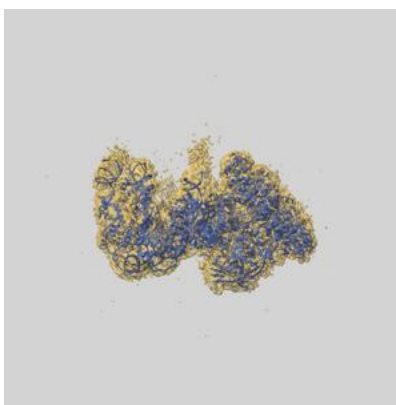
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51229 and PDB model 9GCG. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

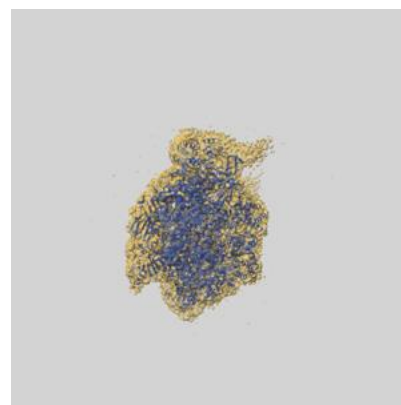
9.1 Map-model overlay [i](#)



X



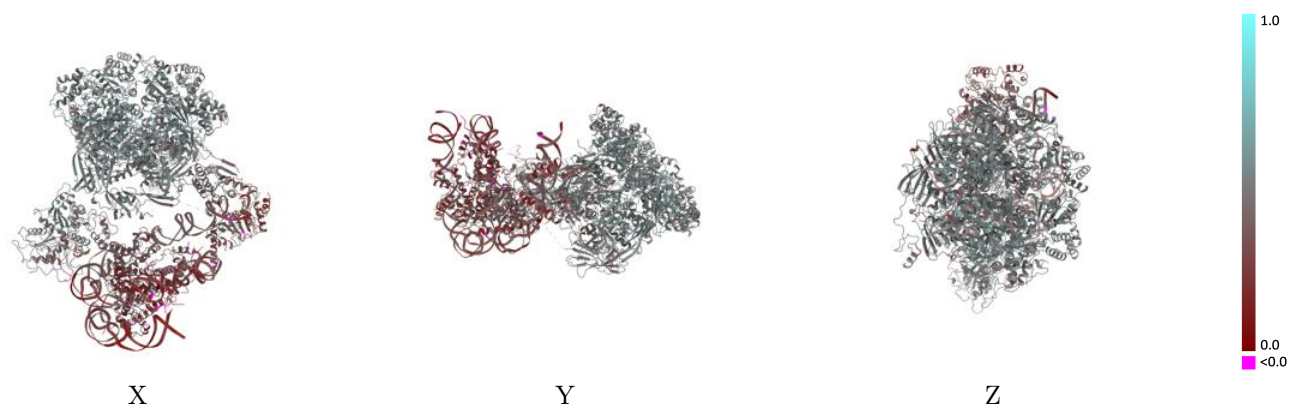
Y



Z

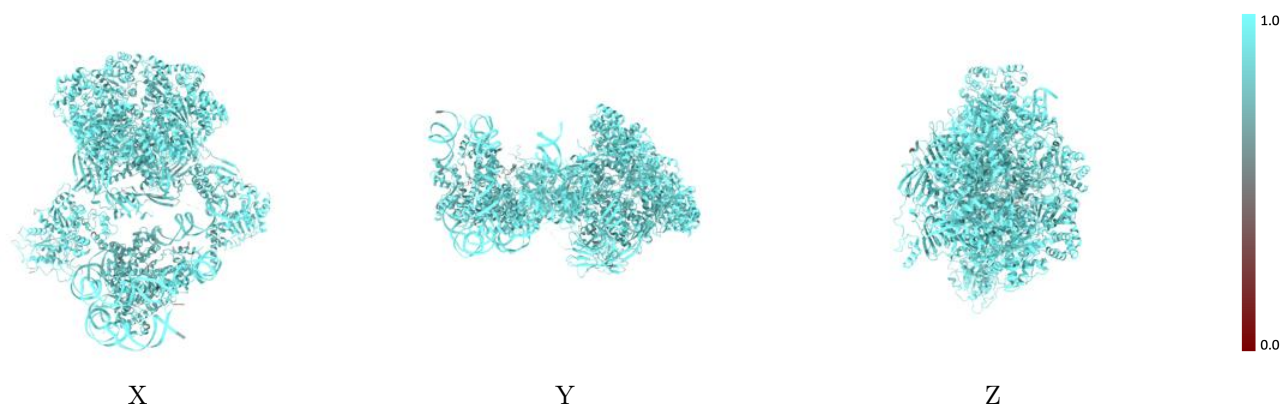
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



