



wwPDB EM Validation Summary Report ⓘ

Apr 20, 2026 – 03:34 PM EDT

PDB ID : 11VE / pdb_000011ve
EMDB ID : EMD-76074
Title : Cryo-EM structure of substrate engaged p97-Ufd1-NPL4-Faf1 complex (State1)
Authors : Liao, Z.; Arkinson, C.; Andreas, M.
Deposited on : 2026-03-13
Resolution : 3.85 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:

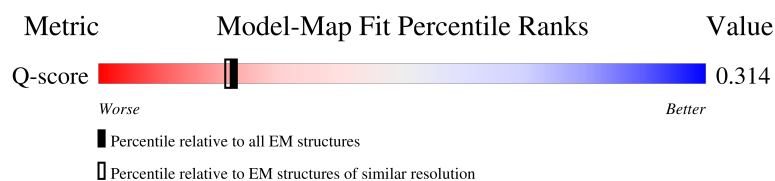
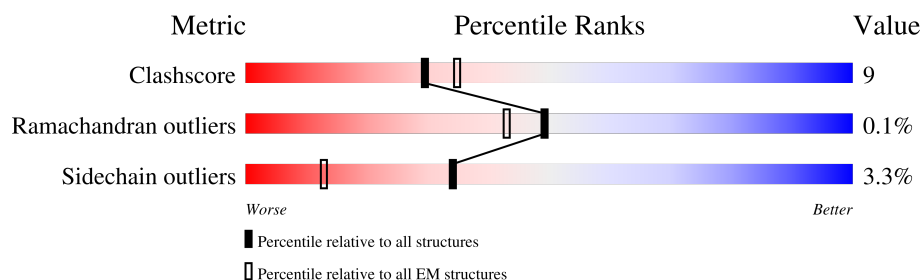
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.85 Å.

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









Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8989 (3.35 - 4.35)

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	G	608	
2	M	173	
2	O	173	
3	P	313	

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Mol	Chain	Length	Quality of chain
4	A	821	
4	B	821	
4	C	821	
4	D	821	
4	E	821	
4	F	821	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 35382 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 Nuclear protein localization protein 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	553	Total	C	N	O	S	0	0
			4397	2791	752	835	19		

- Molecule 2 is a protein called FAS-associated factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	122	Total	C	N	O	S	0	0
			1025	652	177	195	1		
2	O	104	Total	C	N	O		0	0
			861	553	144	164			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	478	PRO	-	expression tag	UNP Q9UNN5
M	479	LEU	-	expression tag	UNP Q9UNN5
M	480	GLY	-	expression tag	UNP Q9UNN5
O	478	PRO	-	expression tag	UNP Q9UNN5
O	479	LEU	-	expression tag	UNP Q9UNN5
O	480	GLY	-	expression tag	UNP Q9UNN5

- Molecule 3 is a protein called Ubiquitin recognition factor in ER-associated degradation protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	P	54	Total	C	N	O	0	0
			420	268	81	71		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	308	HIS	-	expression tag	UNP Q92890
P	309	HIS	-	expression tag	UNP Q92890

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Chain	Residue	Modelled	Actual	Comment	Reference
P	310	HIS	-	expression tag	UNP Q92890
P	311	HIS	-	expression tag	UNP Q92890
P	312	HIS	-	expression tag	UNP Q92890
P	313	HIS	-	expression tag	UNP Q92890

- Molecule 4 is a protein called Transitional endoplasmic reticulum ATPase.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	728	Total	C	N	O	S	0	0
			5201	3248	938	993	22		
4	B	549	Total	C	N	O	S	0	0
			4300	2698	755	825	22		
4	C	726	Total	C	N	O	S	0	0
			5176	3230	934	990	22		
4	D	551	Total	C	N	O	S	0	0
			4201	2646	741	793	21		
4	E	549	Total	C	N	O	S	0	0
			4268	2683	753	810	22		
4	F	727	Total	C	N	O	S	0	0
			5195	3247	935	991	22		

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	807	VAL	-	expression tag	UNP P55072
A	808	ASP	-	expression tag	UNP P55072
A	809	LYS	-	expression tag	UNP P55072
A	810	LEU	-	expression tag	UNP P55072
A	811	ALA	-	expression tag	UNP P55072
A	812	ALA	-	expression tag	UNP P55072
A	813	ALA	-	expression tag	UNP P55072
A	814	LEU	-	expression tag	UNP P55072
A	815	GLU	-	expression tag	UNP P55072
A	816	HIS	-	expression tag	UNP P55072
A	817	HIS	-	expression tag	UNP P55072
A	818	HIS	-	expression tag	UNP P55072
A	819	HIS	-	expression tag	UNP P55072
A	820	HIS	-	expression tag	UNP P55072
A	821	HIS	-	expression tag	UNP P55072
B	807	VAL	-	expression tag	UNP P55072
B	808	ASP	-	expression tag	UNP P55072
B	809	LYS	-	expression tag	UNP P55072

