



## wwPDB EM Validation Summary Report ⓘ

Sep 14, 2024 – 09:44 am BST

PDB ID : 8P4O  
EMDB ID : EMD-17421  
Title : CryoEM structure of a GroEL7-GroES7 cage with encapsulated ordered substrate MetK in the presence of ADP-BeFx  
Authors : Wagner, J.; Beck, F.; Bracher, A.; Caravajal, A.I.; Wan, W.; Bohn, S.; Koenner, R.; Baumeister, W.; Fernandez-Busnadiego, R.; Hartl, F.U.  
Deposited on : 2023-05-23  
Resolution : 3.04 Å (reported)  
Based on initial models : 1SX3, 5OPX

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev112  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.38.2

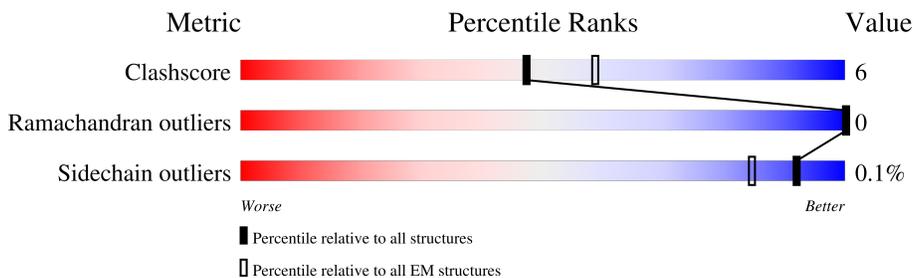
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.04 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	547	
1	B	547	
1	C	547	
1	D	547	
1	E	547	
1	F	547	
1	G	547	
2	O	97	

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Mol	Chain	Length	Quality of chain
2	P	97	<p>20% 78% 20%</p>
2	Q	97	<p>20% 84% 14%</p>
2	R	97	<p>23% 86% 12%</p>
2	S	97	<p>22% 88% 9%</p>
2	T	97	<p>20% 87% 11%</p>
2	U	97	<p>23% 90% 8%</p>
3	1	384	<p>76% 81% 18%</p>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 34605 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 Chaperonin GroEL.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	524	Total 3851	C 2395	N 665	O 771	S 20	0	0
1	B	524	Total 3851	C 2395	N 665	O 771	S 20	0	0
1	C	524	Total 3847	C 2393	N 665	O 769	S 20	0	0
1	D	524	Total 3851	C 2395	N 665	O 771	S 20	0	0
1	E	524	Total 3851	C 2395	N 665	O 771	S 20	0	0
1	F	524	Total 3851	C 2395	N 665	O 771	S 20	0	0
1	G	524	Total 3851	C 2395	N 665	O 771	S 20	0	0

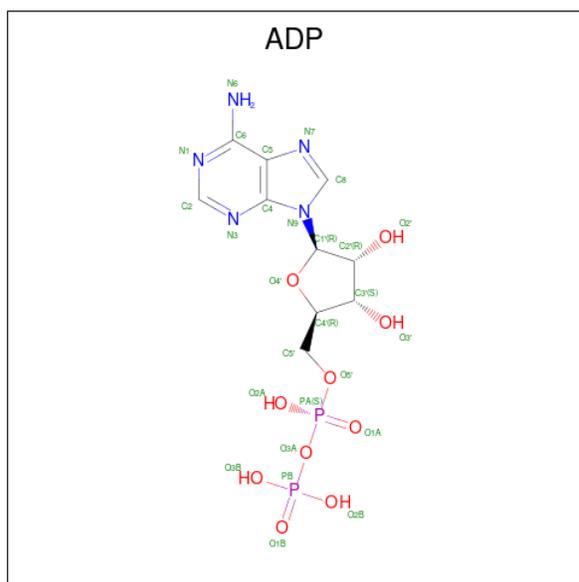
- Molecule 2 is a protein called Co-chaperonin GroES.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	O	95	Total 644	C 404	N 117	O 122	S 1	0	0
2	P	95	Total 644	C 404	N 117	O 122	S 1	0	0
2	Q	95	Total 644	C 404	N 117	O 122	S 1	0	0
2	R	95	Total 644	C 404	N 117	O 122	S 1	0	0
2	S	95	Total 644	C 404	N 117	O 122	S 1	0	0
2	T	95	Total 644	C 404	N 117	O 122	S 1	0	0
2	U	95	Total 644	C 404	N 117	O 122	S 1	0	0

- Molecule 3 is a protein called S-adenosylmethionine synthase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	1	379	2892	1825	492	562	13	0	0

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
4	A	1	27	10	5	10	2	0
4	B	1	27	10	5	10	2	0
4	C	1	27	10	5	10	2	0
4	D	1	27	10	5	10	2	0
4	E	1	27	10	5	10	2	0
4	F	1	27	10	5	10	2	0
4	G	1	27	10	5	10	2	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

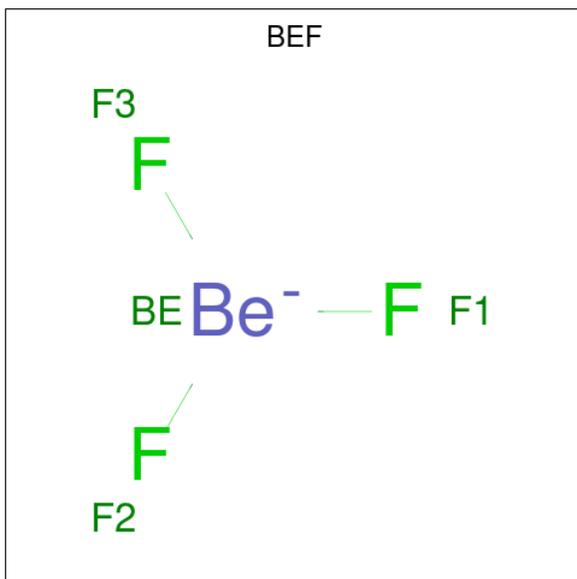
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
5	A	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
5	B	1	Total	Mg	0
			1	1	
5	C	1	Total	Mg	0
			1	1	
5	D	1	Total	Mg	0
			1	1	
5	E	1	Total	Mg	0
			1	1	
5	F	1	Total	Mg	0
			1	1	
5	G	1	Total	Mg	0
			1	1	

- Molecule 6 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF<sub>3</sub>).



Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	Be	F	0
			4	1	3	
6	B	1	Total	Be	F	0
			4	1	3	
6	C	1	Total	Be	F	0
			4	1	3	
6	D	1	Total	Be	F	0
			4	1	3	
6	E	1	Total	Be	F	0
			4	1	3	

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Mol	Chain	Residues	Atoms			AltConf
6	F	1	Total 4	Be 1	F 3	0
6	G	1	Total 4	Be 1	F 3	0

- Molecule 7 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total 1	K 1	0
7	B	1	Total 1	K 1	0
7	C	1	Total 1	K 1	0
7	D	1	Total 1	K 1	0
7	E	1	Total 1	K 1	0
7	F	1	Total 1	K 1	0
7	G	1	Total 1	K 1	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		AltConf
8	A	3	Total 3	O 3	0
8	B	3	Total 3	O 3	0
8	C	3	Total 3	O 3	0
8	D	3	Total 3	O 3	0
8	E	3	Total 3	O 3	0
8	F	3	Total 3	O 3	0
8	G	3	Total 3	O 3	0

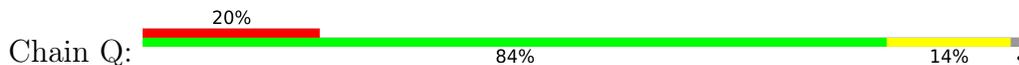




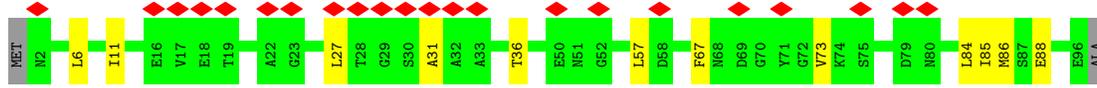
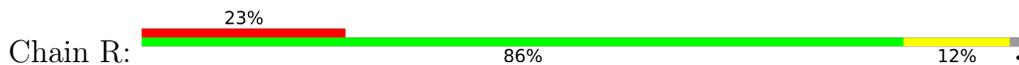




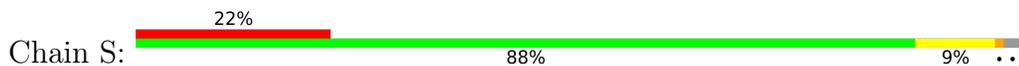
• Molecule 2: Co-chaperonin GroES



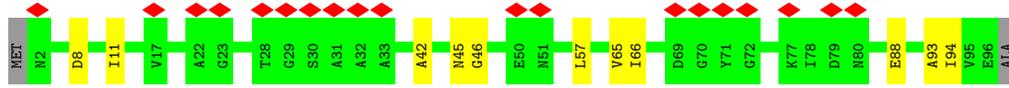
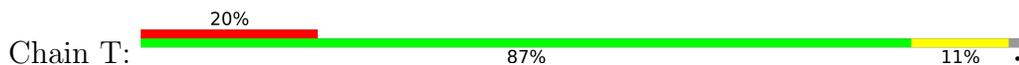
• Molecule 2: Co-chaperonin GroES



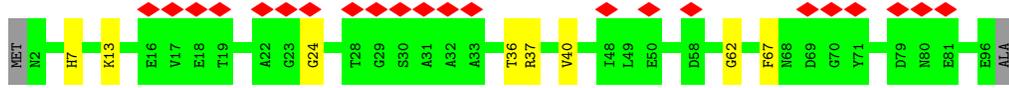
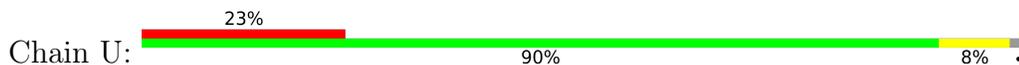
• Molecule 2: Co-chaperonin GroES