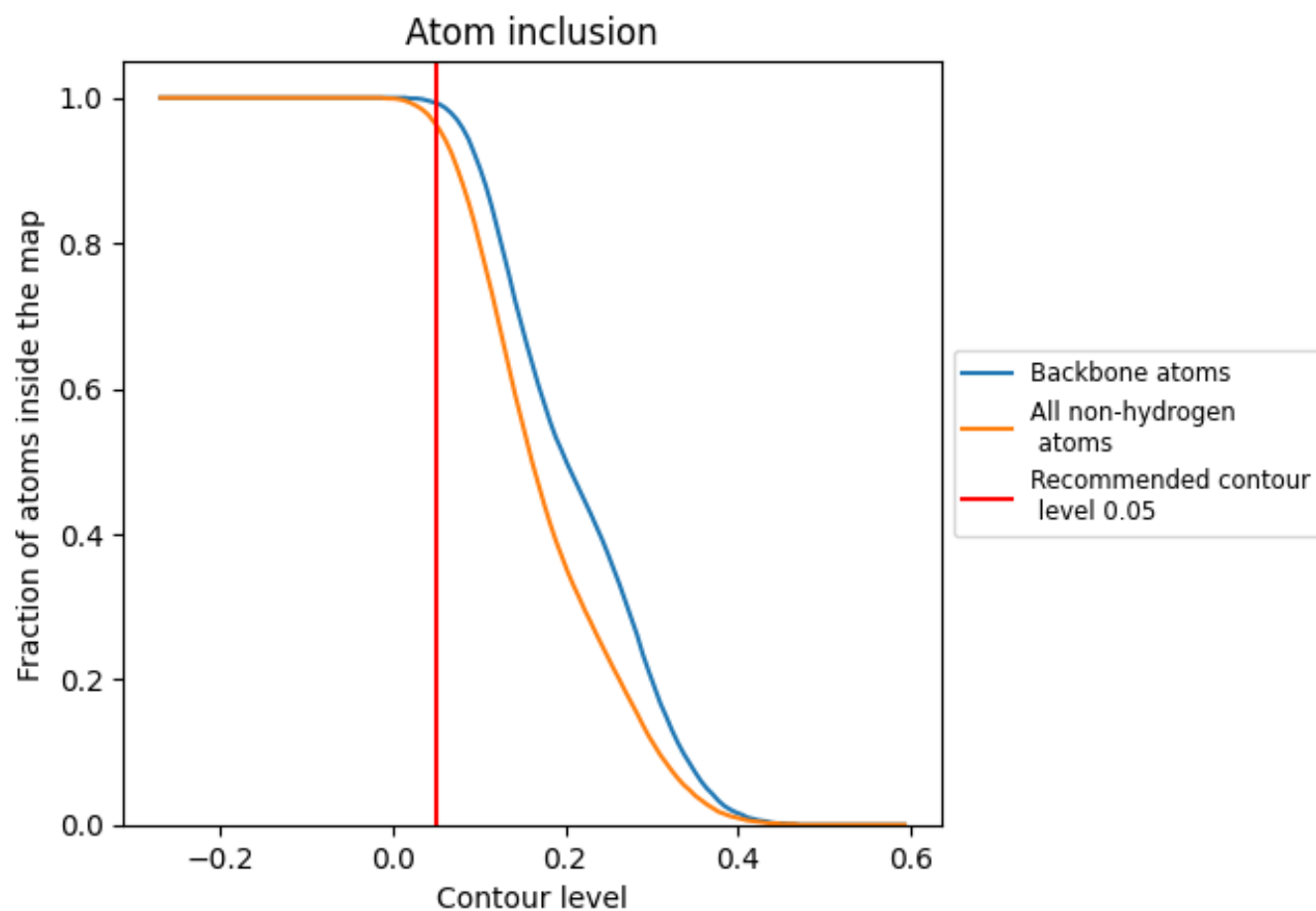
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).











































9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 96% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9640	 0.4240
A	 0.9760	 0.5130
B	 0.9760	 0.5000
C	 0.9780	 0.5050
D	 0.9780	 0.5040
E	 0.9710	 0.4980
F	 0.9760	 0.5090
G	 0.9630	 0.4200
H	 0.9590	 0.3790
I	 0.9390	 0.4440
J	 0.9650	 0.4490
K	 0.9840	 0.2780
L	 0.9910	 0.2830
M	 0.9330	 0.3190
N	 0.9320	 0.3060
O	 0.8720	 0.2420
P	 0.9150	 0.2720
Q	 0.8910	 0.2100
R	 0.9190	 0.2590
S	 0.8600	 0.3420
T	 0.9270	 0.3750