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Chain	Residue	Modelled	Actual	Comment	Reference
B	810	LEU	-	expression tag	UNP P55072
B	811	ALA	-	expression tag	UNP P55072
B	812	ALA	-	expression tag	UNP P55072
B	813	ALA	-	expression tag	UNP P55072
B	814	LEU	-	expression tag	UNP P55072
B	815	GLU	-	expression tag	UNP P55072
B	816	HIS	-	expression tag	UNP P55072
B	817	HIS	-	expression tag	UNP P55072
B	818	HIS	-	expression tag	UNP P55072
B	819	HIS	-	expression tag	UNP P55072
B	820	HIS	-	expression tag	UNP P55072
B	821	HIS	-	expression tag	UNP P55072
C	807	VAL	-	expression tag	UNP P55072
C	808	ASP	-	expression tag	UNP P55072
C	809	LYS	-	expression tag	UNP P55072
C	810	LEU	-	expression tag	UNP P55072
C	811	ALA	-	expression tag	UNP P55072
C	812	ALA	-	expression tag	UNP P55072
C	813	ALA	-	expression tag	UNP P55072
C	814	LEU	-	expression tag	UNP P55072
C	815	GLU	-	expression tag	UNP P55072
C	816	HIS	-	expression tag	UNP P55072
C	817	HIS	-	expression tag	UNP P55072
C	818	HIS	-	expression tag	UNP P55072
C	819	HIS	-	expression tag	UNP P55072
C	820	HIS	-	expression tag	UNP P55072
C	821	HIS	-	expression tag	UNP P55072
D	807	VAL	-	expression tag	UNP P55072
D	808	ASP	-	expression tag	UNP P55072
D	809	LYS	-	expression tag	UNP P55072
D	810	LEU	-	expression tag	UNP P55072
D	811	ALA	-	expression tag	UNP P55072
D	812	ALA	-	expression tag	UNP P55072
D	813	ALA	-	expression tag	UNP P55072
D	814	LEU	-	expression tag	UNP P55072
D	815	GLU	-	expression tag	UNP P55072
D	816	HIS	-	expression tag	UNP P55072
D	817	HIS	-	expression tag	UNP P55072
D	818	HIS	-	expression tag	UNP P55072
D	819	HIS	-	expression tag	UNP P55072
D	820	HIS	-	expression tag	UNP P55072
D	821	HIS	-	expression tag	UNP P55072

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Chain	Residue	Modelled	Actual	Comment	Reference
E	807	VAL	-	expression tag	UNP P55072
E	808	ASP	-	expression tag	UNP P55072
E	809	LYS	-	expression tag	UNP P55072
E	810	LEU	-	expression tag	UNP P55072
E	811	ALA	-	expression tag	UNP P55072
E	812	ALA	-	expression tag	UNP P55072
E	813	ALA	-	expression tag	UNP P55072
E	814	LEU	-	expression tag	UNP P55072
E	815	GLU	-	expression tag	UNP P55072
E	816	HIS	-	expression tag	UNP P55072
E	817	HIS	-	expression tag	UNP P55072
E	818	HIS	-	expression tag	UNP P55072
E	819	HIS	-	expression tag	UNP P55072
E	820	HIS	-	expression tag	UNP P55072
E	821	HIS	-	expression tag	UNP P55072
F	807	VAL	-	expression tag	UNP P55072
F	808	ASP	-	expression tag	UNP P55072
F	809	LYS	-	expression tag	UNP P55072
F	810	LEU	-	expression tag	UNP P55072
F	811	ALA	-	expression tag	UNP P55072
F	812	ALA	-	expression tag	UNP P55072
F	813	ALA	-	expression tag	UNP P55072
F	814	LEU	-	expression tag	UNP P55072
F	815	GLU	-	expression tag	UNP P55072
F	816	HIS	-	expression tag	UNP P55072
F	817	HIS	-	expression tag	UNP P55072
F	818	HIS	-	expression tag	UNP P55072
F	819	HIS	-	expression tag	UNP P55072
F	820	HIS	-	expression tag	UNP P55072
F	821	HIS	-	expression tag	UNP P55072

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

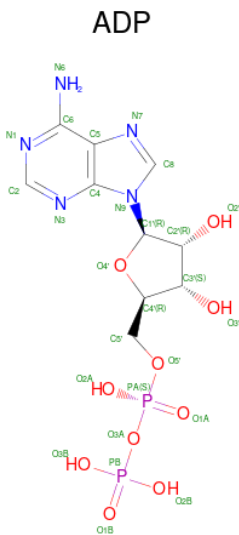
Mol	Chain	Residues	Atoms		AltConf
5	G	2	Total	Zn	0
			2	2	

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).