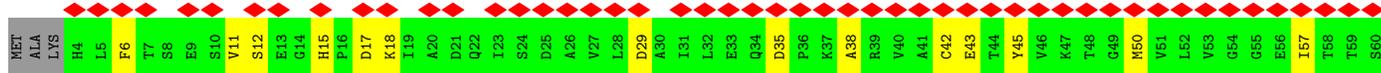
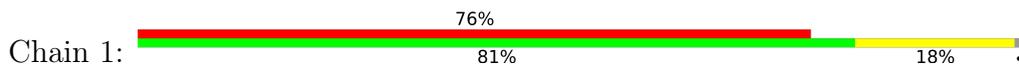
• Molecule 2: Co-chaperonin GroES



• Molecule 2: Co-chaperonin GroES



• Molecule 3: S-adenosylmethionine synthase



A61	A62	A63	A64	A65	A66	A67	A68	A69	A70	A71	A72	A73	A74	A75	A76	A77	A78	A79	A80	A81	A82	A83	A84	A85	A86	A87	A88	A89	A90	A91	A92	A93	A94	A95	A96	A97	A98	A99	A100	A101	A102	A103	A104	A105	A106	A107	A108	A109	A110	A111	A112	A113	A114	A115	A116	A117	A118	A119	A120
G121	L122	M123	F124	G125	Y126	A127	T128	M129	E130	T131	D132	V133	L134	M135	P136	A150	E151	V152	G156	T157	L158	P159	W160	L161	R162	P163	D164	A165	K166	F171	Q172	Y173	D174	D175	G176	K177	I178	V179	G180	I181	D182	V185	L186	S187	T188	Q189	H190	S191	E192	E193	I194	D195	Q196	K197	S198				
L199	Q200	E201	A202	V203	M204	E205	E206	I207	I208	K209	L212	P213	A214	E215	W216	L217	T218	S219	A220	T221	K222	F223	F224	I225	N226	P227	T228	G229	R230	F231	V232	I233	G234	G235	P236	M237	G238	D239	C240	G241	L242	T243	G244	R245	K246	I247	I248	G253	G254	M255	A256	R257	H258	G259	G260	G261	A262		
F263	S264	G265	K266	D267	P268	S269	K270	V271	D272	R273	Y277	R280	A283	K284	N285	G290	L291	A292	D293	R294	C295	E296	I297	Q298	V299	S300	Y301	A302	I303	G304	V305	A306	E307	P308	T309	S310	I311	M312	V313	E314	T315	F316	G317	T318	E319	K320	V321	P322	S323	E324	Q325	L326	T327	L328	L329				
V330	R331	E332	F333	F334	D335	L336	R337	P338	V339	G340	L341	I342	Q343	M344	L345	D346	L347	L348	H349	P350	I351	V352	K353	E354	T355	A356	A357	H360	F361	G362	R363	E364	H365	E369	K370	T371	D372	K373	A374	Q375	L376	L377	R378	D379	A380	A381	G382	LEU	LYS										

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	454545	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 ( $e^-/\text{\AA}^2$ )	55	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	22500	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.948	Depositor
Minimum map value	-2.696	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.157	Depositor
Recommended contour level	0.671	Depositor
Map size ( $\text{\AA}$ )	279.04, 279.04, 279.04	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.09, 1.09, 1.09	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	0.25	0/3879	0.48	0/5238
1	B	0.25	0/3879	0.47	0/5238
1	C	0.24	0/3875	0.49	0/5233
1	D	0.25	0/3879	0.48	0/5238
1	E	0.25	0/3879	0.47	0/5238
1	F	0.25	0/3879	0.48	0/5238
1	G	0.24	0/3879	0.47	0/5238
2	O	0.24	0/647	0.51	0/882
2	P	0.24	0/647	0.49	0/882
2	Q	0.24	0/647	0.50	0/882
2	R	0.24	0/647	0.50	0/882
2	S	0.24	0/647	0.50	0/882
2	T	0.24	0/647	0.50	0/882
2	U	0.24	0/647	0.51	0/882
3	1	0.24	0/2951	0.48	0/4007
All	All	0.24	0/34629	0.48	0/46842

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3851	0	3972	52	0
1	B	3851	0	3972	43	0
1	C	3847	0	3967	41	0
1	D	3851	0	3972	43	0
1	E	3851	0	3972	49	0
1	F	3851	0	3972	43	0
1	G	3851	0	3972	47	0
2	O	644	0	633	12	0
2	P	644	0	633	11	0
2	Q	644	0	633	8	0
2	R	644	0	633	7	0
2	S	644	0	633	7	0
2	T	644	0	633	7	0
2	U	644	0	633	6	0
3	1	2892	0	2831	42	0
4	A	27	0	12	1	0
4	B	27	0	12	1	0
4	C	27	0	12	1	0
4	D	27	0	12	1	0
4	E	27	0	12	1	0
4	F	27	0	12	1	0
4	G	27	0	12	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
6	A	4	0	0	1	0
6	B	4	0	0	1	0
6	C	4	0	0	1	0
6	D	4	0	0	1	0
6	E	4	0	0	1	0
6	F	4	0	0	1	0
6	G	4	0	0	1	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	E	1	0	0	0	0
7	F	1	0	0	0	0
7	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	3	0	0	0	0
8	B	3	0	0	0	0
8	C	3	0	0	0	0
8	D	3	0	0	0	0
8	E	3	0	0	0	0
8	F	3	0	0	0	0
8	G	3	0	0	0	0
All	All	34605	0	35145	407	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 407 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)
2:Q:11:ILE:HG22	2:Q:85:ILE:HG12	1.72	0.72
1:B:193:MET:HG3	1:B:371:LYS:HG2	1.71	0.71
2:P:11:ILE:HG22	2:P:85:ILE:HG12	1.72	0.71
1:G:284:ARG:HH22	1:G:368:ARG:HD2	1.57	0.69
1:D:23:LEU:HD23	1:D:74:VAL:HG13	1.74	0.69

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	522/547 (95%)	519 (99%)	3 (1%)	0	100	100
1	B	522/547 (95%)	517 (99%)	5 (1%)	0	100	100
1	C	522/547 (95%)	517 (99%)	5 (1%)	0	100	100
1	D	522/547 (95%)	516 (99%)	6 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	522/547 (95%)	516 (99%)	6 (1%)	0	100	100
1	F	522/547 (95%)	518 (99%)	4 (1%)	0	100	100
1	G	522/547 (95%)	520 (100%)	2 (0%)	0	100	100
2	O	93/97 (96%)	92 (99%)	1 (1%)	0	100	100
2	P	93/97 (96%)	91 (98%)	2 (2%)	0	100	100
2	Q	93/97 (96%)	92 (99%)	1 (1%)	0	100	100
2	R	93/97 (96%)	92 (99%)	1 (1%)	0	100	100
2	S	93/97 (96%)	91 (98%)	2 (2%)	0	100	100
2	T	93/97 (96%)	91 (98%)	2 (2%)	0	100	100
2	U	93/97 (96%)	92 (99%)	1 (1%)	0	100	100
3	1	377/384 (98%)	369 (98%)	8 (2%)	0	100	100
All	All	4682/4892 (96%)	4633 (99%)	49 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	403/414 (97%)	403 (100%)	0	100	100
1	B	403/414 (97%)	403 (100%)	0	100	100
1	C	402/414 (97%)	400 (100%)	2 (0%)	86	93
1	D	403/414 (97%)	403 (100%)	0	100	100
1	E	403/414 (97%)	402 (100%)	1 (0%)	92	96
1	F	403/414 (97%)	403 (100%)	0	100	100
1	G	403/414 (97%)	403 (100%)	0	100	100
2	O	62/80 (78%)	62 (100%)	0	100	100
2	P	62/80 (78%)	62 (100%)	0	100	100
2	Q	62/80 (78%)	62 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	R	62/80 (78%)	62 (100%)	0	100	100
2	S	62/80 (78%)	61 (98%)	1 (2%)	58	79
2	T	62/80 (78%)	62 (100%)	0	100	100
2	U	62/80 (78%)	62 (100%)	0	100	100
3	1	304/312 (97%)	303 (100%)	1 (0%)	91	95
All	All	3558/3770 (94%)	3553 (100%)	5 (0%)	92	97

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	82	ASN
1	C	226	LYS
1	E	82	ASN
2	S	68	ASN
3	1	129	ASN

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

Mol	Chain	Res	Type
1	A	348	GLN
1	F	453	GLN
2	S	68	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 28 ligands modelled in this entry, 14 are monoatomic - leaving 14 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
4	ADP	C	1600	6,7,5	24,29,29	0.92	1 (4%)	29,45,45	1.41	4 (13%)
4	ADP	G	1600	6,7,5	24,29,29	0.92	1 (4%)	29,45,45	1.40	4 (13%)
4	ADP	F	1600	7,5	24,29,29	0.93	1 (4%)	29,45,45	1.43	4 (13%)
6	BEF	G	1602	4	0,3,3	-	-	-	-	-
4	ADP	E	1600	6,7,5	24,29,29	0.93	1 (4%)	29,45,45	1.42	4 (13%)
6	BEF	E	1602	4	0,3,3	-	-	-	-	-
4	ADP	A	1600	6,7,5	24,29,29	0.93	1 (4%)	29,45,45	1.43	4 (13%)
6	BEF	A	1602	4	0,3,3	-	-	-	-	-
6	BEF	F	1602	-	0,3,3	-	-	-	-	-
6	BEF	B	1602	4	0,3,3	-	-	-	-	-
6	BEF	C	1602	4	0,3,3	-	-	-	-	-
4	ADP	D	1600	7,5	24,29,29	0.93	1 (4%)	29,45,45	1.43	4 (13%)
4	ADP	B	1600	6,7,5	24,29,29	0.93	1 (4%)	29,45,45	1.42	4 (13%)
6	BEF	D	1602	-	0,3,3	-	-	-	-	-

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
4	ADP	C	1600	6,7,5	-	5/12/32/32	0/3/3/3
4	ADP	G	1600	6,7,5	-	5/12/32/32	0/3/3/3
4	ADP	F	1600	7,5	-	5/12/32/32	0/3/3/3
4	ADP	E	1600	6,7,5	-	4/12/32/32	0/3/3/3
4	ADP	A	1600	6,7,5	-	4/12/32/32	0/3/3/3
4	ADP	D	1600	7,5	-	5/12/32/32	0/3/3/3
4	ADP	B	1600	6,7,5	-	5/12/32/32	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1600	ADP	C5-C4	2.45	1.47	1.40
4	B	1600	ADP	C5-C4	2.44	1.47	1.40
4	F	1600	ADP	C5-C4	2.43	1.47	1.40
4	C	1600	ADP	C5-C4	2.42	1.47	1.40
4	G	1600	ADP	C5-C4	2.41	1.47	1.40

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1600	ADP	C3'-C2'-C1'	3.31	105.96	100.98
4	C	1600	ADP	N3-C2-N1	-3.27	123.57	128.68
4	E	1600	ADP	N3-C2-N1	-3.25	123.59	128.68
4	E	1600	ADP	C3'-C2'-C1'	3.25	105.87	100.98
4	B	1600	ADP	N3-C2-N1	-3.25	123.60	128.68

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1600	ADP	PA-O3A-PB-O2B
4	B	1600	ADP	PA-O3A-PB-O3B
4	C	1600	ADP	PA-O3A-PB-O2B
4	C	1600	ADP	O4'-C4'-C5'-O5'
4	D	1600	ADP	O4'-C4'-C5'-O5'

There are no ring outliers.

