



wwPDB EM Validation Summary Report ⓘ

Jul 3, 2024 – 05:20 am BST

PDB ID : 7NJN
EMDB ID : EMD-12392
Title : Mycobacterium smegmatis ATP synthase state 1d
Authors : Montgomery, M.G.; Petri, J.; Spikes, T.E.; Walker, J.E.
Deposited on : 2021-02-17
Resolution : 2.64 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:

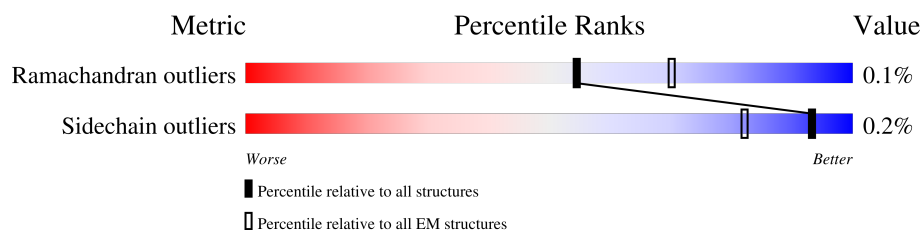
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.64 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	548	91% 8% 7%
1	B	548	92% 8% 7%
1	C	548	98% . 7%
2	D	475	98% . 7%
2	E	475	97% . 7%
2	F	475	99% . 7%
3	G	307	95% 5% 10%
4	H	121	97% .. 38%
5	L	86	97% . 15%

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Mol	Chain	Length	Quality of chain
5	M	86	<div> <div>16%</div> <div>99%</div> <div>.</div> </div>
5	N	86	<div> <div>14%</div> <div>98%</div> <div>.</div> </div>
5	O	86	<div> <div>13%</div> <div>99%</div> <div>.</div> </div>
5	P	86	<div> <div>17%</div> <div>99%</div> <div>.</div> </div>
5	Q	86	<div> <div>13%</div> <div>95%</div> <div>5%</div> </div>
5	R	86	<div> <div>16%</div> <div>98%</div> <div>.</div> </div>
5	S	86	<div> <div>17%</div> <div>98%</div> <div>.</div> </div>
5	T	86	<div> <div>13%</div> <div>97%</div> <div>.</div> </div>
6	a	252	<div> <div>42%</div> <div>94%</div> <div>6%</div> </div>
7	b	180	<div> <div>59%</div> <div>81%</div> <div>19%</div> </div>
8	d	445	<div> <div>55%</div> <div>97%</div> <div>..</div> </div>

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 74620 atoms, of which 37371 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 ATP synthase subunit alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	503	Total	C	H	N	O	S	0	0
			7631	2395	3820	660	746	10		
1	B	505	Total	C	H	N	O	S	0	0
			7639	2398	3823	659	749	10		
1	C	536	Total	C	H	N	O	S	1	0
			8129	2551	4065	701	802	10		

- Molecule 2 is a protein called ATP synthase subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	D	468	Total	C	H	N	O	S	2	0
			7162	2265	3573	616	695	13		
2	E	464	Total	C	H	N	O	S	0	0
			7087	2243	3533	609	689	13		
2	F	469	Total	C	H	N	O	S	0	0
			7166	2266	3577	616	694	13		

- Molecule 3 is a protein called ATP synthase gamma chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	G	293	Total	C	H	N	O	S	0	0
			4513	1401	2263	408	435	6		

- Molecule 4 is a protein called ATP synthase epsilon chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	H	118	Total	C	H	N	O	S	0	0
			1802	565	891	161	184	1		

- Molecule 5 is a protein called ATP synthase subunit c.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	L	83	Total	C	H	N	O	S	0	0
			1175	382	595	94	102	2		
5	M	85	Total	C	H	N	O	S	0	0
			1204	391	607	97	107	2		
5	N	84	Total	C	H	N	O	S	0	0
			1192	387	603	96	104	2		
5	O	85	Total	C	H	N	O	S	0	0
			1204	391	607	97	107	2		
5	P	85	Total	C	H	N	O	S	0	0
			1204	391	607	97	107	2		
5	Q	82	Total	C	H	N	O	S	0	0
			1156	376	584	93	101	2		
5	R	84	Total	C	H	N	O	S	0	0
			1187	386	599	95	105	2		
5	S	84	Total	C	H	N	O	S	0	0
			1192	387	603	96	104	2		
5	T	83	Total	C	H	N	O	S	0	0
			1175	382	595	94	102	2		

- Molecule 6 is a protein called ATP synthase subunit a.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	a	238	Total	C	H	N	O	S	0	0
			3767	1252	1916	292	301	6		

- Molecule 7 is a protein called ATP synthase subunit b.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	b	145	Total	C	H	N	O	S	0	0
			2172	667	1095	194	214	2		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	171	HIS	-	expression tag	UNP A0R204
b	172	HIS	-	expression tag	UNP A0R204
b	173	HIS	-	expression tag	UNP A0R204
b	174	HIS	-	expression tag	UNP A0R204
b	175	HIS	-	expression tag	UNP A0R204
b	176	HIS	-	expression tag	UNP A0R204
b	177	HIS	-	expression tag	UNP A0R204
b	178	HIS	-	expression tag	UNP A0R204
b	179	HIS	-	expression tag	UNP A0R204

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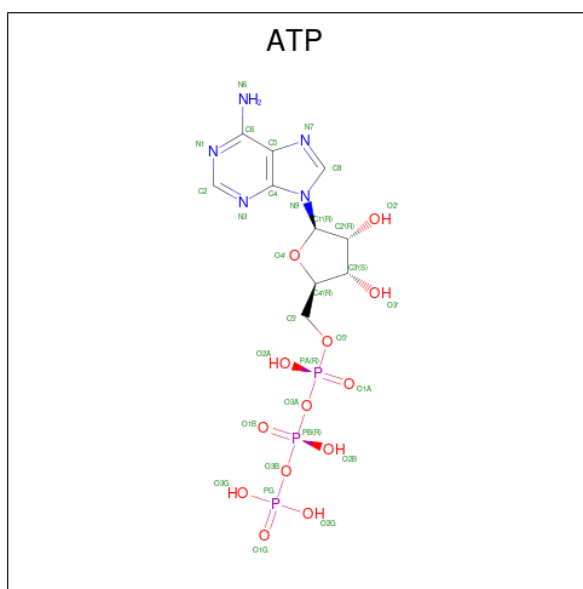
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Chain	Residue	Modelled	Actual	Comment	Reference
b	180	HIS	-	expression tag	UNP A0R204

- Molecule 8 is a protein called ATP synthase subunit b-delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	d	433	Total	C	H	N	O	S	
			6592	2014	3343	592	638	5	0
									0

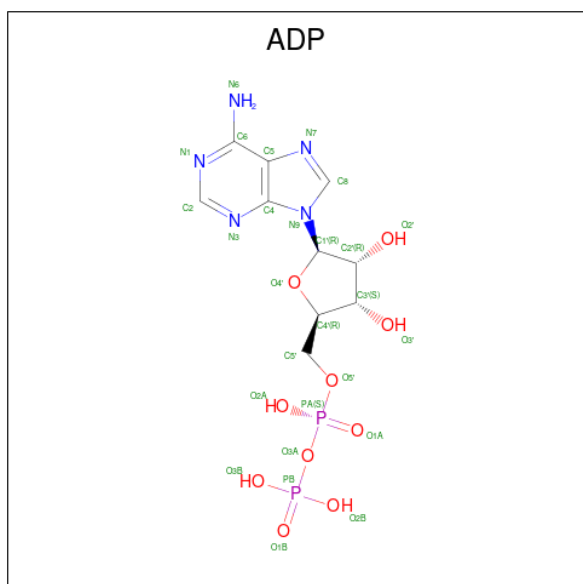
- Molecule 9 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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Mol	Chain	Residues	Atoms		AltConf
10	B	1	Total	Mg	0
			1	1	
10	C	1	Total	Mg	0
			1	1	
10	D	1	Total	Mg	0
			1	1	
10	F	1	Total	Mg	0
			1	1	

- Molecule 11 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms						AltConf
11	D	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
11	E	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		AltConf
12	A	3	Total	O	0
			3	3	
12	B	3	Total	O	0
			3	3	
12	C	3	Total	O	0
			3	3	

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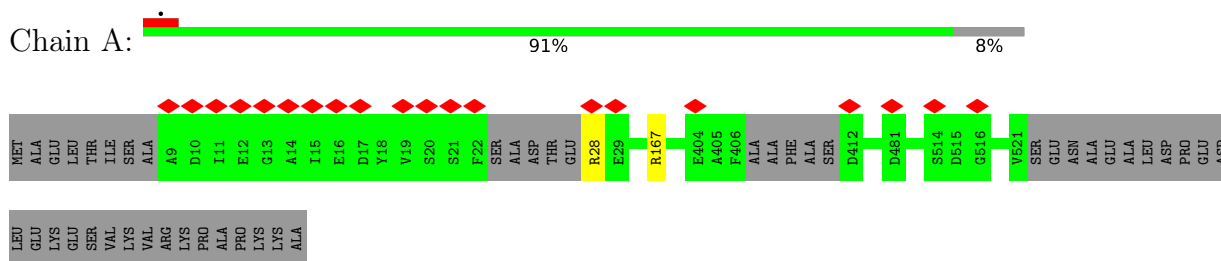
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Mol	Chain	Residues	Atoms		AltConf
12	D	4	Total	O	0
			4	4	
12	F	3	Total	O	0
			3	3	