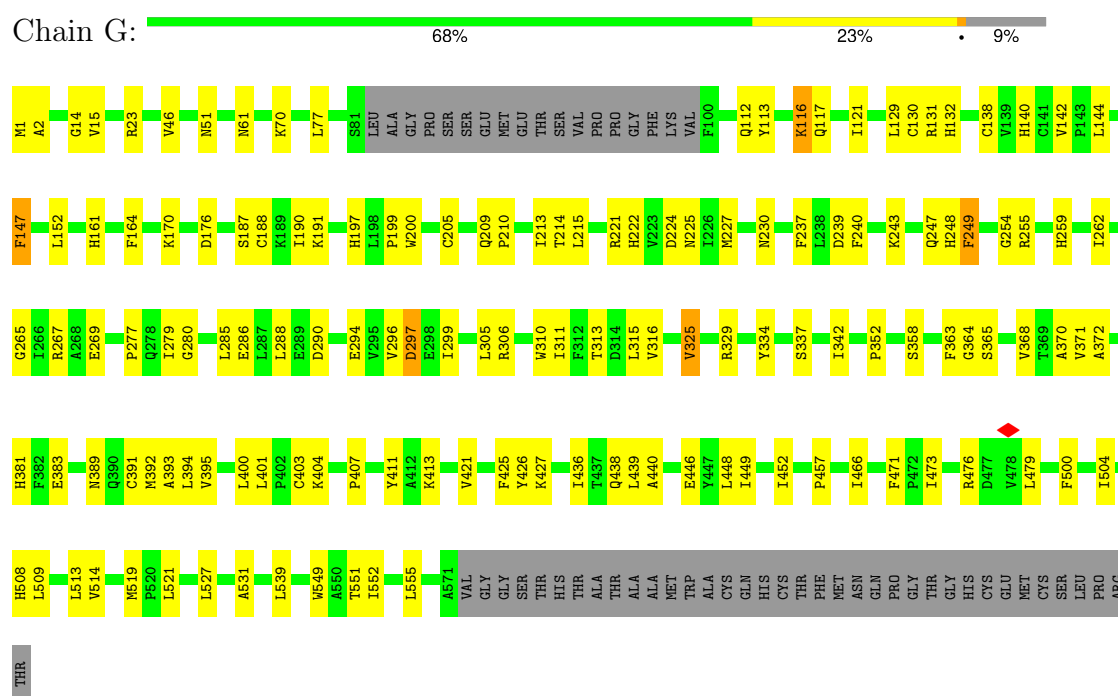


Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total 27	C 10	N 5	O 10	P 2	0
7	B	1	Total 27	C 10	N 5	O 10	P 2	0
7	C	1	Total 27	C 10	N 5	O 10	P 2	0
7	D	1	Total 27	C 10	N 5	O 10	P 2	0
7	D	1	Total 27	C 10	N 5	O 10	P 2	0
7	E	1	Total 27	C 10	N 5	O 10	P 2	0
7	E	1	Total 27	C 10	N 5	O 10	P 2	0
7	F	1	Total 27	C 10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

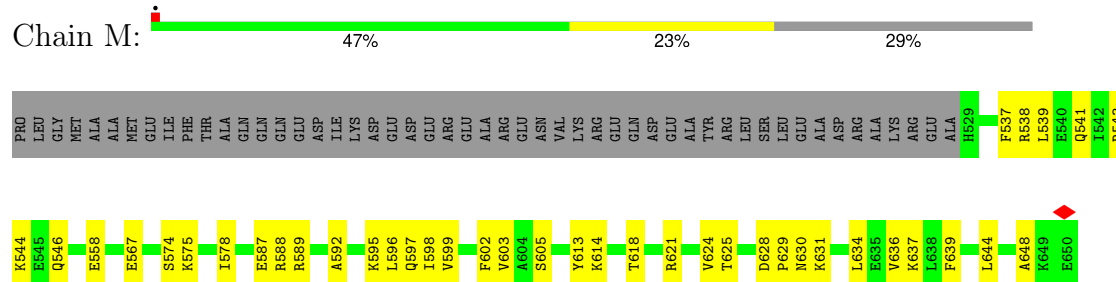
3 Residue-property plots

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: Nuclear protein localization protein 4 homolog

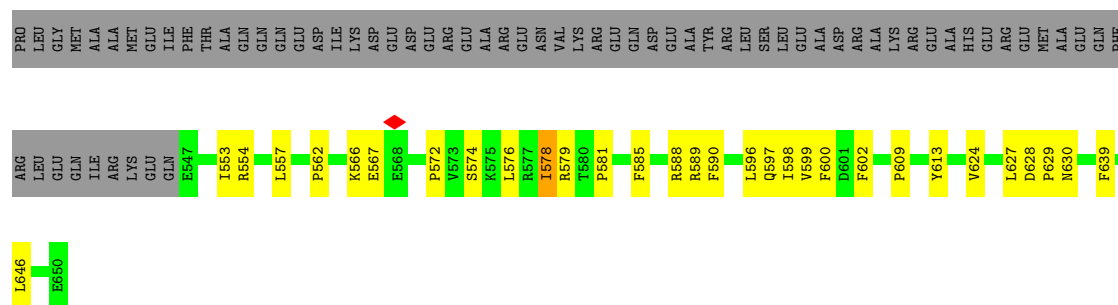


- Molecule 2: FAS-associated factor 1



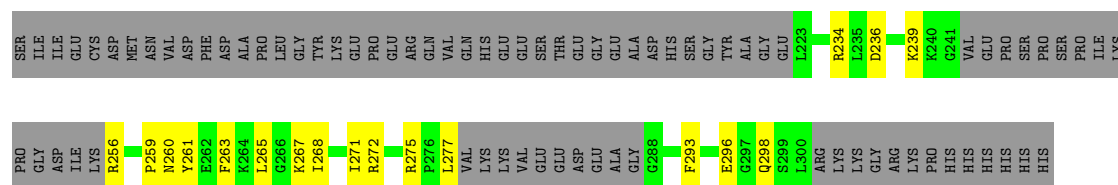
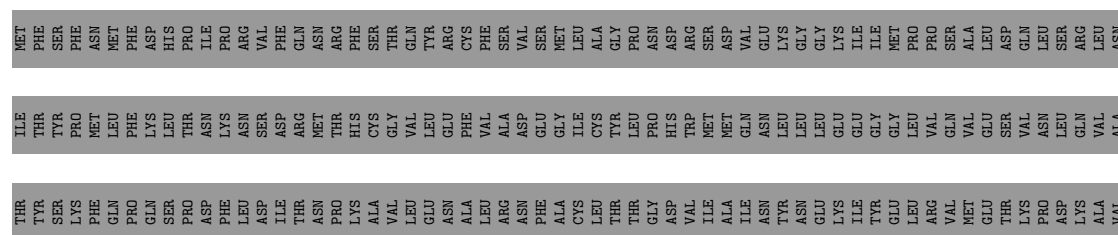
- Molecule 2: FAS-associated factor 1