14 monomers are involved in 7 short contacts:

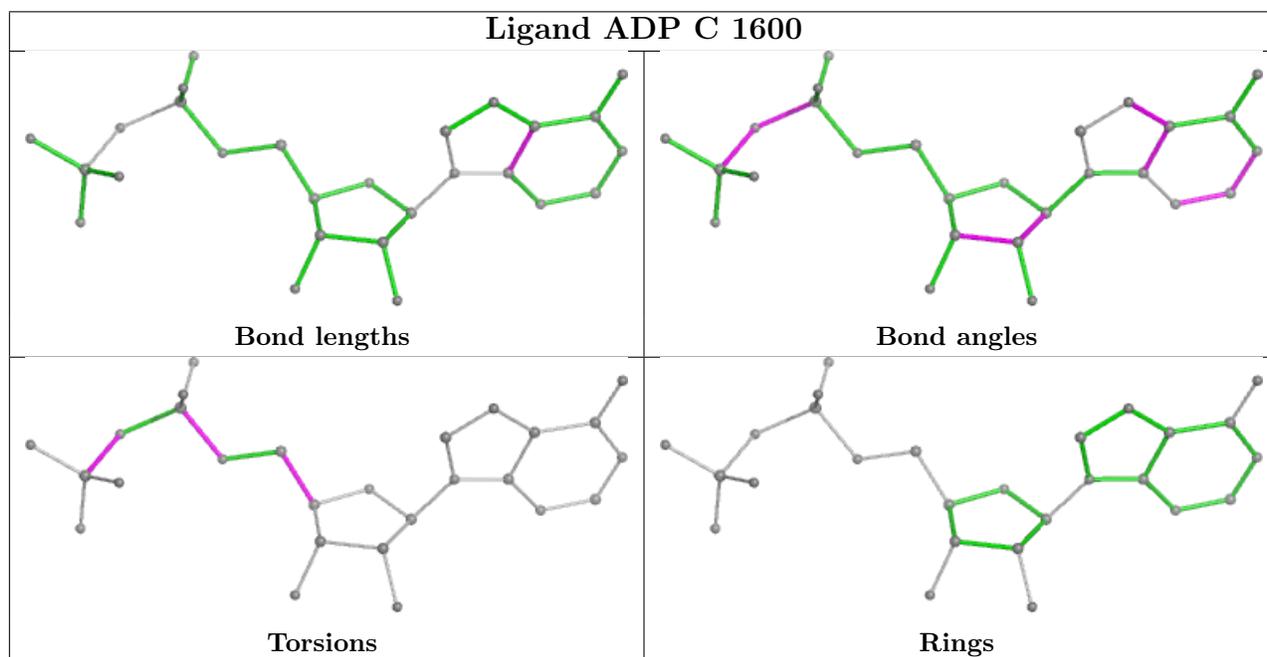
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1600	ADP	1	0
4	G	1600	ADP	1	0
4	F	1600	ADP	1	0
6	G	1602	BEF	1	0
4	E	1600	ADP	1	0
6	E	1602	BEF	1	0
4	A	1600	ADP	1	0
6	A	1602	BEF	1	0
6	F	1602	BEF	1	0
6	B	1602	BEF	1	0
6	C	1602	BEF	1	0