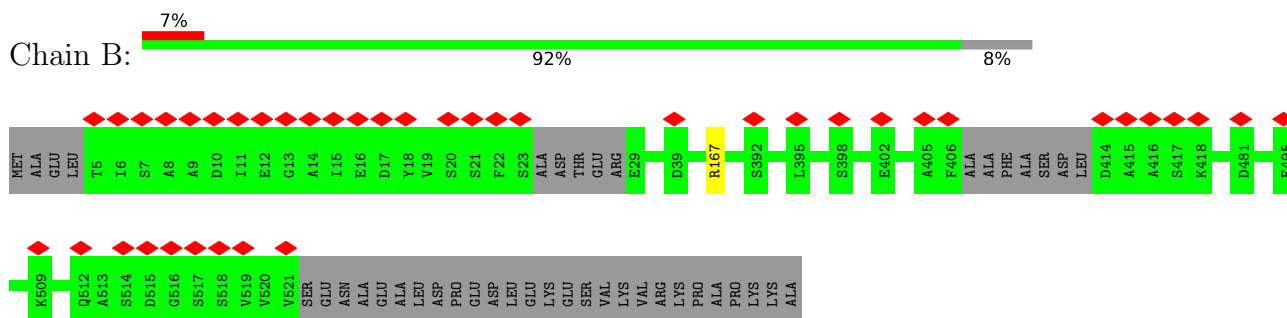
3 Residue-property plots [i](#)

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.

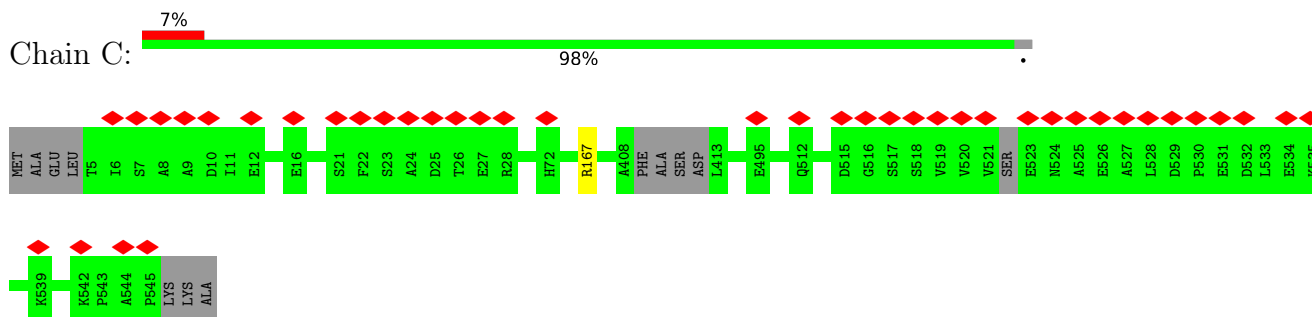
- Molecule 1: ATP synthase subunit alpha



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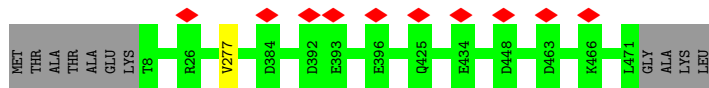


- Molecule 2: ATP synthase subunit beta

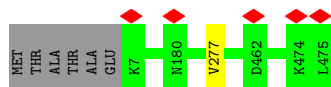




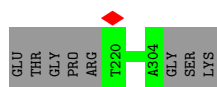
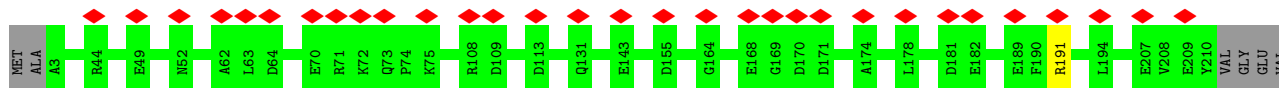
- Molecule 2: ATP synthase subunit beta



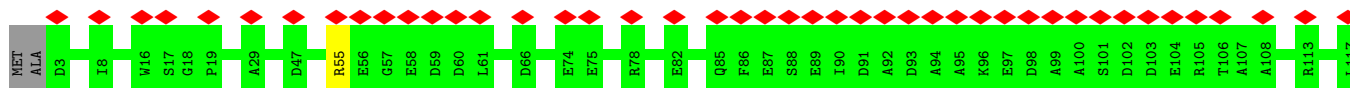
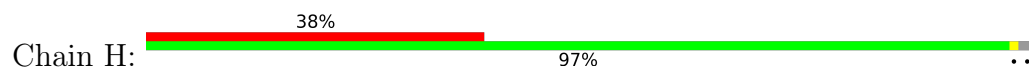
- Molecule 2: ATP synthase subunit beta



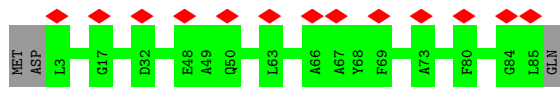
- Molecule 3: ATP synthase gamma chain



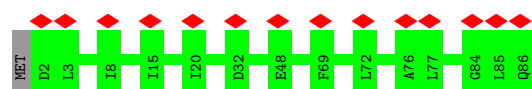
- Molecule 4: ATP synthase epsilon chain



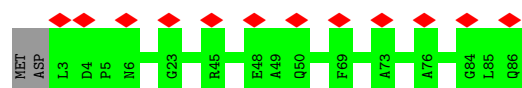
- Molecule 5: ATP synthase subunit c



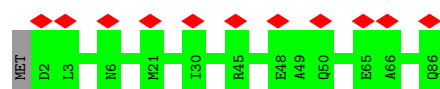
- Molecule 5: ATP synthase subunit c



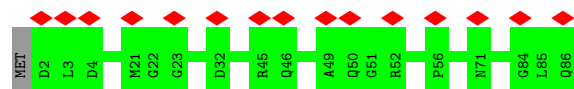
- Molecule 5: ATP synthase subunit c



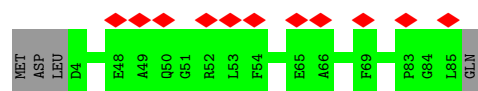
- Molecule 5: ATP synthase subunit c



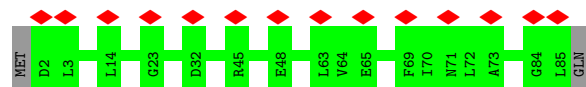
- Molecule 5: ATP synthase subunit c



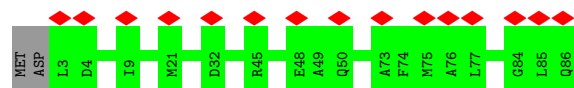
- Molecule 5: ATP synthase subunit c



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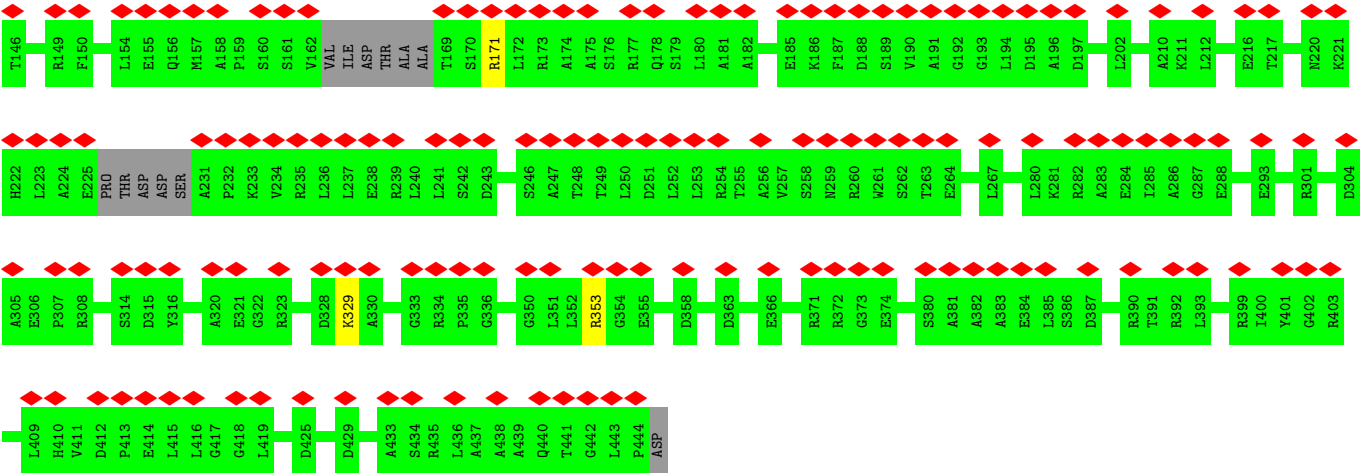


The diagram shows a linear sequence of 120 residues, represented by a horizontal bar divided into 120 segments. The residues are labeled as follows: MET, ASP, L3, D4, I9, A13, M21, I30, G31, D32, G62, A67, A73, A76, L85, and GLN. The residues L3, D4, I9, A13, I30, G31, D32, G62, A67, A73, A76, and L85 are highlighted in red, while MET, ASP, M21, and GLN are in grey. Red diamond markers are placed above each of the 12 highlighted residues.