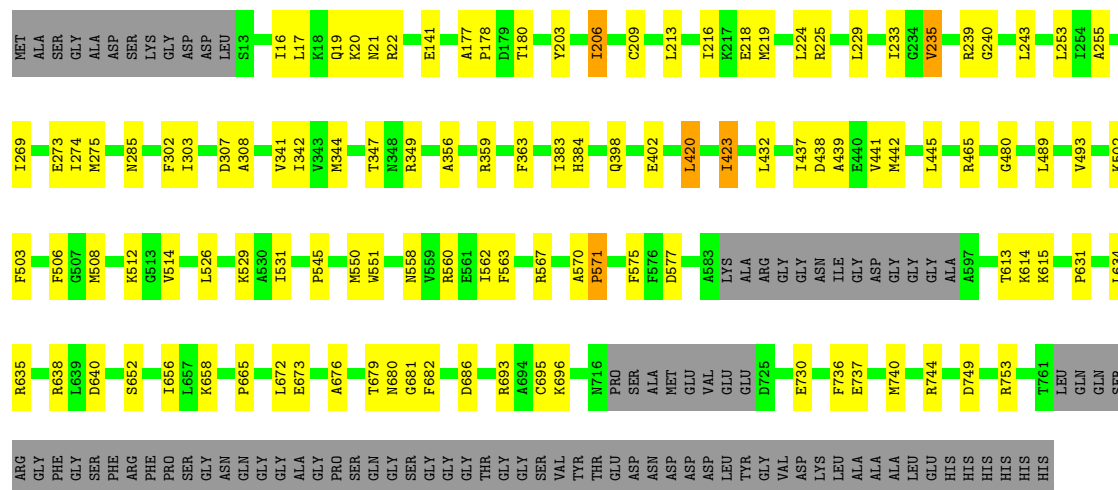
- Molecule 3: Ubiquitin recognition factor in ER-associated degradation protein 1

Chain P: 12% 6% 83%



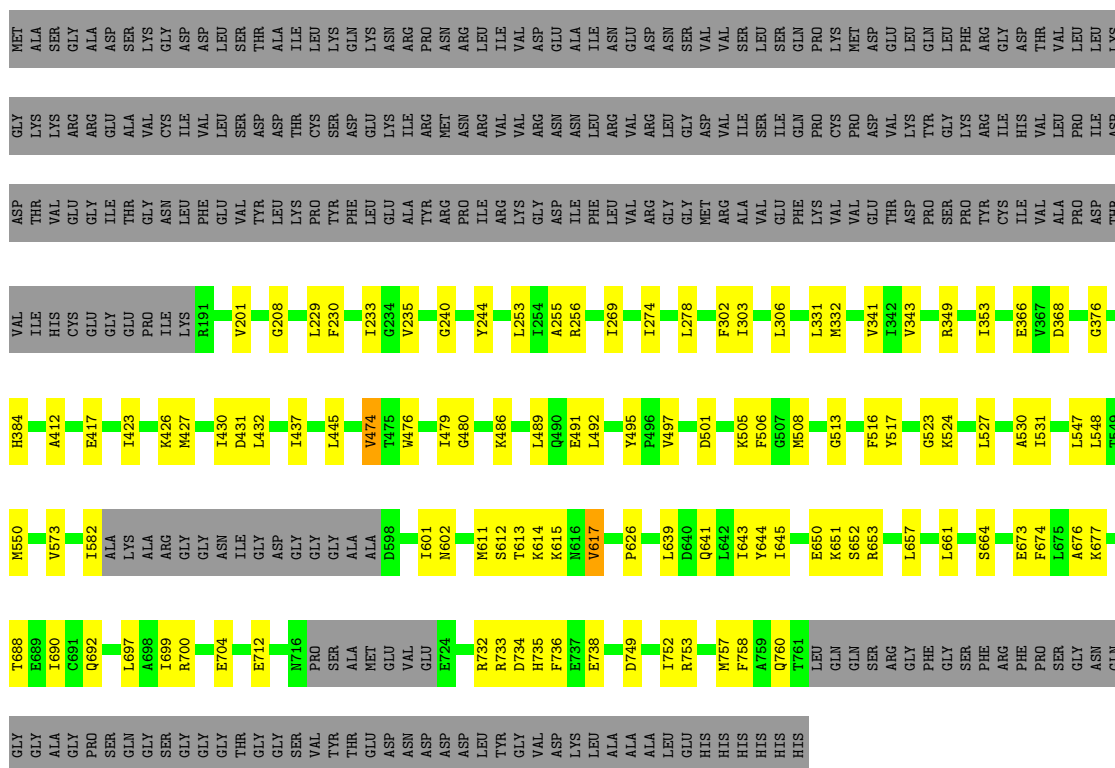
- Molecule 4: Transitional endoplasmic reticulum ATPase