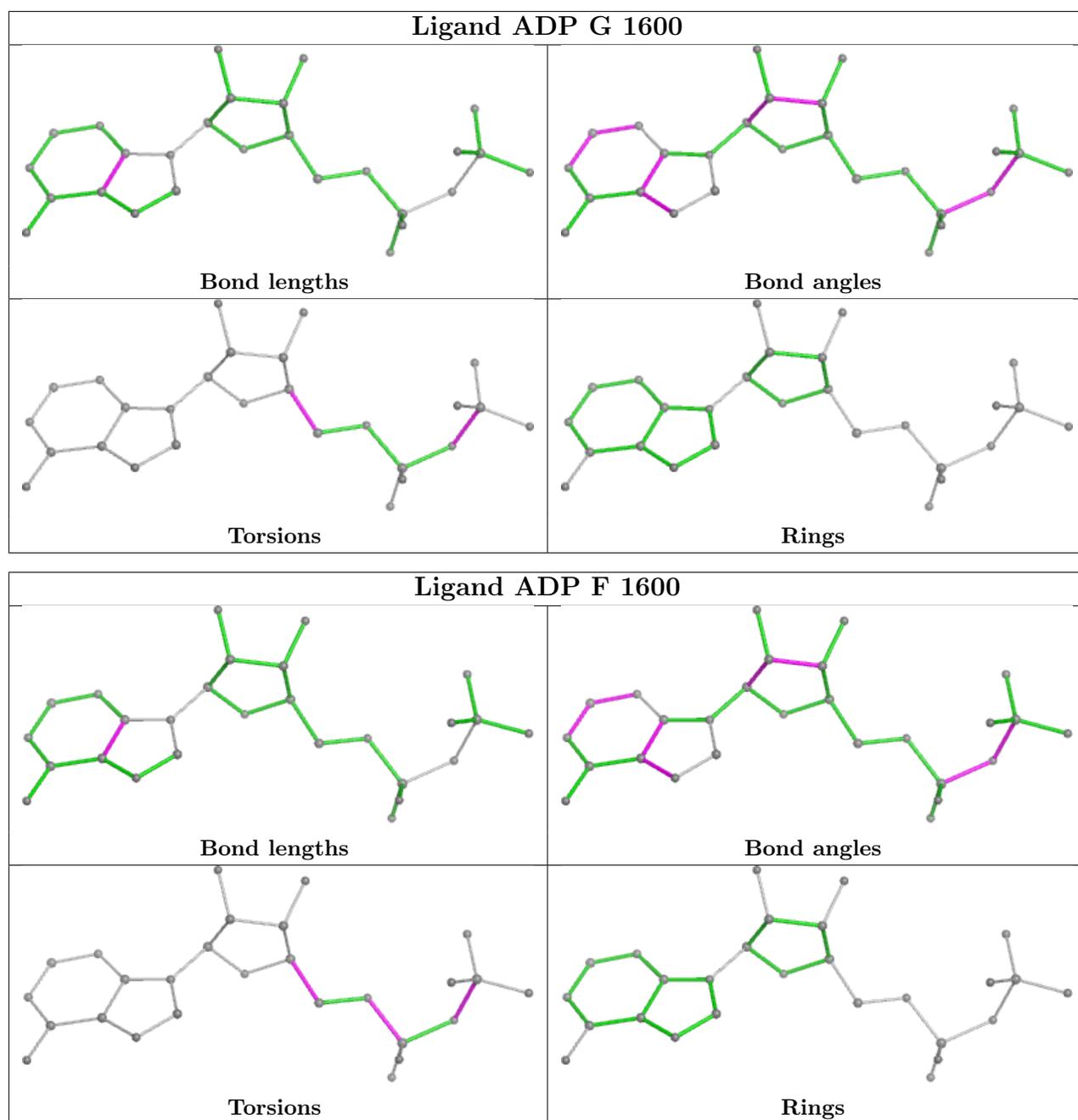
*Continued on next page...*

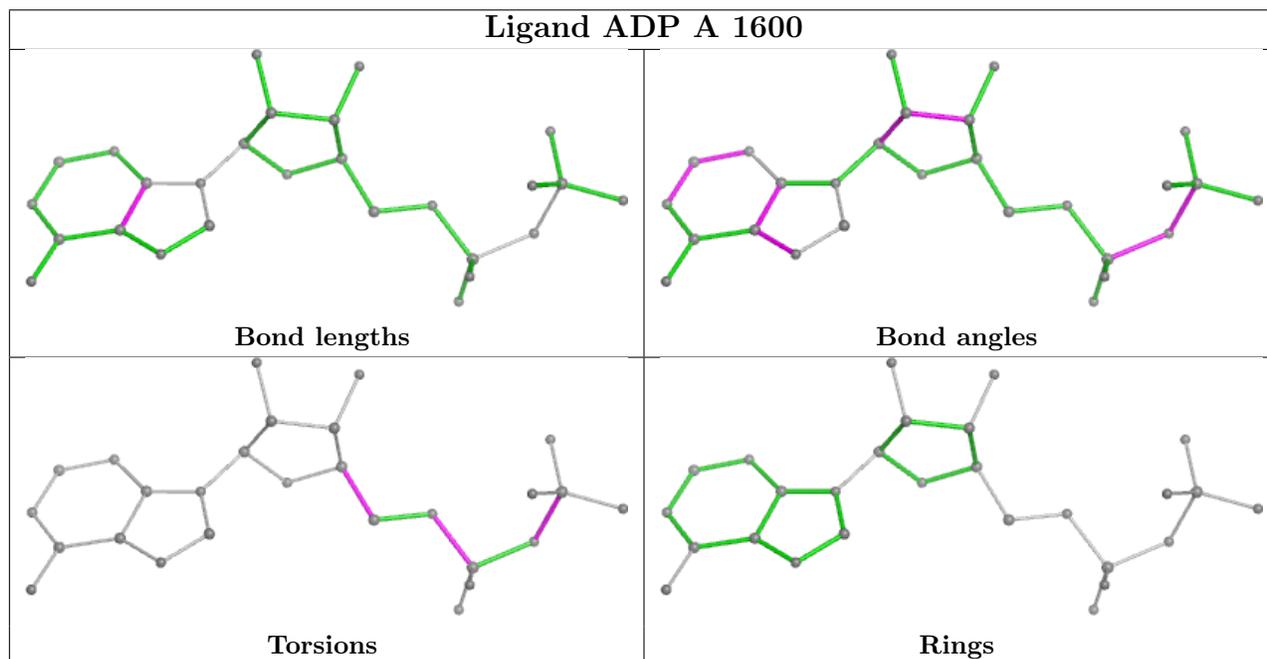
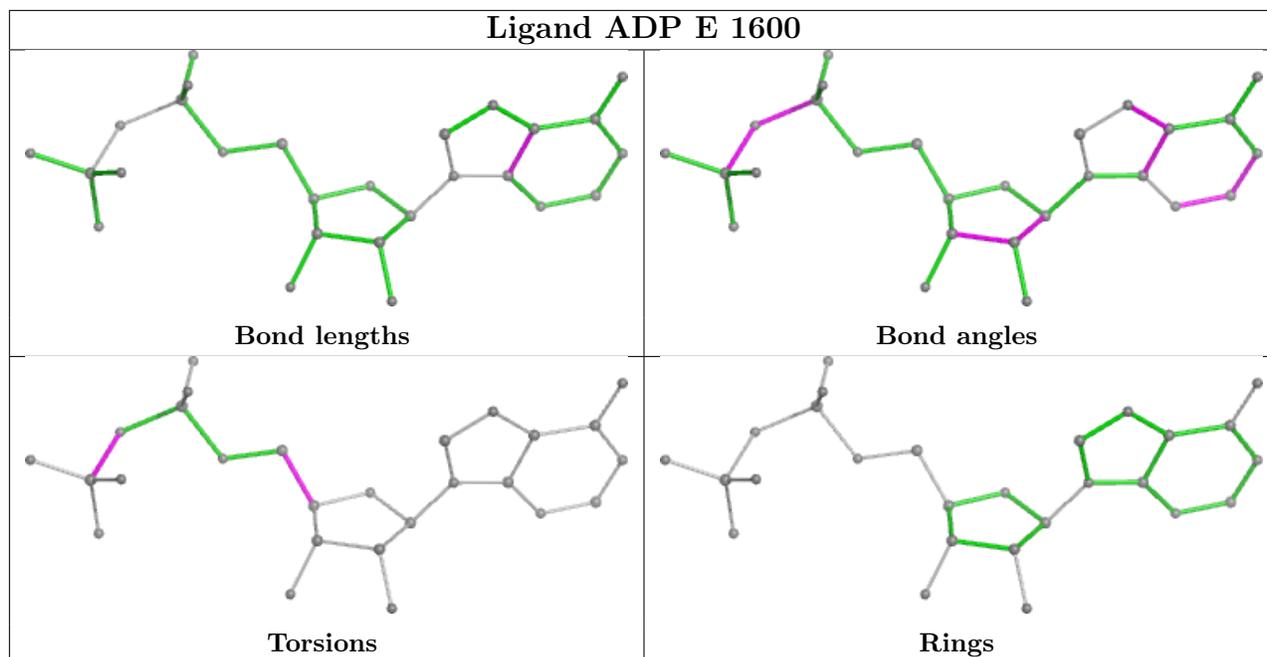
*Continued from previous page...*

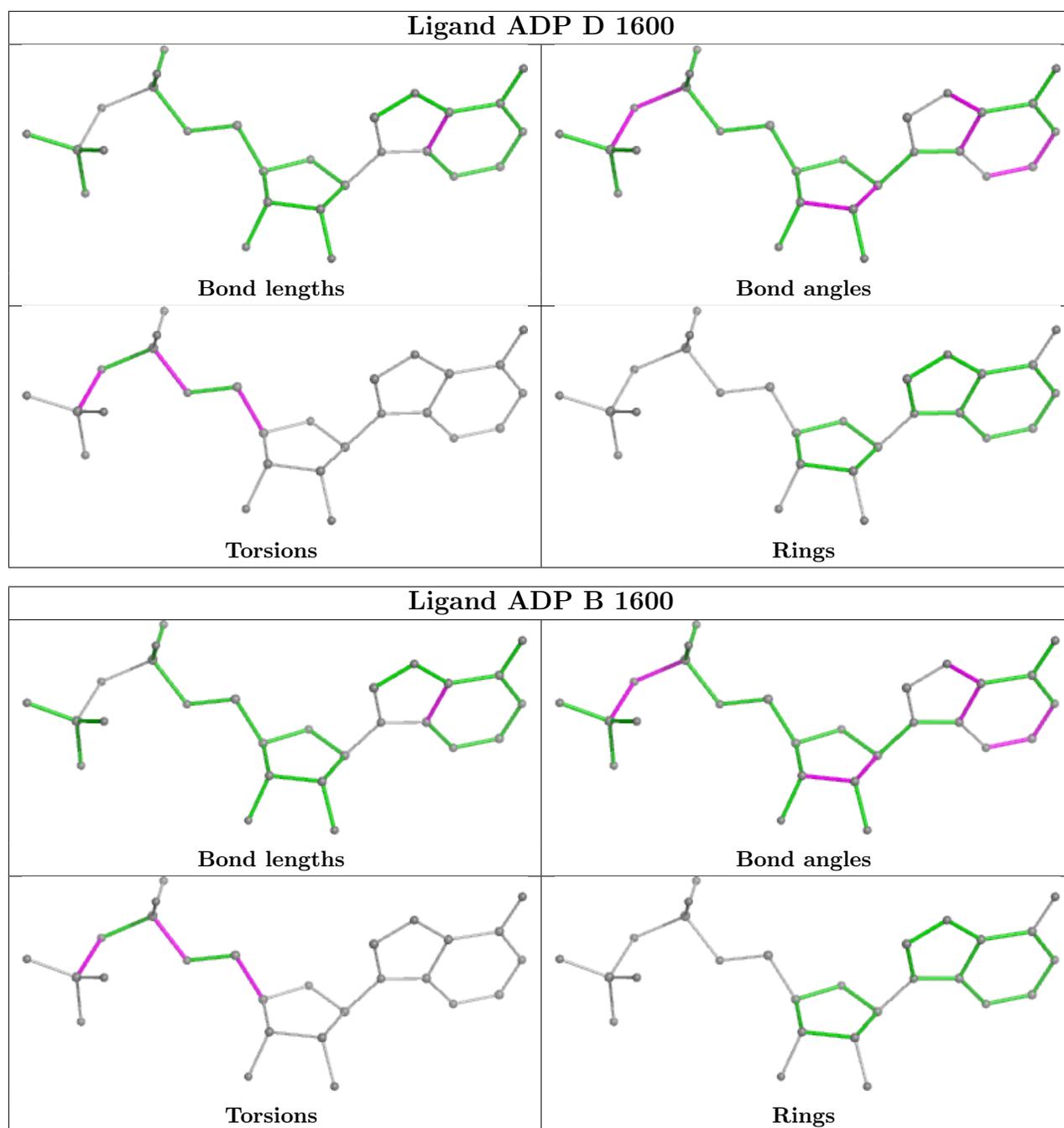
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1600	ADP	1	0
4	B	1600	ADP	1	0
6	D	1602	BEF	1	0

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.

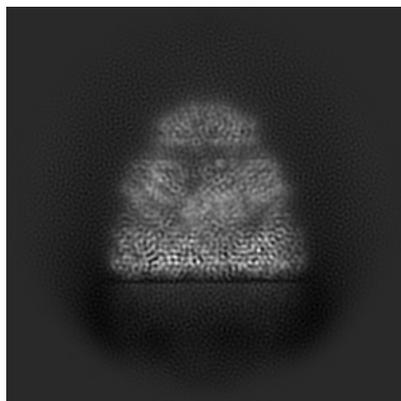
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17421. These allow visual inspection of the internal detail of the map and identification of artifacts.

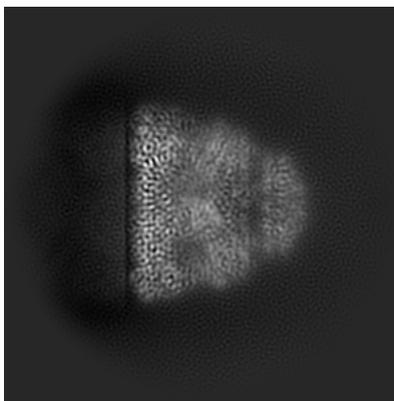
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