G165	G166	V167	A168	F169	L170	A171	M174	E177	E178	L179	R188	L189	M192	G197	W208	Y209	I210	Q211	W212	F213	A216	D222	L223	F224	L227	F231	L236	L239	E246	L247	ASP	GLU	HIS	ASP	HIS																			
F65	W66	E67	E78	G79	S80	I81	G82	M83	K84	I85	F88	W89	L90	V108	L109	P110	L111	Q112	Y113	G114	G115	A116	D117	G118	A119	A120	A121	E122	L123	Y124	K125	A128	S129	D130	L139	F140	V143	G144	Y145	A146	A147	R152	R153	G154	I155	V156	G157	H158	P159	I160	Y164			
ME1	LEU	ALA	ALA	GLU	GLU	GLY	GLY	ALA	A10	I11	H12	V13	G14	H15	H16	L17	V19	F20	E21	L22	F23	G24	M25	T26	F27	D30	L33	A34	T35	A36	V37	T38	A39	V40	I41	V42	I43	A44	L45	A46	F47	Y48	L49	R50	A51	K52	V53	T54	S55	T56	G57	V58	P59	V62

[illegible]

E68	S69	E70	K71	V72	T73	E74	E75	A76	K77	Q78	D79	S80	E81	B82	A85	Q86	E89	Q90	R97	A100	Q104	L108	Q112	R115	G120	L121	Q122	A123	E124	A125	V126	N127	K128	A129	A130	E131	I132	V133	R134	A135	H136	V137	A138	D139	Q141	A142	Q143	S144	A145					
M1	F4	I5	G6	Q7	L8	I9	G10	F11	A12	V13	I14	I17	I18	V23	R27	T28	L29	K30	R31	N32	Q33	Q34	E35	A36	V37	R38	A39	A40	L41	A42	E43	S44	A45	E46	A47	A48	K49	K50	L51	A52	D53	A54	D55	A56	H57	H58	A59	K60	A61	L62	A63	D64	A65	K66



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21966	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 ($e^-/\text{\AA}^2$)	59.86	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.076	Depositor
Minimum map value	0.000	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0141	Depositor
Map size (Å)	415.0, 415.0, 415.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0.29	0/3868	0.49	0/5233
1	B	0.28	0/3873	0.49	0/5241
1	C	0.28	0/4125	0.49	0/5583
2	D	0.29	0/3659	0.50	0/4961
2	E	0.28	0/3619	0.50	0/4908
2	F	0.30	0/3654	0.50	0/4953
3	G	0.27	0/2279	0.52	0/3080
4	H	0.25	0/922	0.54	0/1252
5	L	0.27	0/591	0.44	0/802
5	M	0.27	0/608	0.45	0/825
5	N	0.27	0/600	0.47	0/814
5	O	0.26	0/608	0.44	0/825
5	P	0.28	0/608	0.48	0/825
5	Q	0.28	0/583	0.47	0/791
5	R	0.27	0/599	0.46	0/813
5	S	0.27	0/600	0.45	0/814
5	T	0.27	0/591	0.45	0/802
6	a	0.27	0/1905	0.43	0/2602
7	b	0.24	0/1086	0.47	0/1467
8	d	0.24	0/3276	0.48	0/4433
All	All	0.28	0/37654	0.49	0/51024

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

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	497/548 (91%)	488 (98%)	9 (2%)	0	100	100
1	B	499/548 (91%)	484 (97%)	15 (3%)	0	100	100
1	C	531/548 (97%)	518 (98%)	13 (2%)	0	100	100
2	D	468/475 (98%)	459 (98%)	8 (2%)	1 (0%)	47	64
2	E	462/475 (97%)	456 (99%)	5 (1%)	1 (0%)	47	64
2	F	467/475 (98%)	458 (98%)	8 (2%)	1 (0%)	47	64
3	G	289/307 (94%)	287 (99%)	2 (1%)	0	100	100
4	H	116/121 (96%)	114 (98%)	2 (2%)	0	100	100
5	L	81/86 (94%)	79 (98%)	2 (2%)	0	100	100
5	M	83/86 (96%)	79 (95%)	4 (5%)	0	100	100
5	N	82/86 (95%)	80 (98%)	2 (2%)	0	100	100
5	O	83/86 (96%)	82 (99%)	1 (1%)	0	100	100
5	P	83/86 (96%)	78 (94%)	5 (6%)	0	100	100
5	Q	80/86 (93%)	77 (96%)	3 (4%)	0	100	100
5	R	82/86 (95%)	75 (92%)	7 (8%)	0	100	100
5	S	82/86 (95%)	78 (95%)	4 (5%)	0	100	100
5	T	81/86 (94%)	76 (94%)	5 (6%)	0	100	100
6	a	236/252 (94%)	225 (95%)	11 (5%)	0	100	100
7	b	143/180 (79%)	138 (96%)	5 (4%)	0	100	100
8	d	427/445 (96%)	424 (99%)	3 (1%)	0	100	100
All	All	4872/5148 (95%)	4755 (98%)	114 (2%)	3 (0%)	54	69

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	277	VAL
2	D	277	VAL
2	F	277	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	406/441 (92%)	404 (100%)	2 (0%)	88	94
1	B	407/441 (92%)	406 (100%)	1 (0%)	93	97
1	C	433/441 (98%)	432 (100%)	1 (0%)	93	97
2	D	384/388 (99%)	384 (100%)	0	100	100
2	E	381/388 (98%)	381 (100%)	0	100	100
2	F	384/388 (99%)	384 (100%)	0	100	100
3	G	228/238 (96%)	227 (100%)	1 (0%)	91	95
4	H	94/96 (98%)	93 (99%)	1 (1%)	73	85
5	L	53/56 (95%)	53 (100%)	0	100	100
5	M	55/56 (98%)	55 (100%)	0	100	100
5	N	54/56 (96%)	54 (100%)	0	100	100
5	O	55/56 (98%)	55 (100%)	0	100	100
5	P	55/56 (98%)	55 (100%)	0	100	100
5	Q	52/56 (93%)	52 (100%)	0	100	100
5	R	54/56 (96%)	54 (100%)	0	100	100
5	S	54/56 (96%)	54 (100%)	0	100	100
5	T	53/56 (95%)	53 (100%)	0	100	100
6	a	191/200 (96%)	191 (100%)	0	100	100
7	b	111/134 (83%)	111 (100%)	0	100	100
8	d	337/347 (97%)	334 (99%)	3 (1%)	78	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3841/4006 (96%)	3832 (100%)	9 (0%)	93 97

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	d	329	LYS
8	d	353	ARG
1	C	167	ARG
3	G	191	ARG
4	H	55	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
5	M	71	ASN
5	O	71	ASN
5	S	71	ASN
6	a	192	ASN
7	b	131	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 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
9	ATP	C	600	10	26,33,33	0.68	0	31,52,52	1.08	3 (9%)
9	ATP	F	600	10	26,33,33	0.67	0	31,52,52	1.05	2 (6%)
11	ADP	D	600	10	24,29,29	0.95	1 (4%)	29,45,45	1.34	4 (13%)
11	ADP	E	600	-	24,29,29	0.94	1 (4%)	29,45,45	1.52	4 (13%)
9	ATP	B	600	10	26,33,33	0.66	0	31,52,52	1.08	3 (9%)
9	ATP	A	600	10	26,33,33	0.68	0	31,52,52	1.11	4 (12%)

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
9	ATP	C	600	10	-	0/18/38/38	0/3/3/3
9	ATP	F	600	10	-	1/18/38/38	0/3/3/3
11	ADP	D	600	10	-	5/12/32/32	0/3/3/3
11	ADP	E	600	-	-	1/12/32/32	0/3/3/3
9	ATP	B	600	10	-	1/18/38/38	0/3/3/3
9	ATP	A	600	10	-	1/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	E	600	ADP	C5-C4	2.34	1.47	1.40
11	D	600	ADP	C5-C4	2.17	1.46	1.40

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	E	600	ADP	PA-O3A-PB	-3.74	120.00	132.83
11	D	600	ADP	N3-C2-N1	-3.66	122.95	128.68
11	E	600	ADP	N3-C2-N1	-3.61	123.04	128.68
11	E	600	ADP	C3'-C2'-C1'	3.41	106.11	100.98
11	D	600	ADP	PA-O3A-PB	-3.33	121.39	132.83

There are no chirality outliers.