Chain A: 75% 13% 11%

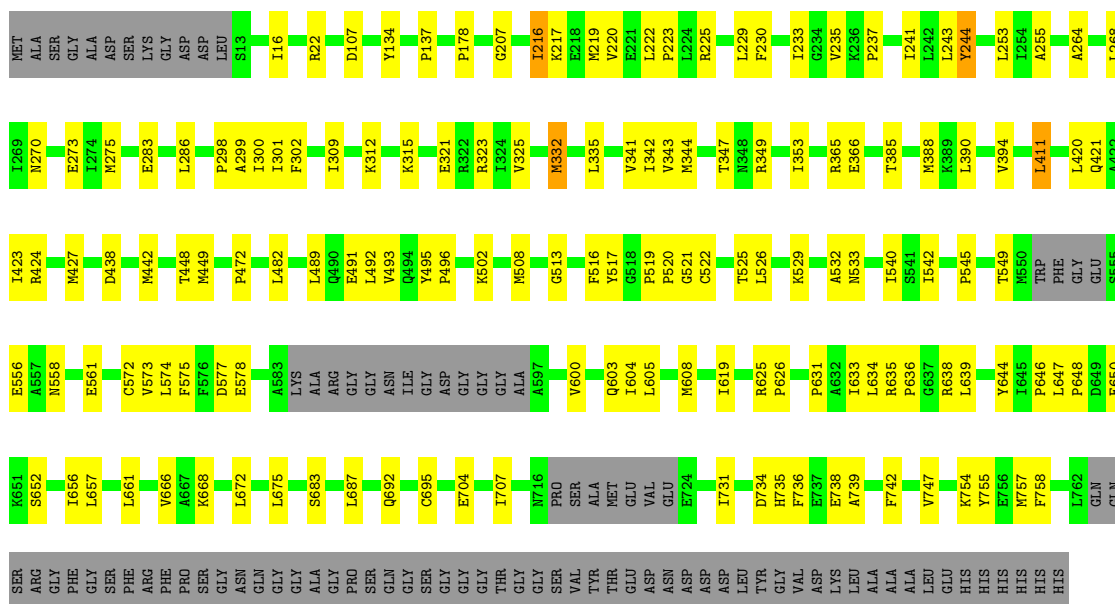


- Molecule 4: Transitional endoplasmic reticulum ATPase

Chain B: 54% 13% 33%



- Molecule 4: Transitional endoplasmic reticulum ATPase



- Molecule 4: Transitional endoplasmic reticulum ATPase





PRO	SER	GLN	GLY	SER	GLY	GLY	GLY	THR	GLY	GLY	SER	VAL	SER	TYR	THR	GLU	ASP	ASN	ASP	ASP	ASP	TYR	GLY	VAL	ASP	LYS	LEU	ALA	ALA	LEU	GLU	HIS	HIS	HIS	HIS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

● Molecule 4: Transitional endoplasmic reticulum ATPase



SER	PHE	ARG	PHE	PRO	SER	GLY	ASN	GLN	GLY	GLY	ALA	PRO	SER	GLN	GLY	SER	GLY	GLY	GLY	THR	GLY	GLY	SER	VAL	THR	GLU	ASP	ASN	ASP	ASP	ASP	LEU	GLY	VAL	GLY	LYS	LEU	ALA	ALA	LEU	GLU	HIS	HIS	HIS	HIS	HIS
K668	E673	E673	K677	L687	T688	E689	I690	C691	C692	C695	K696	L697	R700	I703	E706	R709	E710	R711	E712	R713	Q714	T715	ASN	PRO	SER	ALA	MET	GLU	VAL	GLU	E724	F736	M740	D749	I752	M757	Q760	T761	LEU	GLN	GLN	SER	ARG	GLY	PHE	GLY
A566	R567	V573	L574	I582	A583	LYS	ALA	ARG	GLY	GLY	ASN	ILE	GLY	ASP	GLY	D598	R599	V600	I604	L605	M608	M611	S612	T613	K614	K615	F618	P626	D630	I633	P636	L639	D640	E650	K651	S652	L657	L661	V666	A667						
D438	V441	L456	R465	V469	W476	E483	K486	L489	Q490	E491	L492	V493	Q494	Y495	P496	F503	F506	G507	M508	K512	G513	Y517	G523	K524	T525	L526	L527	K529	A530	E534	I542	K543	G544	L548	W551	N558	E561	I562								
E273	I274	M275	S276	A297	P298	A299	I300	I301	F302	I303	E483	T316	R322	R323	I324	M332	L335	V341	I342	V343	M344	L357	R358	R359	R362	F363	E366	L378	H384	M388	K389	K529	A530	E534	E402	T403	H404	V407	C415	I423	E433	I437				
MET	ALA	SER	GLY	ALA	ASP	SER	LYS	GLY	ASP	ASP	LEU	SER	THR	L17	I27	P118	T127	G156	I182	G186	Y203	I206	G207	L213	A214	Q215	I216	K217	E218	M219	I233	G234	V235	P246	P247	G248	T249	G250	A255	T262	I269	N270	G271	P272		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	99404	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.855	Depositor
Minimum map value	-0.328	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.0682	Depositor
Map size (\AA)	378.24, 378.24, 378.24	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.4775, 1.4775, 1.4775	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: ZN, 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	G	0.11	0/4501	0.33	0/6100
2	M	0.10	0/1046	0.31	0/1406
2	O	0.10	0/880	0.31	0/1187
3	P	0.15	0/426	0.42	0/560
4	A	0.12	0/5280	0.34	0/7175
4	B	0.12	0/4368	0.33	0/5896
4	C	0.12	0/5251	0.36	0/7134
4	D	0.12	0/4268	0.35	0/5773
4	E	0.13	0/4336	0.34	0/5855
4	F	0.12	0/5274	0.35	0/7167
All	All	0.12	0/35630	0.34	0/48253

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	4397	0	4306	96	0
2	M	1025	0	1023	24	0
2	O	861	0	865	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	P	420	0	428	16	0
4	A	5201	0	4779	73	0
4	B	4300	0	4310	74	0
4	C	5176	0	4761	105	0
4	D	4201	0	4157	89	0
4	E	4268	0	4283	96	0
4	F	5195	0	4777	91	0
5	G	2	0	0	0	0
6	A	31	0	12	2	0
6	B	31	0	12	1	0
6	C	31	0	12	2	0
7	A	27	0	12	0	0
7	B	27	0	12	3	0
7	C	27	0	12	3	0
7	D	54	0	24	6	0
7	E	54	0	24	2	0
7	F	54	0	24	4	0
All	All	35382	0	33833	636	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 9.