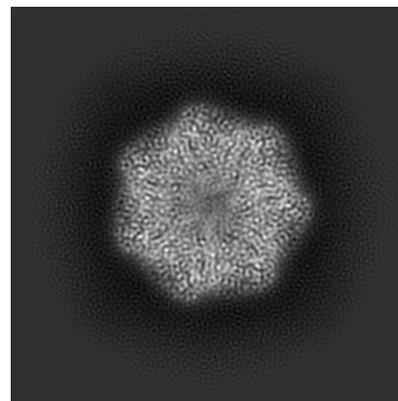
#### 6.1.1 Primary map



X

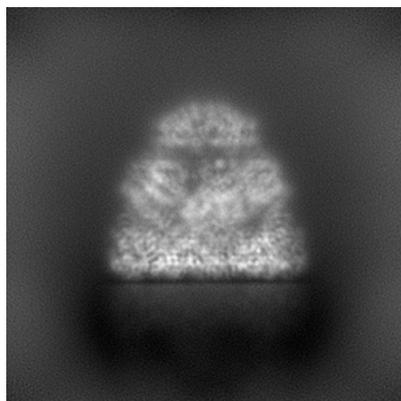


Y

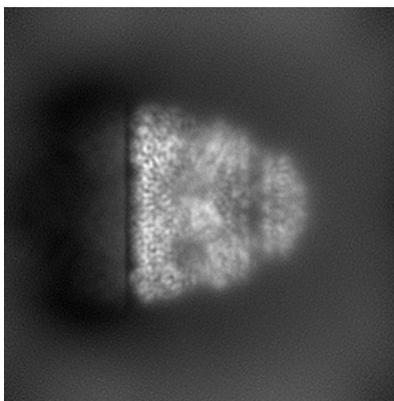


Z

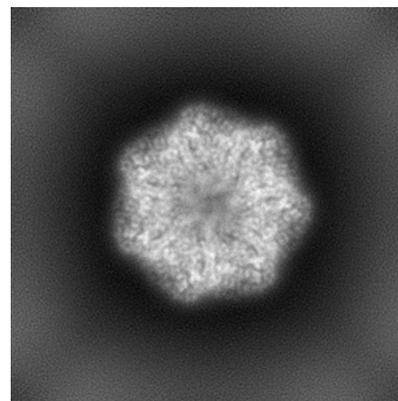
#### 6.1.2 Raw map



X



Y

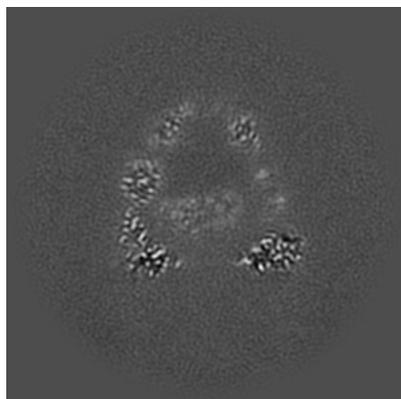


Z

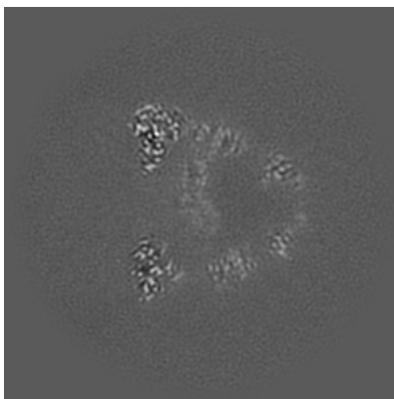
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

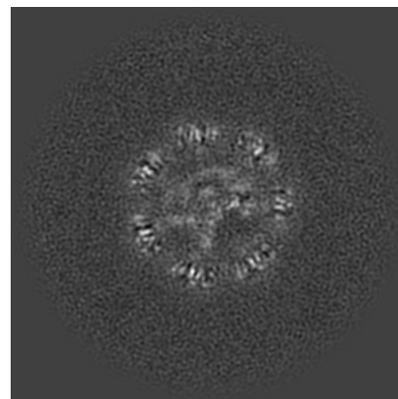
### 6.2.1 Primary map



X Index: 128

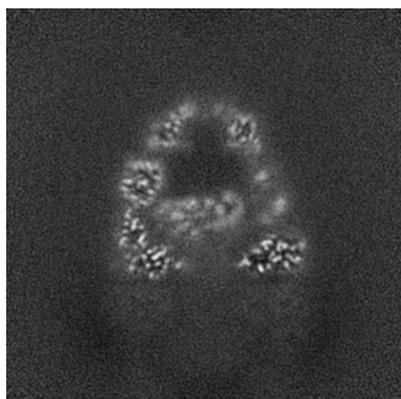


Y Index: 128

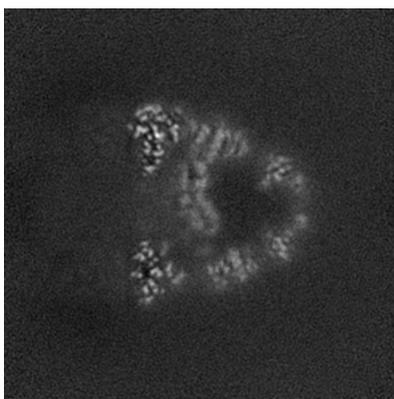


Z Index: 128

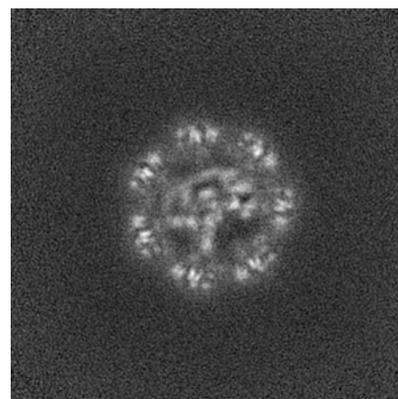
### 6.2.2 Raw map



X Index: 128



Y Index: 128

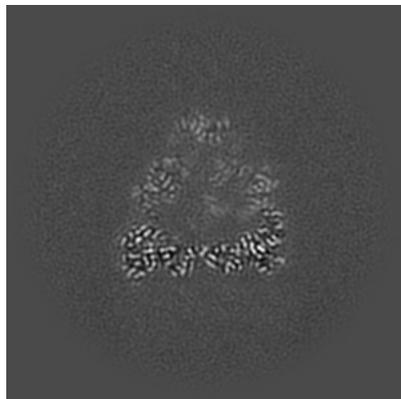


Z Index: 128

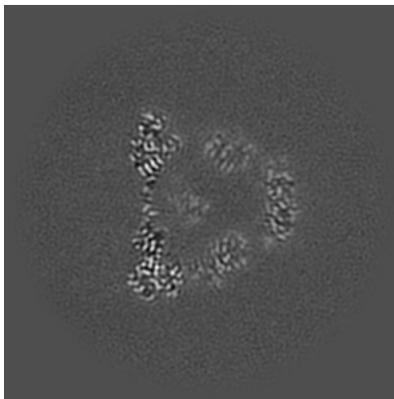
The images above show central slices of the map in three orthogonal directions.

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

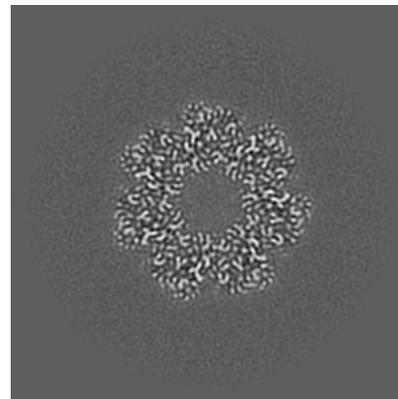
### 6.3.1 Primary map



X Index: 157

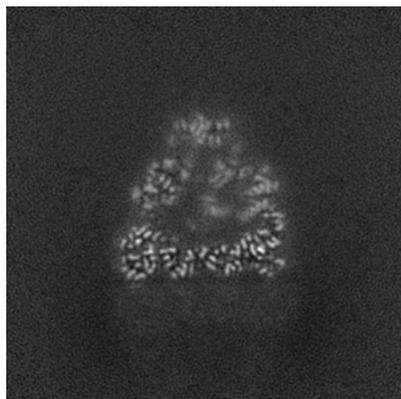


Y Index: 108

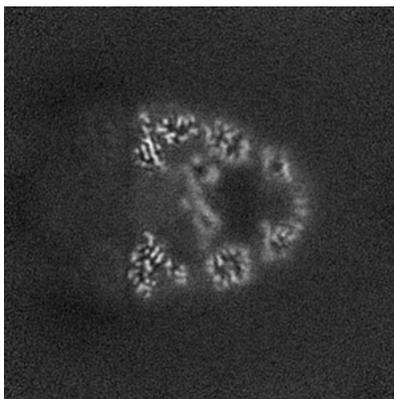


Z Index: 94

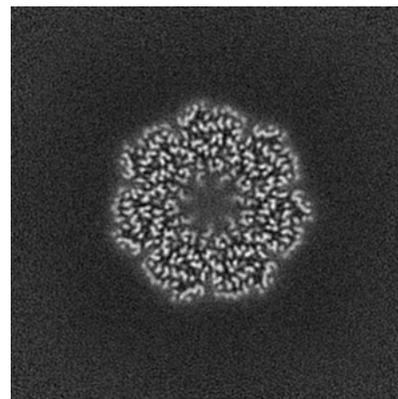
### 6.3.2 Raw map



X Index: 157



Y Index: 135

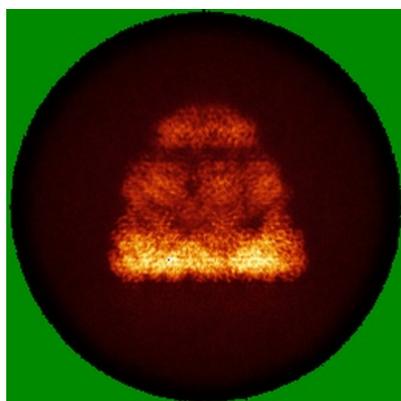


Z Index: 91

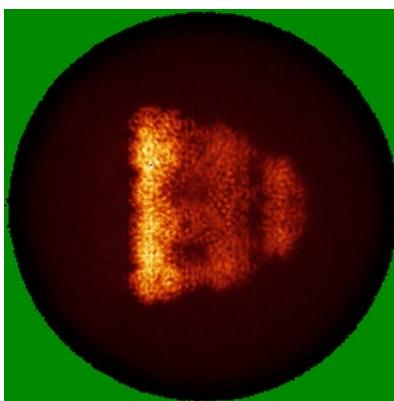
The images above show the largest variance slices of the map in three orthogonal directions.