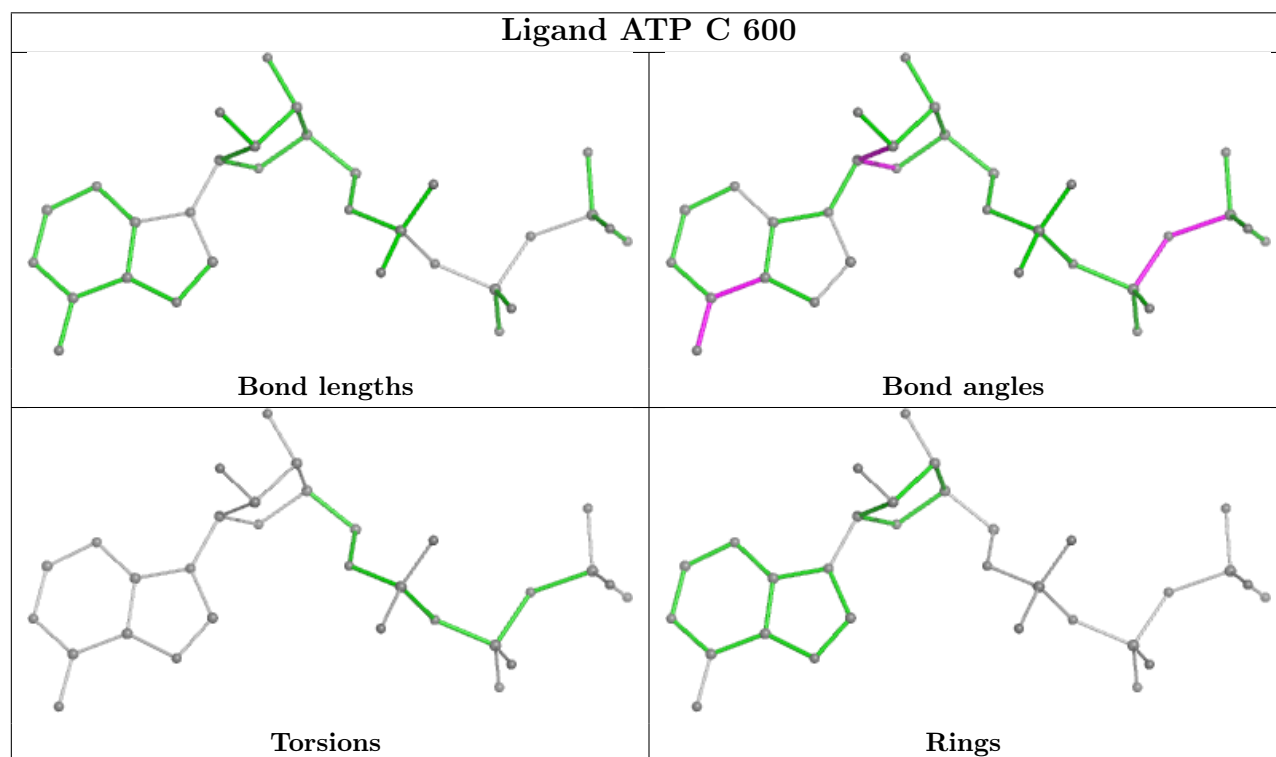
5 of 9 torsion outliers are listed below:

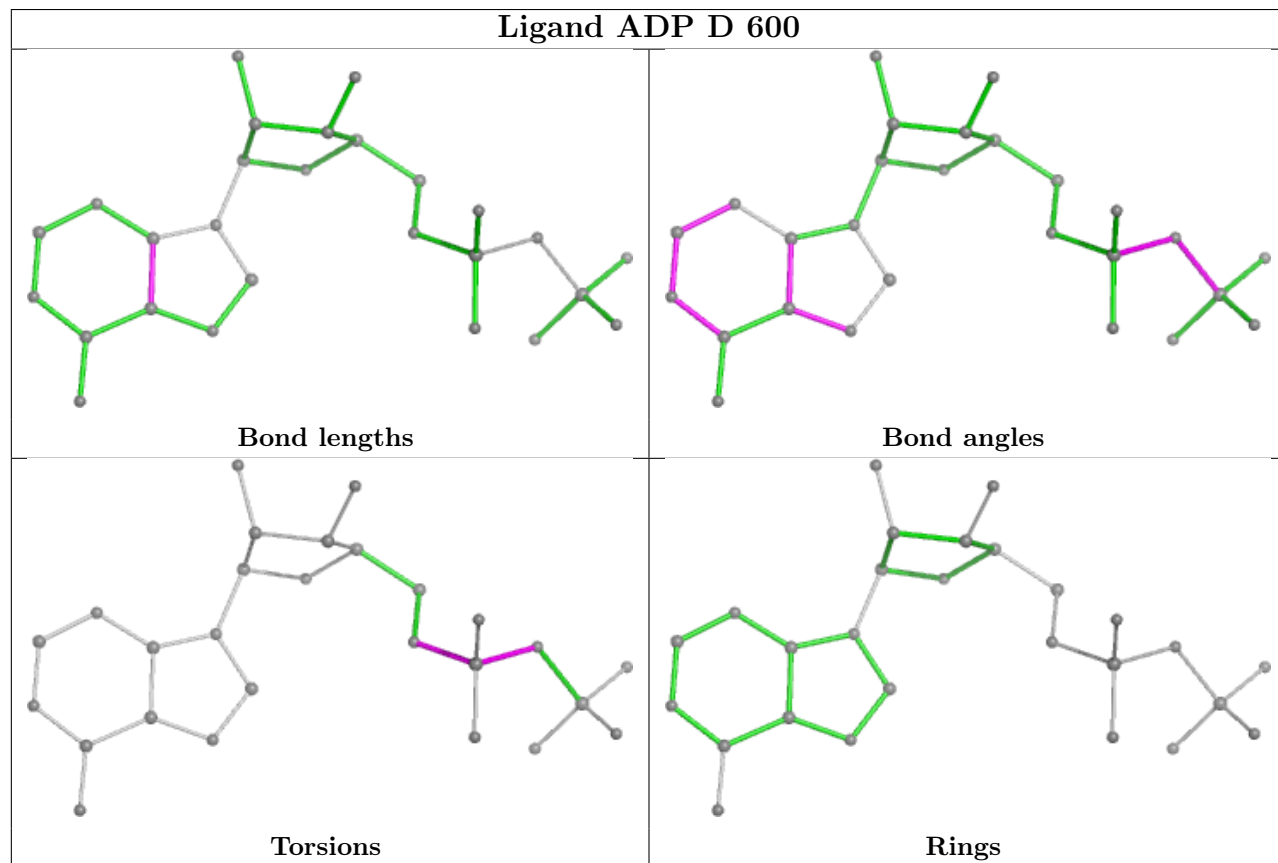
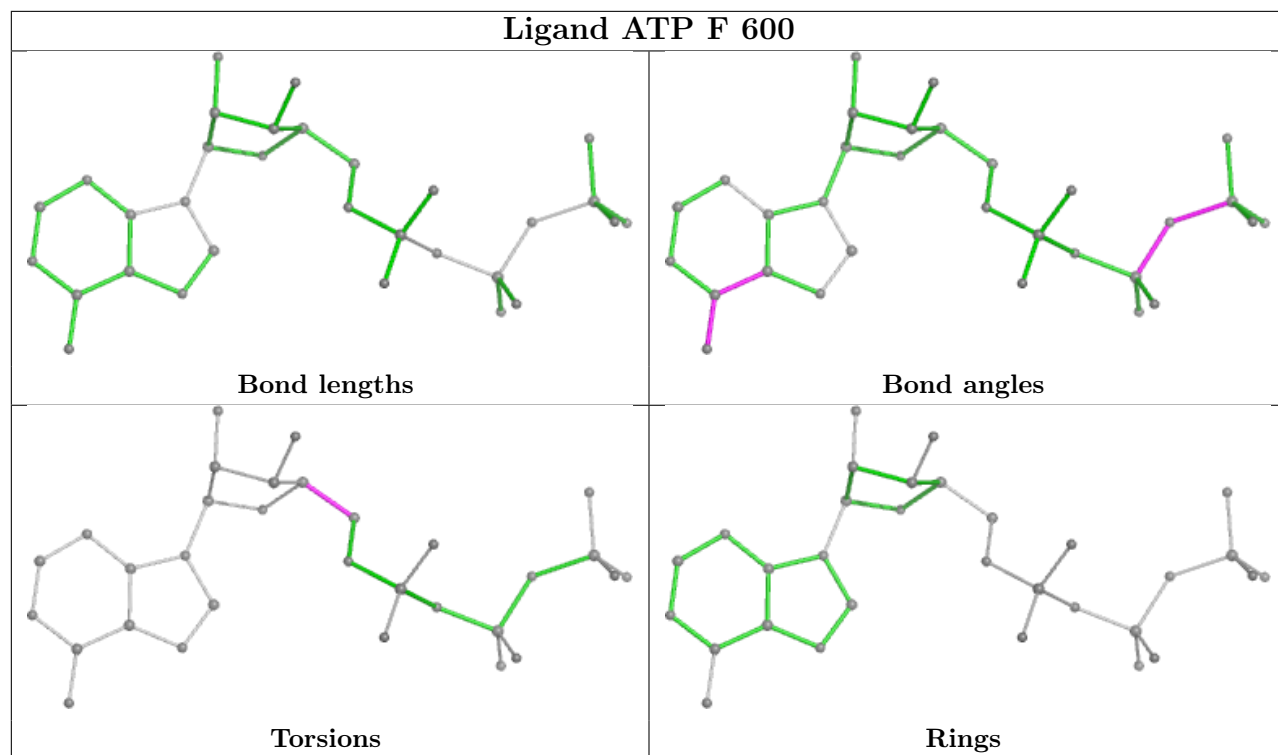
Mol	Chain	Res	Type	Atoms
11	D	600	ADP	C5'-O5'-PA-O3A
9	F	600	ATP	C3'-C4'-C5'-O5'
9	B	600	ATP	C5'-O5'-PA-O3A
11	D	600	ADP	C5'-O5'-PA-O1A
11	D	600	ADP	C5'-O5'-PA-O2A