The worst 5 of 636 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:E:515:LEU:HG	4:E:639:LEU:HD21	1.42	1.00
1:G:138:CYS:SG	1:G:140:HIS:CE1	2.71	0.81
4:D:316:THR:HB	4:D:321:GLU:HG3	1.63	0.81
4:F:402:GLU:HG2	4:F:456:LEU:HD21	1.63	0.79
1:G:225:ASN:HB3	1:G:267:ARG:HG3	1.65	0.78

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	G	549/608 (90%)	520 (95%)	29 (5%)	0	100	100
2	M	120/173 (69%)	114 (95%)	6 (5%)	0	100	100
2	O	102/173 (59%)	96 (94%)	6 (6%)	0	100	100
3	P	48/313 (15%)	40 (83%)	8 (17%)	0	100	100
4	A	722/821 (88%)	681 (94%)	39 (5%)	2 (0%)	36	69
4	B	543/821 (66%)	516 (95%)	27 (5%)	0	100	100
4	C	718/821 (88%)	663 (92%)	55 (8%)	0	100	100
4	D	545/821 (66%)	517 (95%)	27 (5%)	1 (0%)	43	74
4	E	543/821 (66%)	522 (96%)	21 (4%)	0	100	100
4	F	721/821 (88%)	674 (94%)	46 (6%)	1 (0%)	48	80
All	All	4611/6193 (74%)	4343 (94%)	264 (6%)	4 (0%)	49	80

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	571	PRO
4	D	337	GLN
4	A	640	ASP
4	F	27	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	487/531 (92%)	473 (97%)	14 (3%)	37	58
2	M	113/155 (73%)	112 (99%)	1 (1%)	70	75
2	O	96/155 (62%)	94 (98%)	2 (2%)	47	65
3	P	42/273 (15%)	41 (98%)	1 (2%)	43	63
4	A	472/690 (68%)	456 (97%)	16 (3%)	32	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	B	462/690 (67%)	450 (97%)	12 (3%)	40	61
4	C	470/690 (68%)	454 (97%)	16 (3%)	32	56
4	D	431/690 (62%)	412 (96%)	19 (4%)	25	49
4	E	453/690 (66%)	439 (97%)	14 (3%)	35	57
4	F	471/690 (68%)	452 (96%)	19 (4%)	28	52
All	All	3497/5254 (67%)	3383 (97%)	114 (3%)	34	56

5 of 114 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	C	542	ILE
4	F	548	LEU
4	D	420	LEU
4	F	527	LEU
4	F	341	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
4	B	327	GLN
4	E	533	ASN
4	B	460	ASN
4	D	458	GLN
4	B	458	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 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
6	ATP	A	901	-	32,33,33	0.34	0	48,52,52	0.37	0
7	ADP	D	901	-	28,29,29	1.39	4 (14%)	43,45,45	1.91	8 (18%)
7	ADP	E	902	-	28,29,29	1.41	4 (14%)	43,45,45	1.82	9 (20%)
7	ADP	A	902	-	28,29,29	1.43	5 (17%)	43,45,45	1.86	8 (18%)
7	ADP	D	902	-	28,29,29	1.44	5 (17%)	43,45,45	1.90	8 (18%)
7	ADP	E	901	-	28,29,29	1.38	4 (14%)	43,45,45	1.83	9 (20%)
6	ATP	B	901	-	32,33,33	0.31	0	48,52,52	0.34	0
7	ADP	F	901	-	28,29,29	1.40	4 (14%)	43,45,45	1.84	8 (18%)
7	ADP	C	902	-	28,29,29	1.42	4 (14%)	43,45,45	1.88	8 (18%)
7	ADP	B	902	-	28,29,29	1.43	5 (17%)	43,45,45	1.95	8 (18%)
7	ADP	F	902	-	28,29,29	1.40	4 (14%)	43,45,45	1.87	8 (18%)
6	ATP	C	901	-	32,33,33	0.32	0	48,52,52	0.33	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ATP	A	901	-	-	4/22/38/38	0/3/3/3
7	ADP	D	901	-	-	5/16/32/32	0/3/3/3
7	ADP	E	902	-	-	6/16/32/32	0/3/3/3
7	ADP	A	902	-	-	1/16/32/32	0/3/3/3
7	ADP	D	902	-	-	3/16/32/32	0/3/3/3
7	ADP	E	901	-	-	2/16/32/32	0/3/3/3
6	ATP	B	901	-	-	2/22/38/38	0/3/3/3
7	ADP	F	901	-	-	6/16/32/32	0/3/3/3
7	ADP	C	902	-	-	6/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	ADP	B	902	-	-	5/16/32/32	0/3/3/3
7	ADP	F	902	-	-	4/16/32/32	0/3/3/3
6	ATP	C	901	-	-	4/22/38/38	0/3/3/3