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

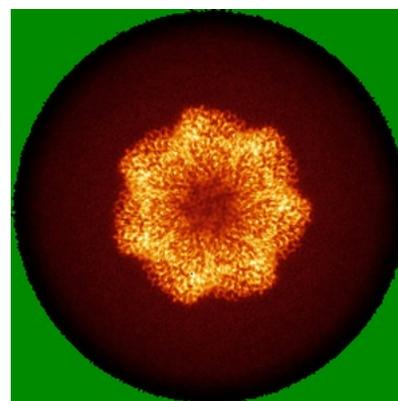
### 6.4.1 Primary map



X

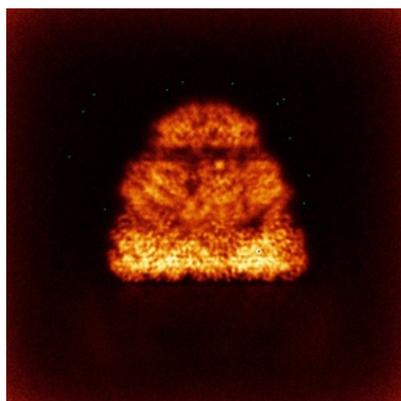


Y

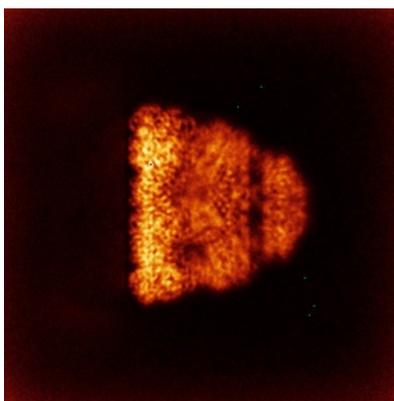


Z

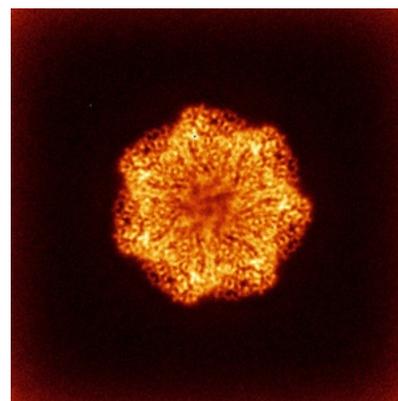
### 6.4.2 Raw map



X



Y

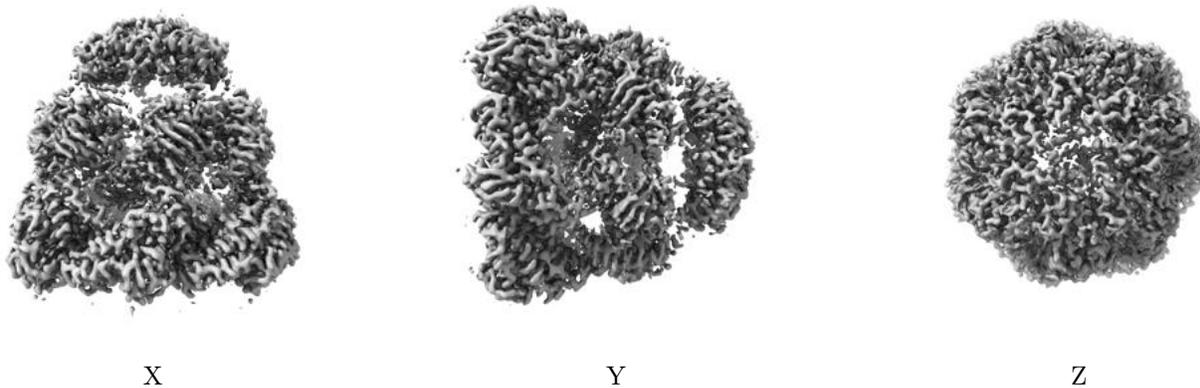


Z

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.

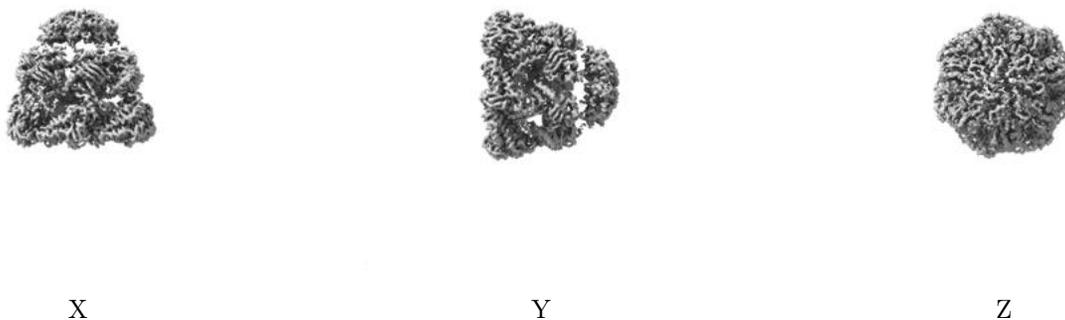
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.671. 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



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.

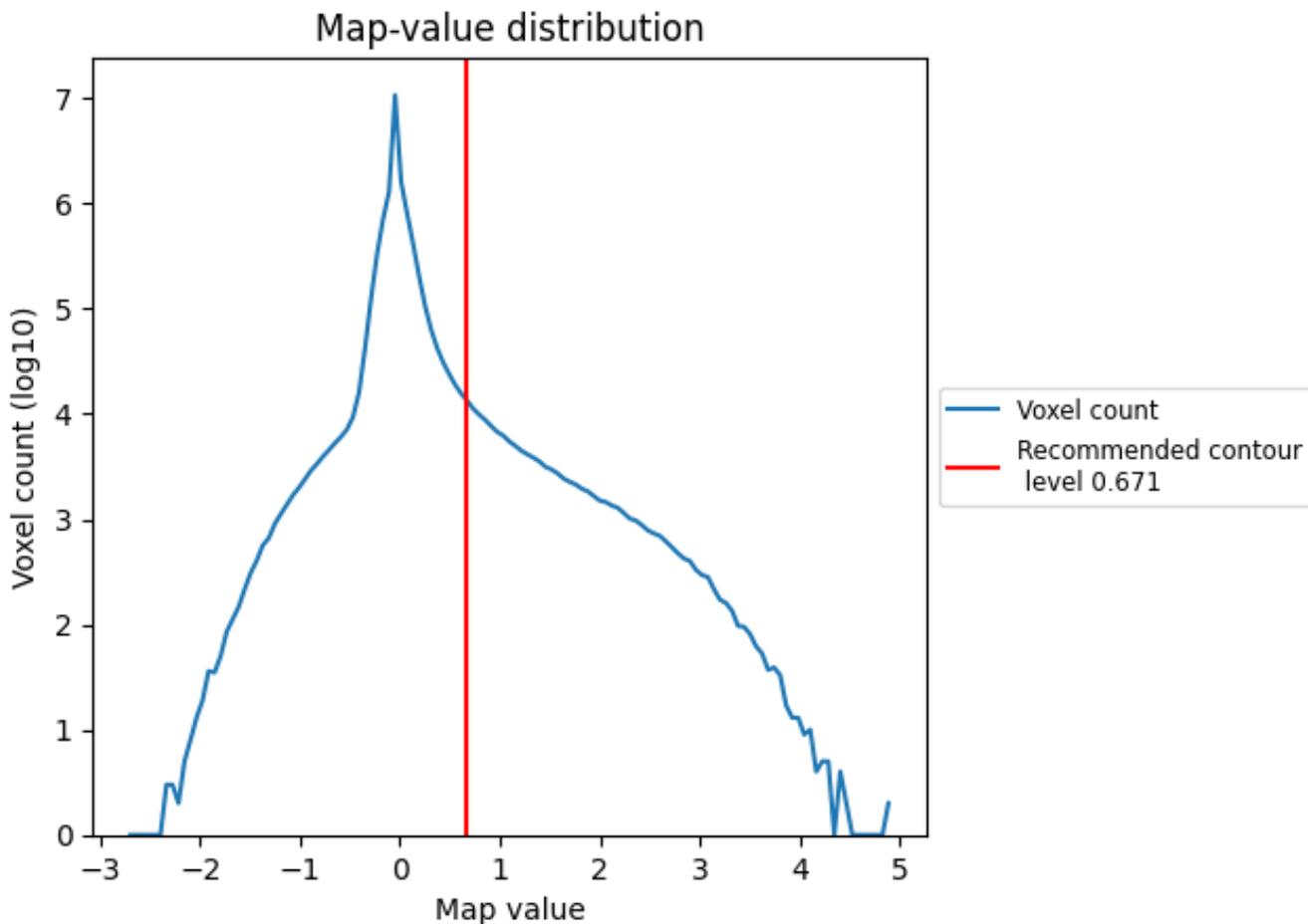
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