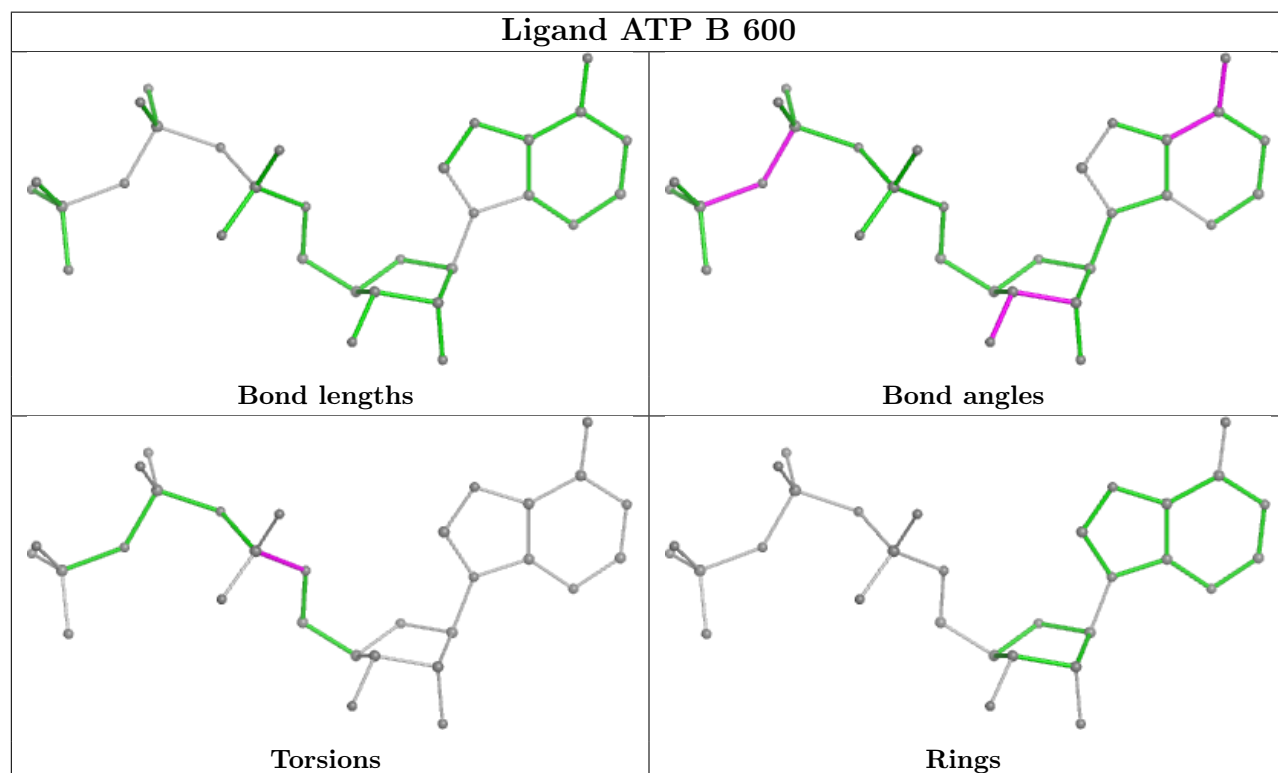
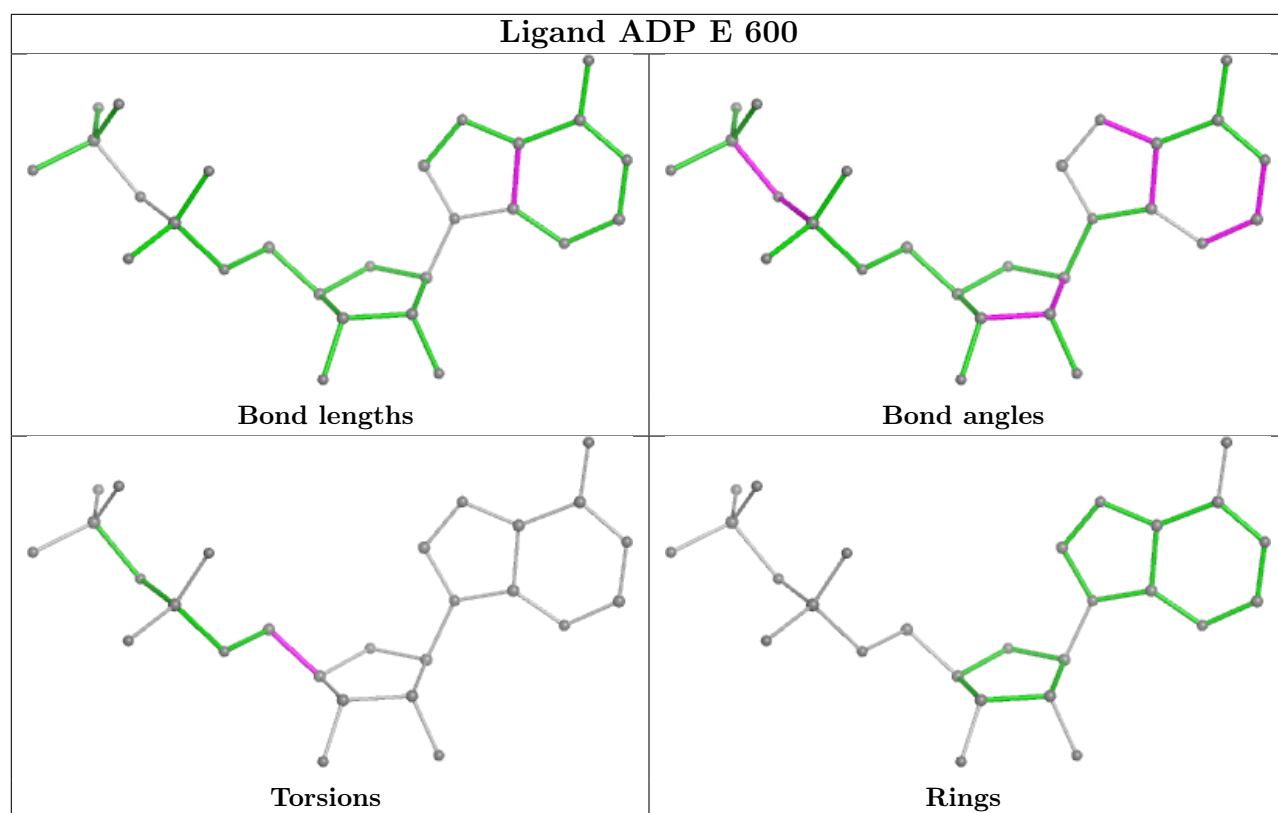
There are no ring outliers.

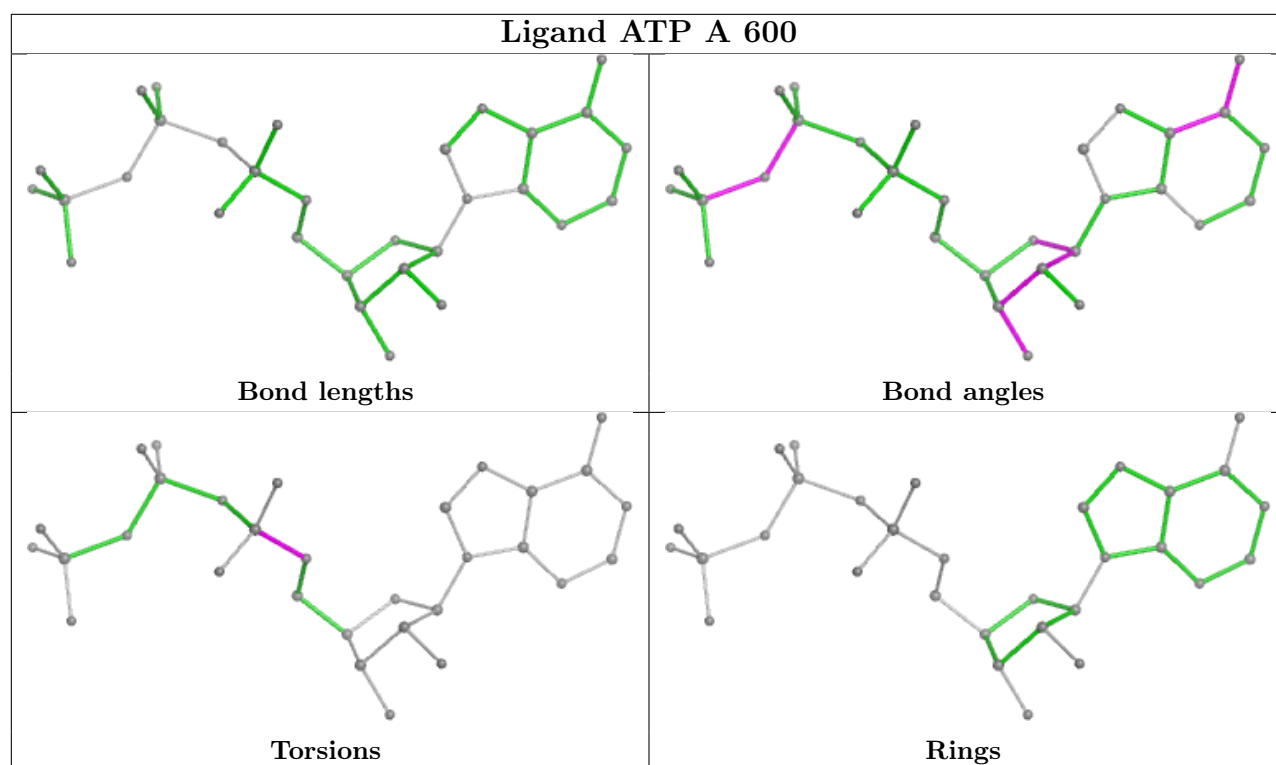
No monomer is involved in short contacts.