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	902	ADP	C5-C4	4.82	1.47	1.39
7	B	902	ADP	C5-C4	4.81	1.47	1.39
7	F	902	ADP	C5-C4	4.77	1.47	1.39
7	D	901	ADP	C5-C4	4.73	1.47	1.39
7	E	902	ADP	C5-C4	4.71	1.47	1.39

The worst 5 of 74 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	901	ADP	C5-C4-N3	-6.51	117.75	126.72
7	D	902	ADP	C5-C4-N3	-6.51	117.76	126.72
7	B	902	ADP	C5-C4-N3	-6.50	117.76	126.72
7	C	902	ADP	C5-C4-N3	-6.39	117.92	126.72
7	F	902	ADP	C5-C4-N3	-6.16	118.23	126.72

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	901	ATP	C5'-O5'-PA-O2A
6	A	901	ATP	C5'-O5'-PA-O3A
6	C	901	ATP	PB-O3B-PG-O2G
7	B	902	ADP	C5'-O5'-PA-O1A
7	C	902	ADP	C5'-O5'-PA-O1A

There are no ring outliers.

9 monomers are involved in 23 short contacts:

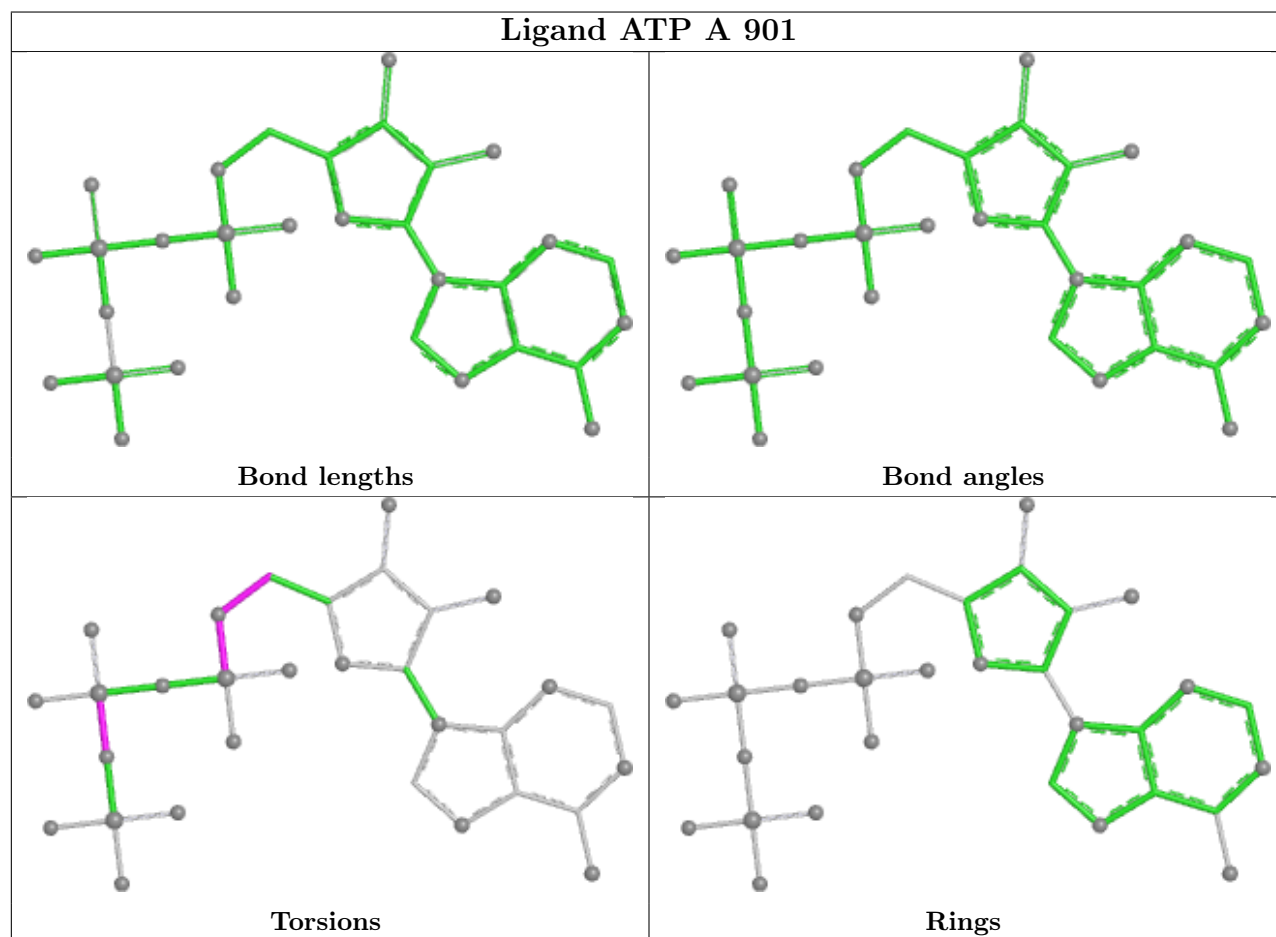
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	901	ATP	2	0
7	D	902	ADP	6	0
7	E	901	ADP	2	0
6	B	901	ATP	1	0