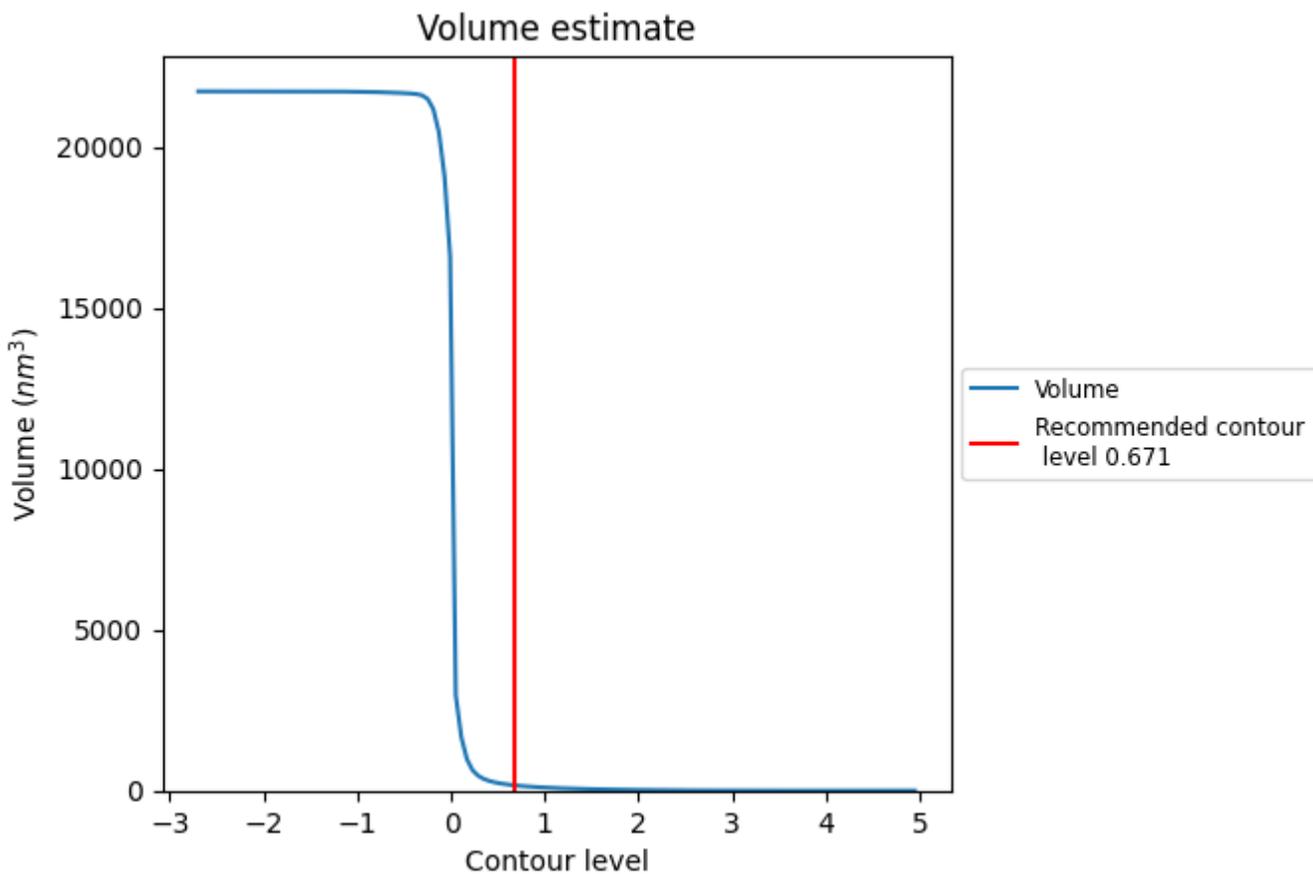
This section contains the results of statistical analysis of the map.

### 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.

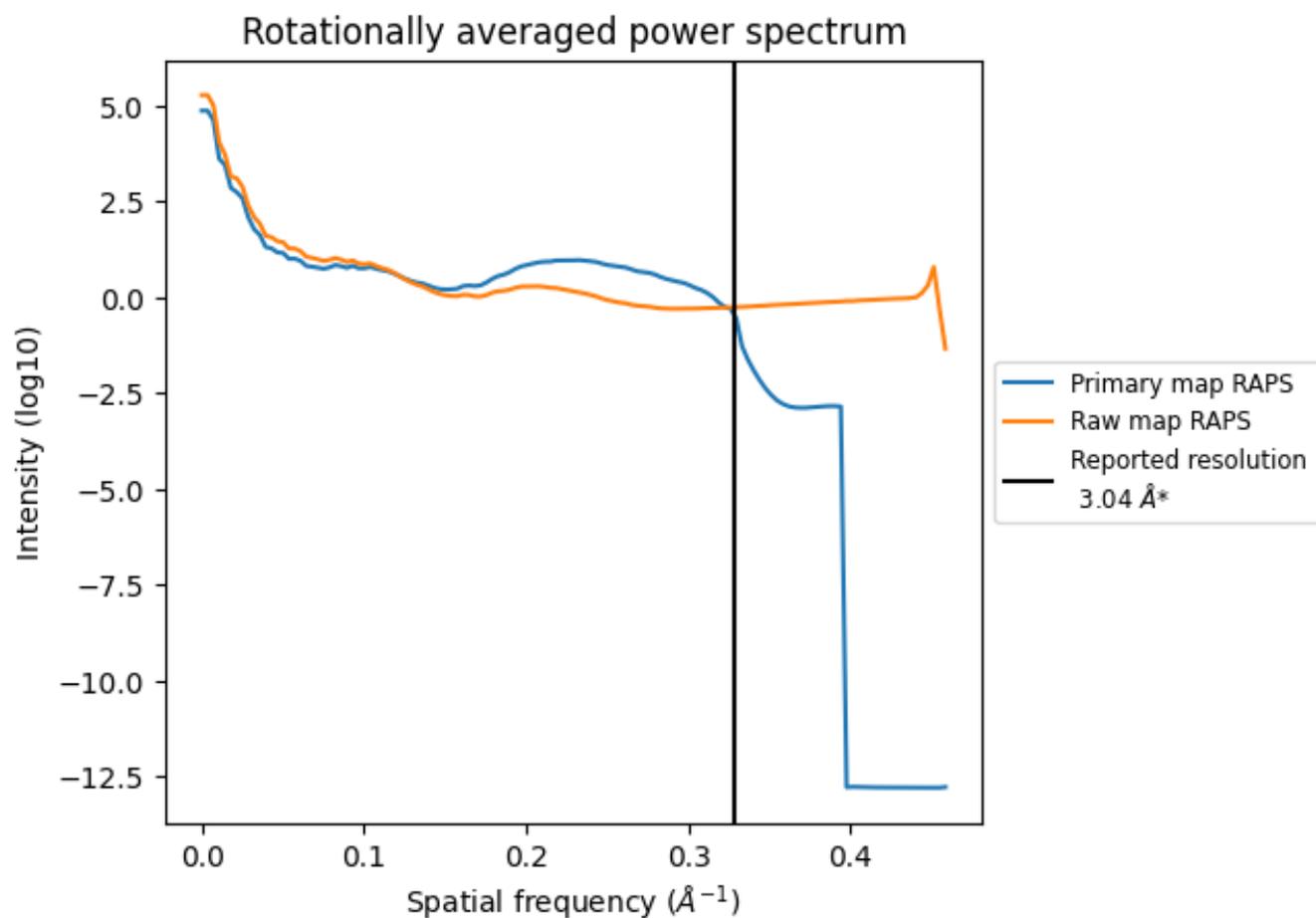
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 167 nm<sup>3</sup>; this corresponds to an approximate mass of 151 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](#)

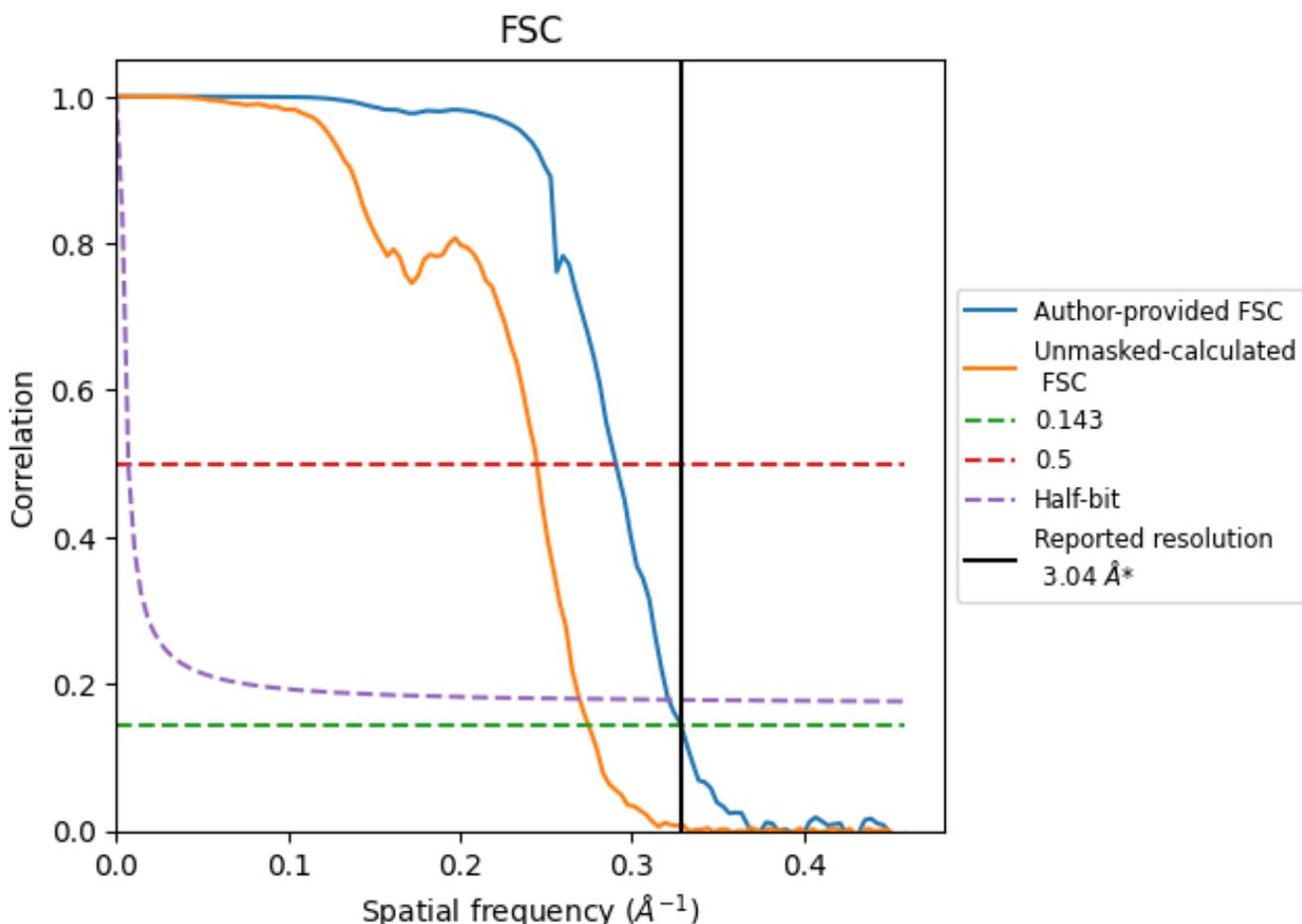


\*Reported resolution corresponds to spatial frequency of 0.329 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.329 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