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

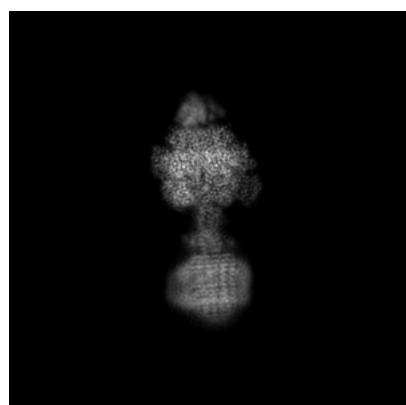
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12392. These allow visual inspection of the internal detail of the map and identification of artifacts.

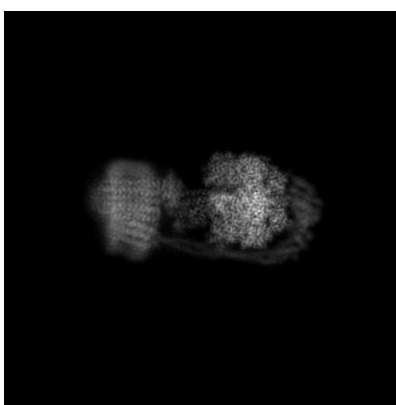
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

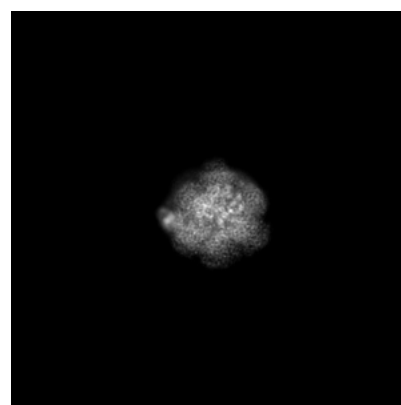
6.1.1 Primary map



X



Y

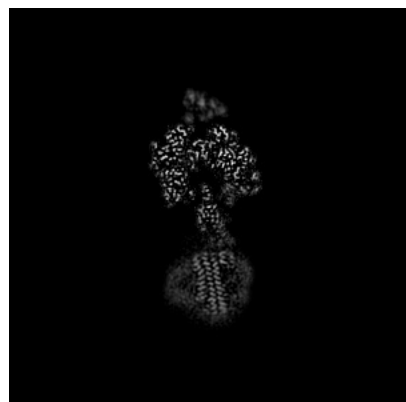


Z

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

6.2 Central slices [i](#)

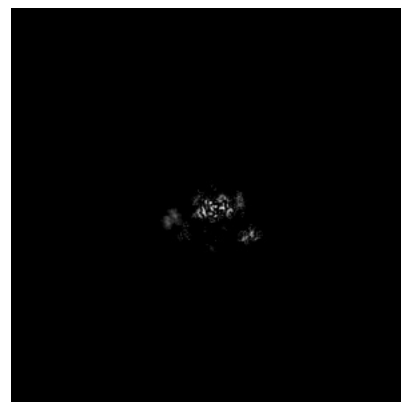
6.2.1 Primary map



X Index: 250



Y Index: 250

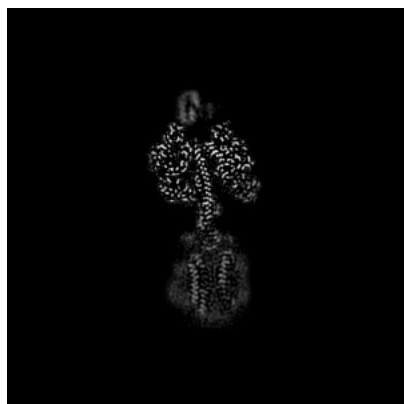


Z Index: 250

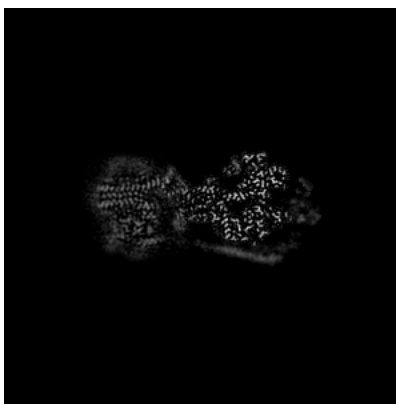
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

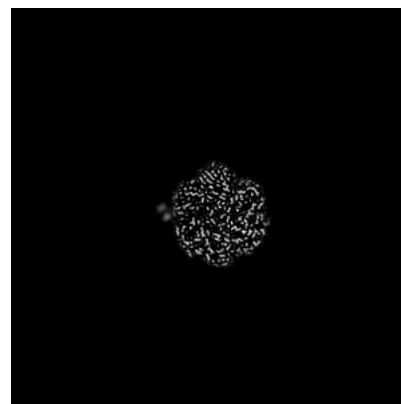
6.3.1 Primary map



X Index: 263



Y Index: 247

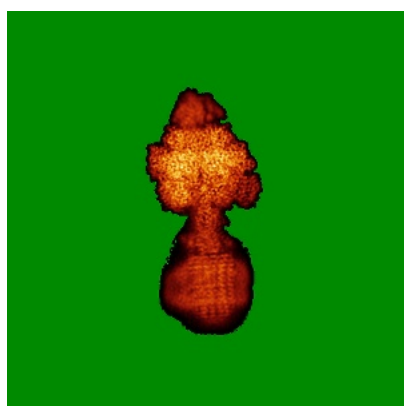


Z Index: 314

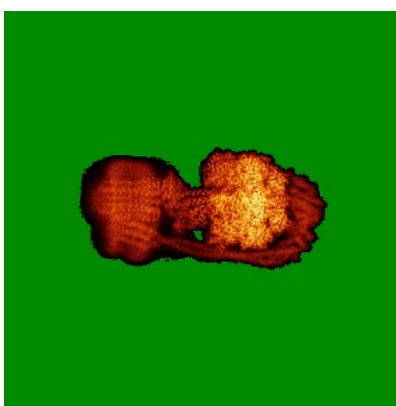
The images above show the largest variance slices of the map in three orthogonal directions.

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

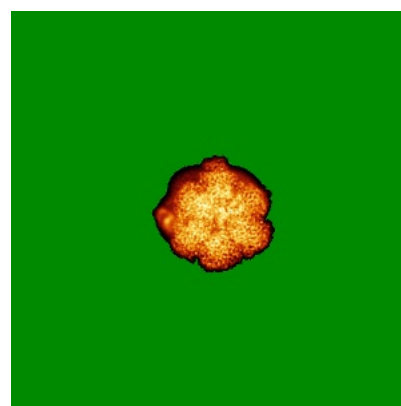
6.4.1 Primary map



X



Y



Z

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](#)

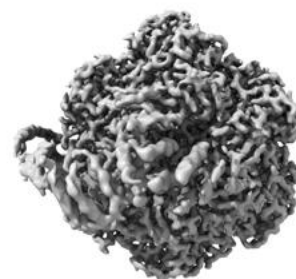
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0141. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

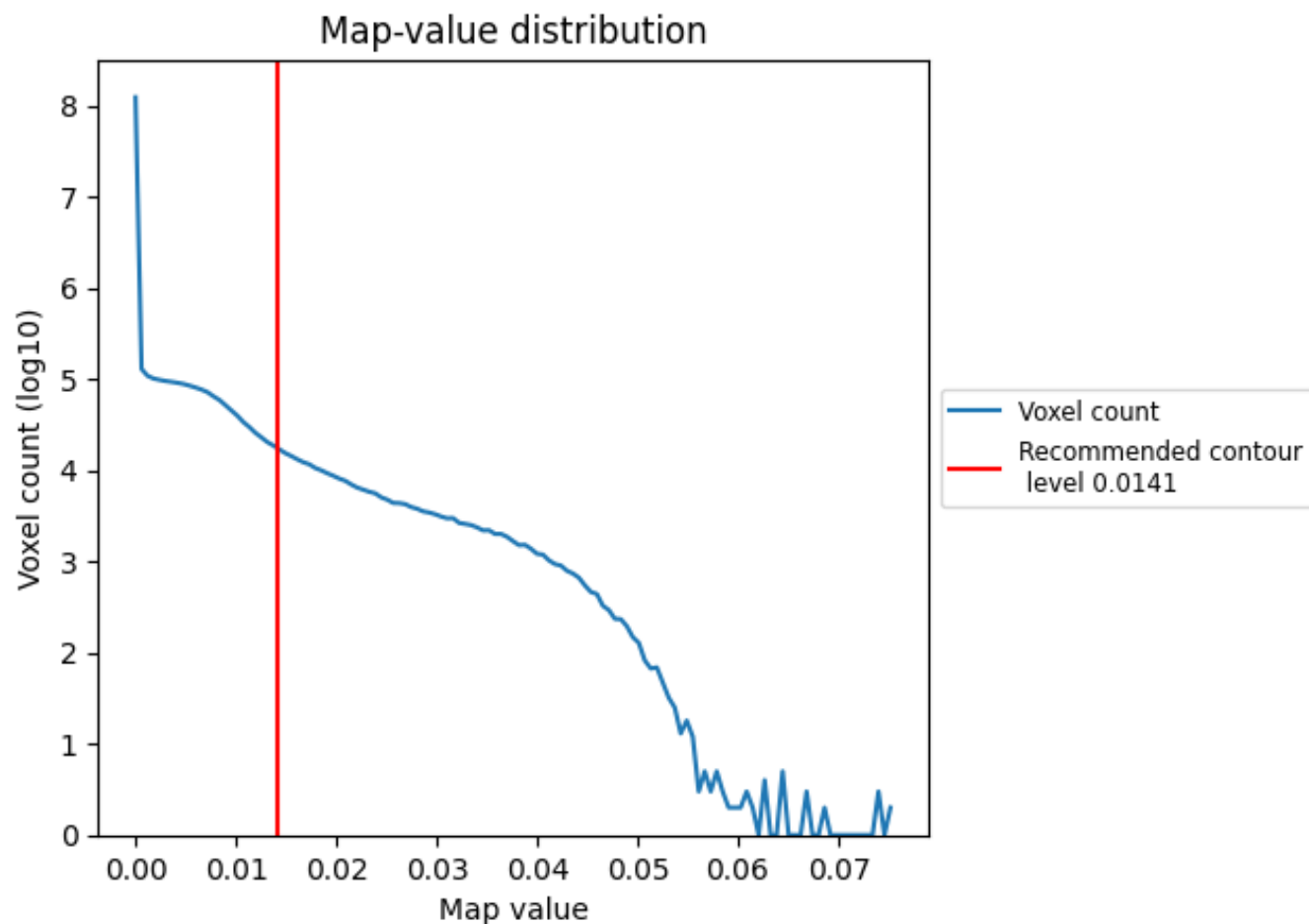
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

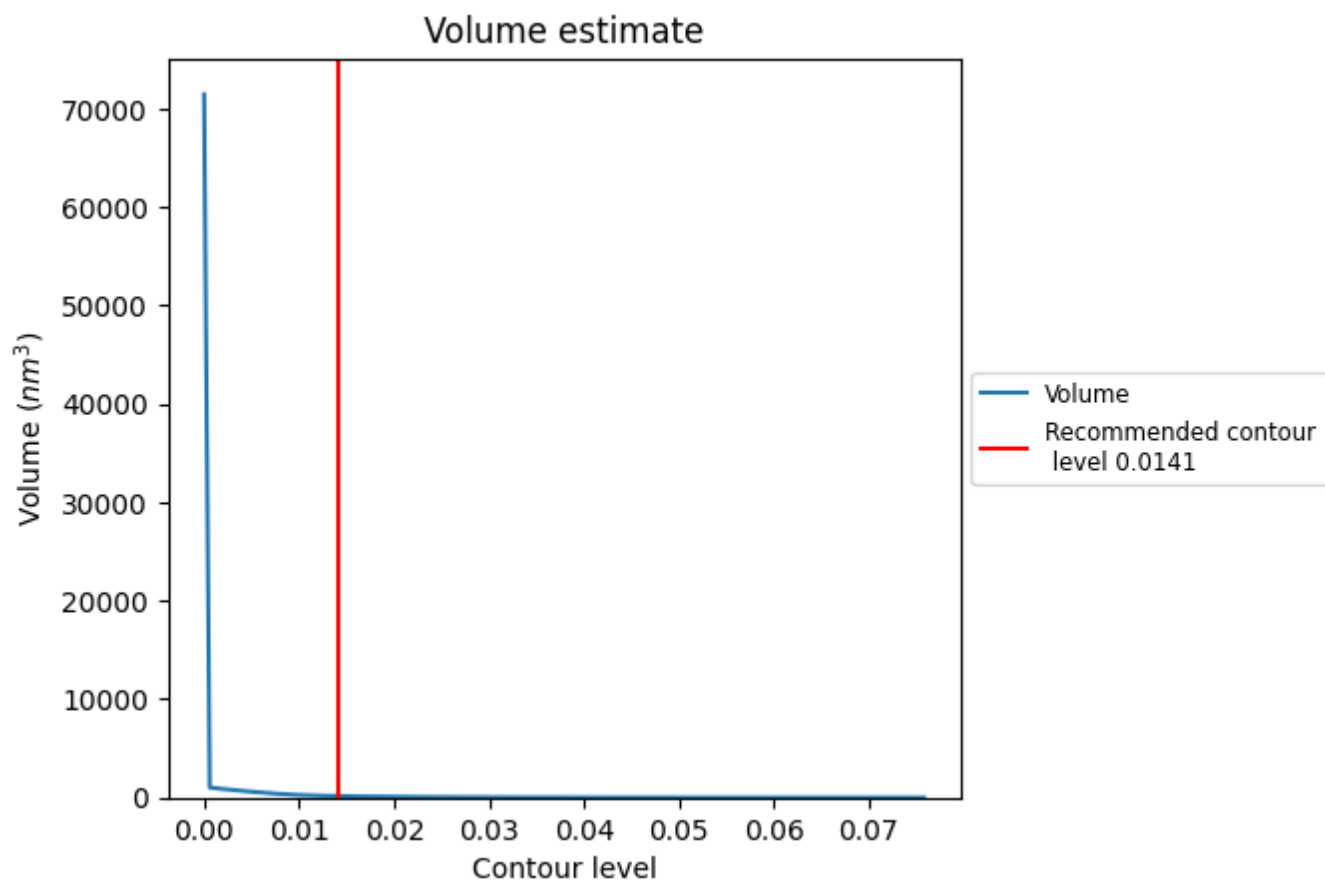
This section contains the results of statistical analysis of the map.

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.

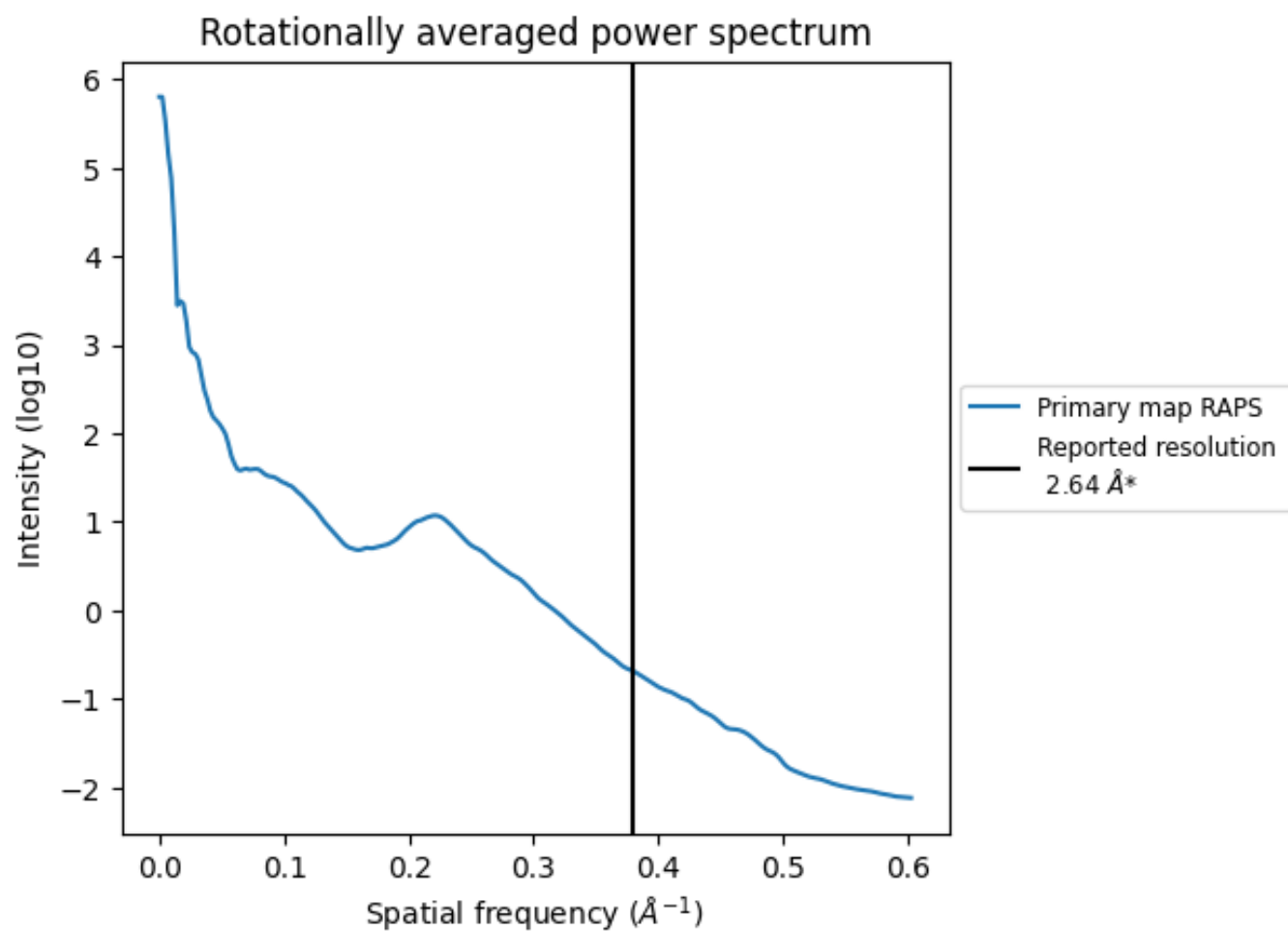
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 151 nm³; this corresponds to an approximate mass of 136 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 0.379 Å⁻¹

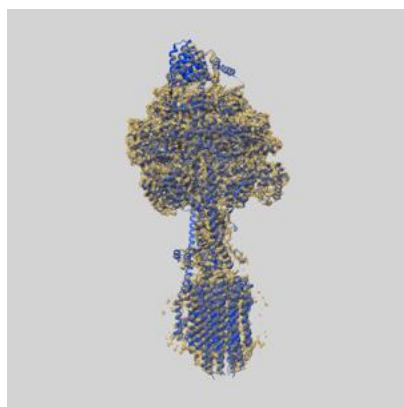
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

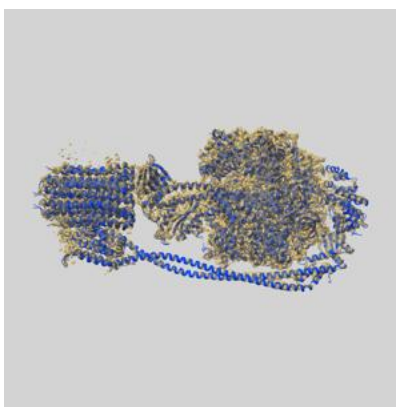
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12392 and PDB model 7NJN. Per-residue inclusion information can be found in section [3](#) on page [9](#).