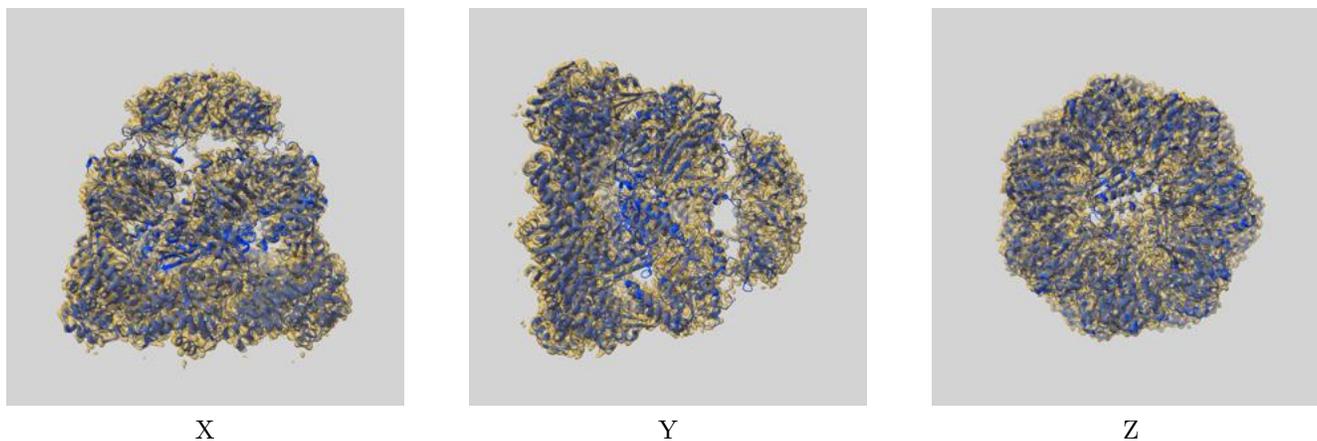
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.04	-	-
Author-provided FSC curve	3.04	3.44	3.11
Unmasked-calculated*	3.64	4.09	3.71

\*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 3.64 differs from the reported value 3.04 by more than 10 %

## 9 Map-model fit [i](#)

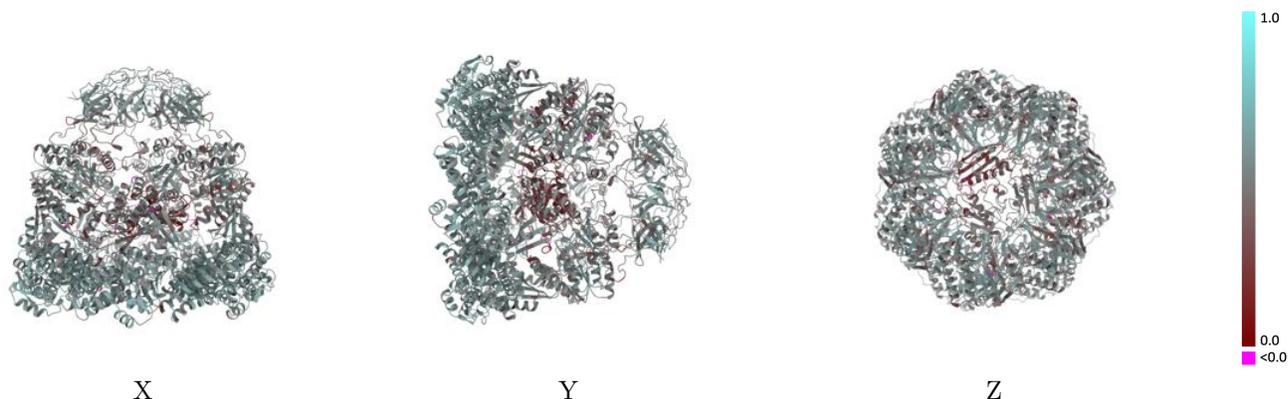
This section contains information regarding the fit between EMDB map EMD-17421 and PDB model 8P4O. Per-residue inclusion information can be found in section 3 on page 8.

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



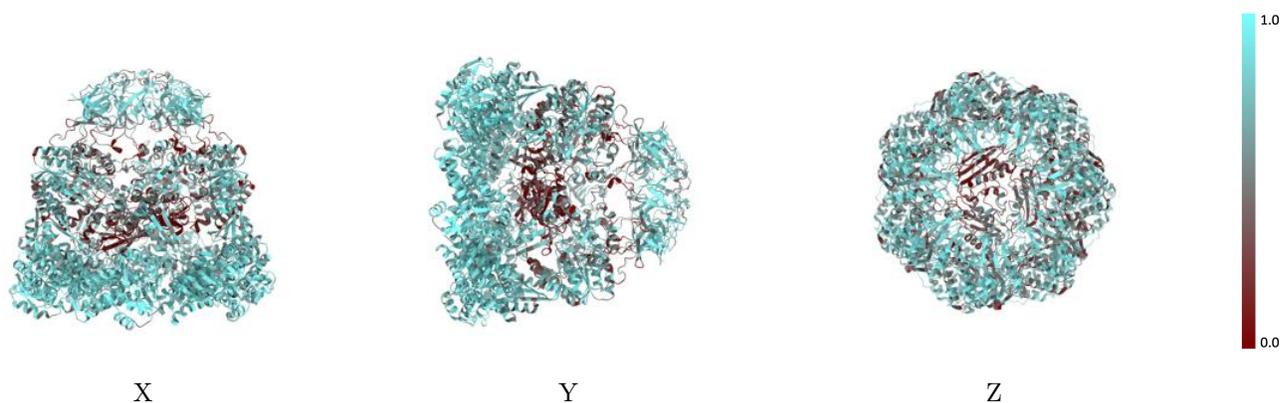
The images above show the 3D surface view of the map at the recommended contour level 0.671 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



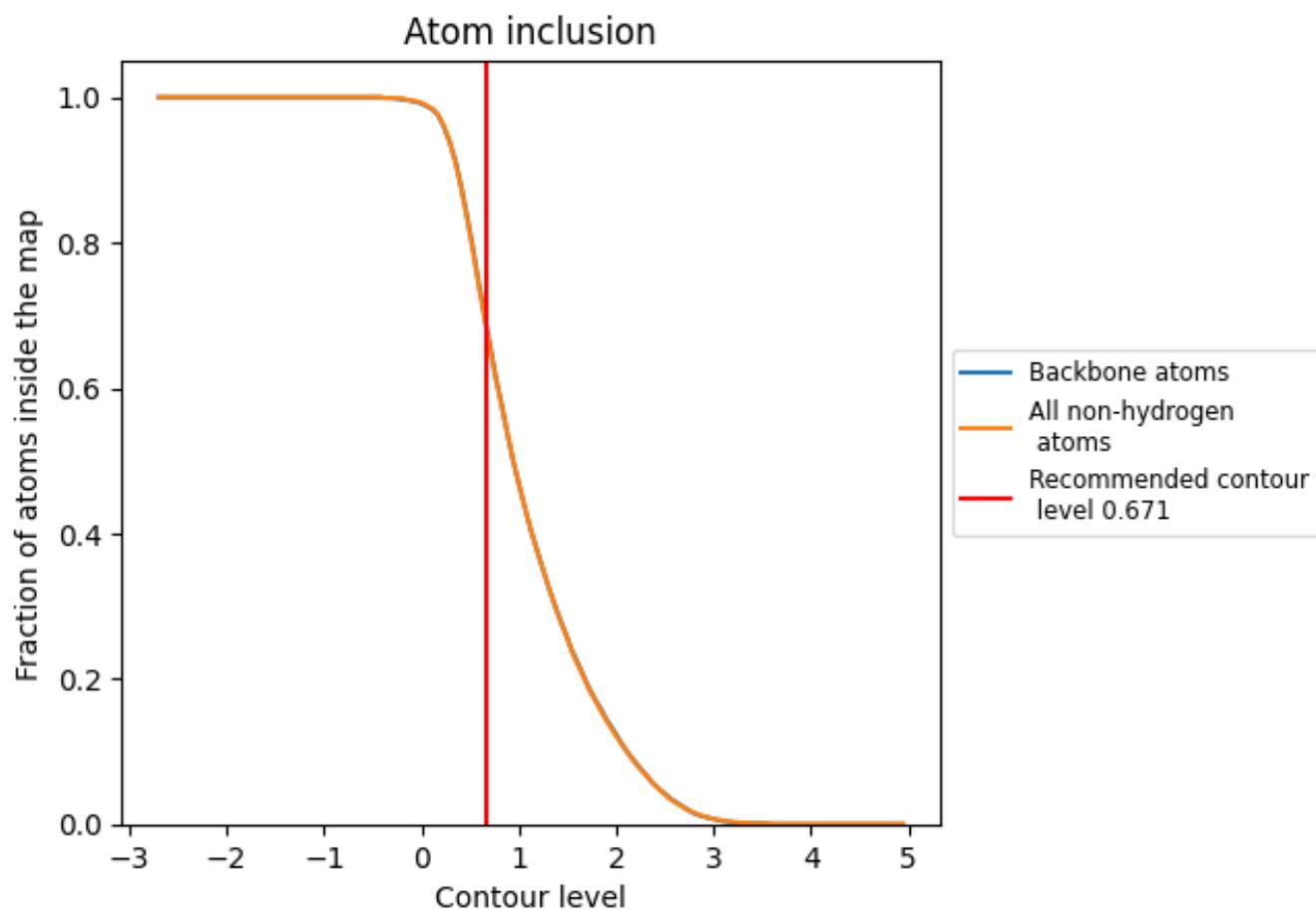
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.671).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 68% 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 (0.671) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6790	 0.5030
1	 0.2340	 0.3270
A	 0.7320	 0.5170
B	 0.7330	 0.5230
C	 0.7170	 0.5140
D	 0.7160	 0.5150
E	 0.7540	 0.5310
F	 0.7550	 0.5290
G	 0.7490	 0.5280
O	 0.6450	 0.4930
P	 0.6480	 0.5040
Q	 0.6480	 0.4920
R	 0.6370	 0.5000
S	 0.6510	 0.5030
T	 0.6680	 0.5000
U	 0.6480	 0.4900