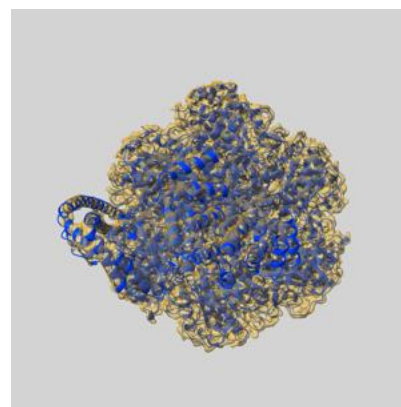
9.1 Map-model overlay [i](#)



X



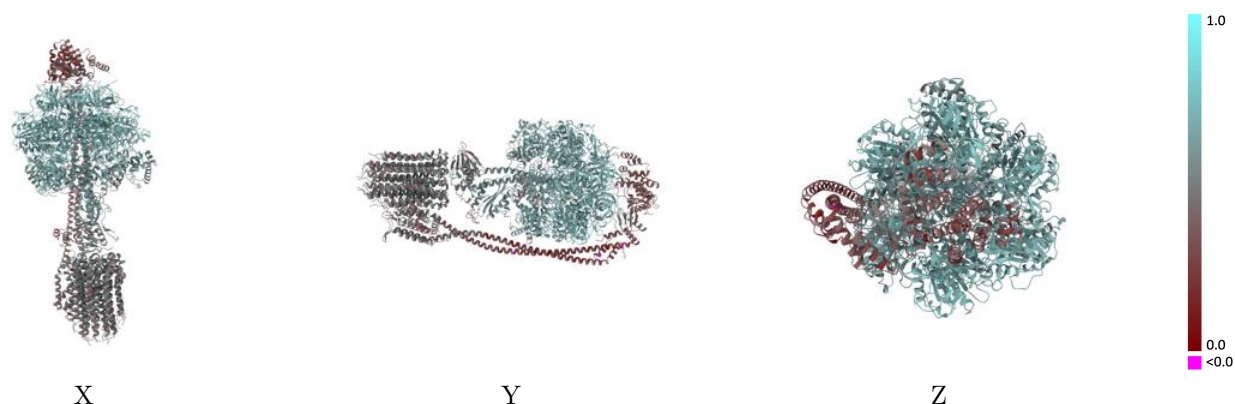
Y



Z

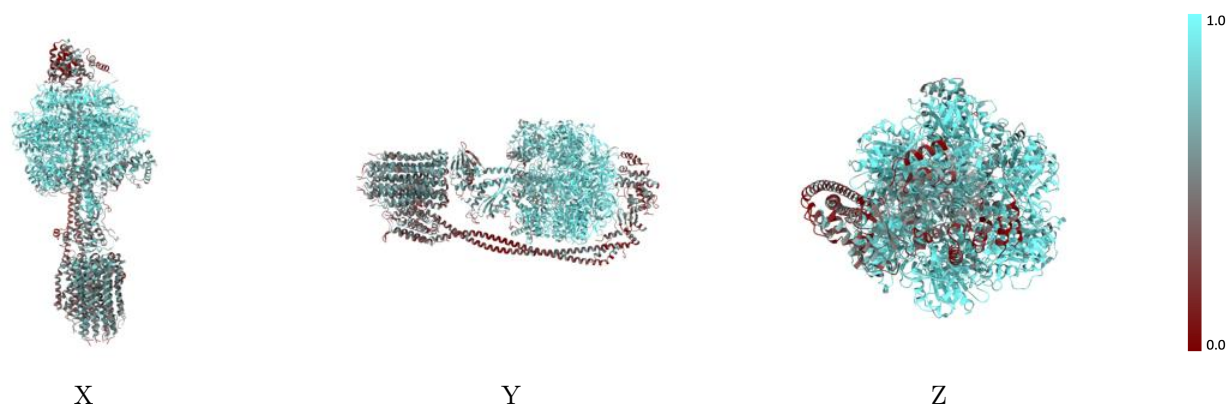
The images above show the 3D surface view of the map at the recommended contour level 0.0141 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



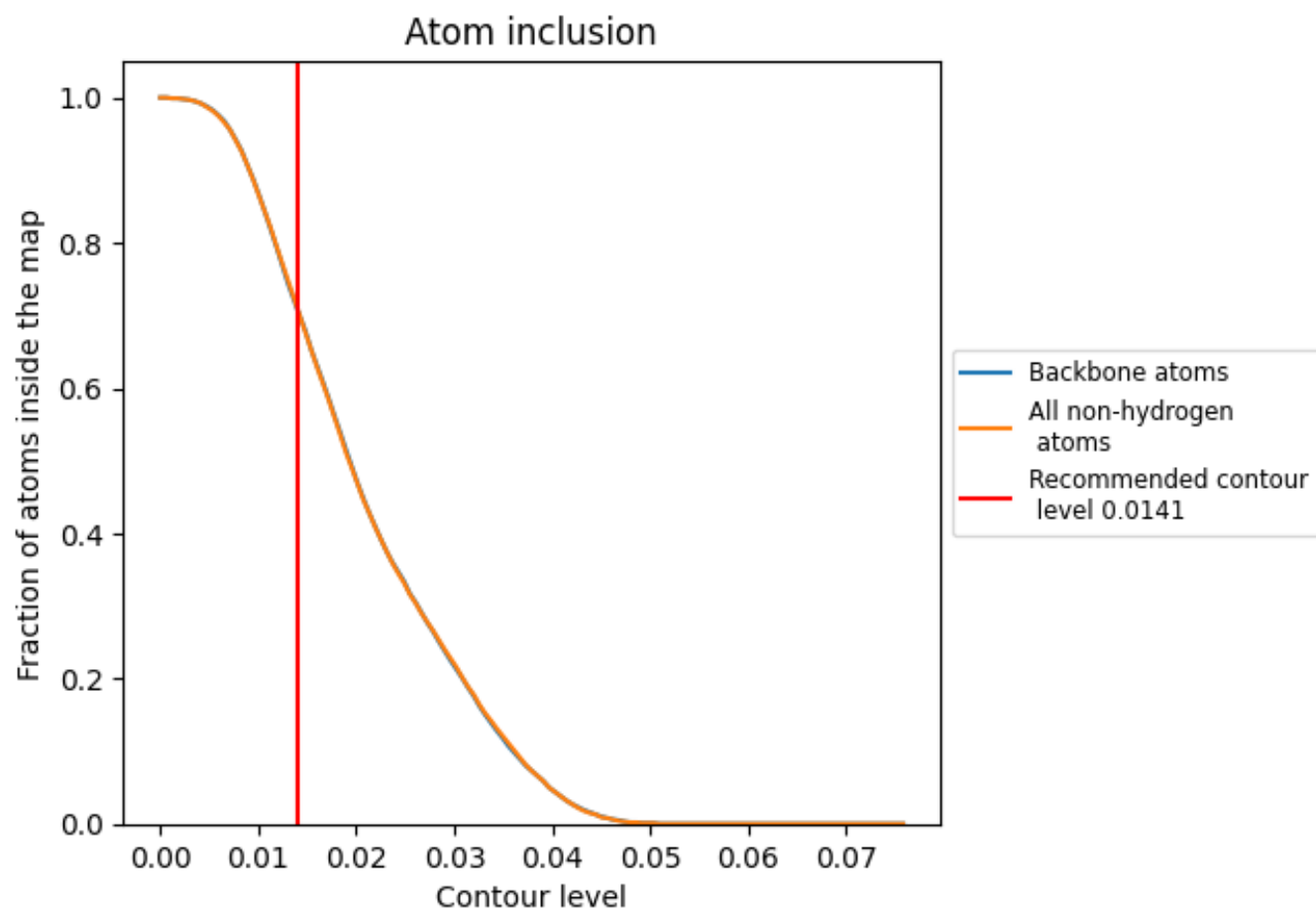
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0141).











































9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 70% 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 (0.0141) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7050	 0.5600
A	 0.8570	 0.6430
B	 0.8110	 0.6220
C	 0.8180	 0.6230
D	 0.8980	 0.6590
E	 0.8430	 0.6380
F	 0.8980	 0.6600
G	 0.7020	 0.5640
H	 0.4600	 0.4510
L	 0.5560	 0.4770
M	 0.5370	 0.4790
N	 0.5390	 0.4690
O	 0.5590	 0.4760
P	 0.5420	 0.4700
Q	 0.5520	 0.4740
R	 0.5440	 0.4710
S	 0.5360	 0.4700
T	 0.5600	 0.4660
a	 0.4230	 0.4280
b	 0.2840	 0.3290
d	 0.3480	 0.3260