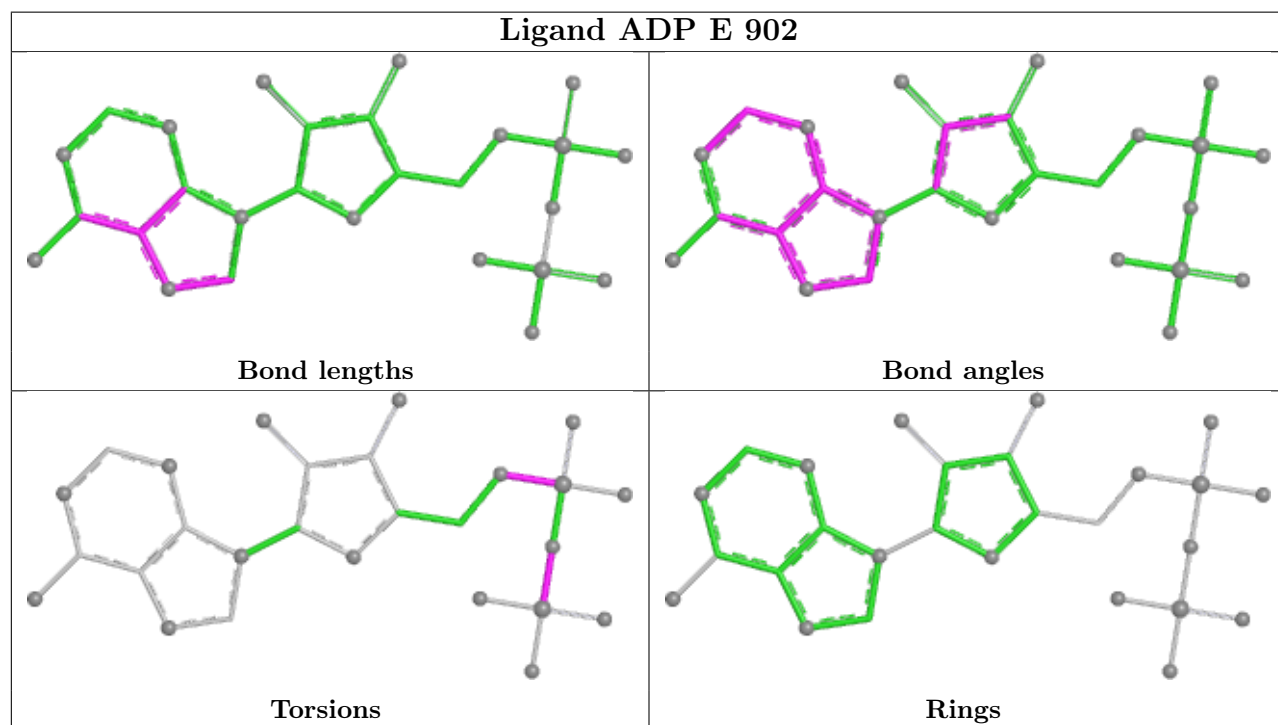
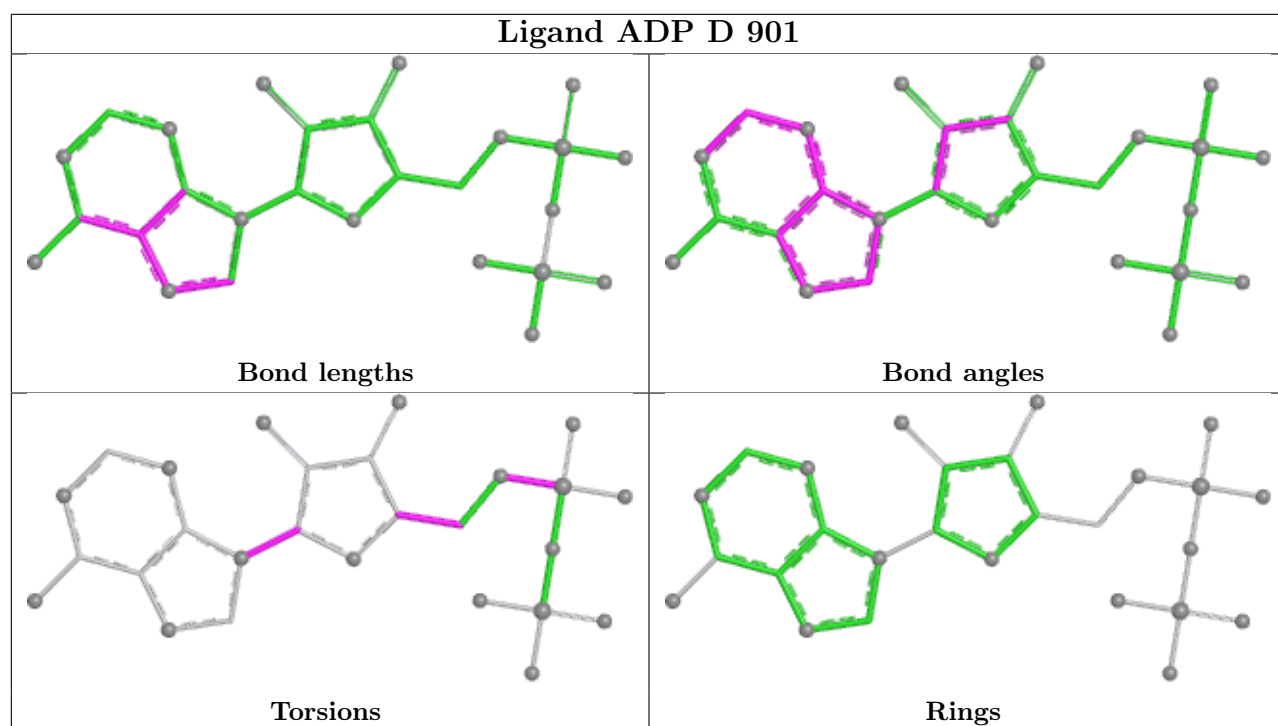
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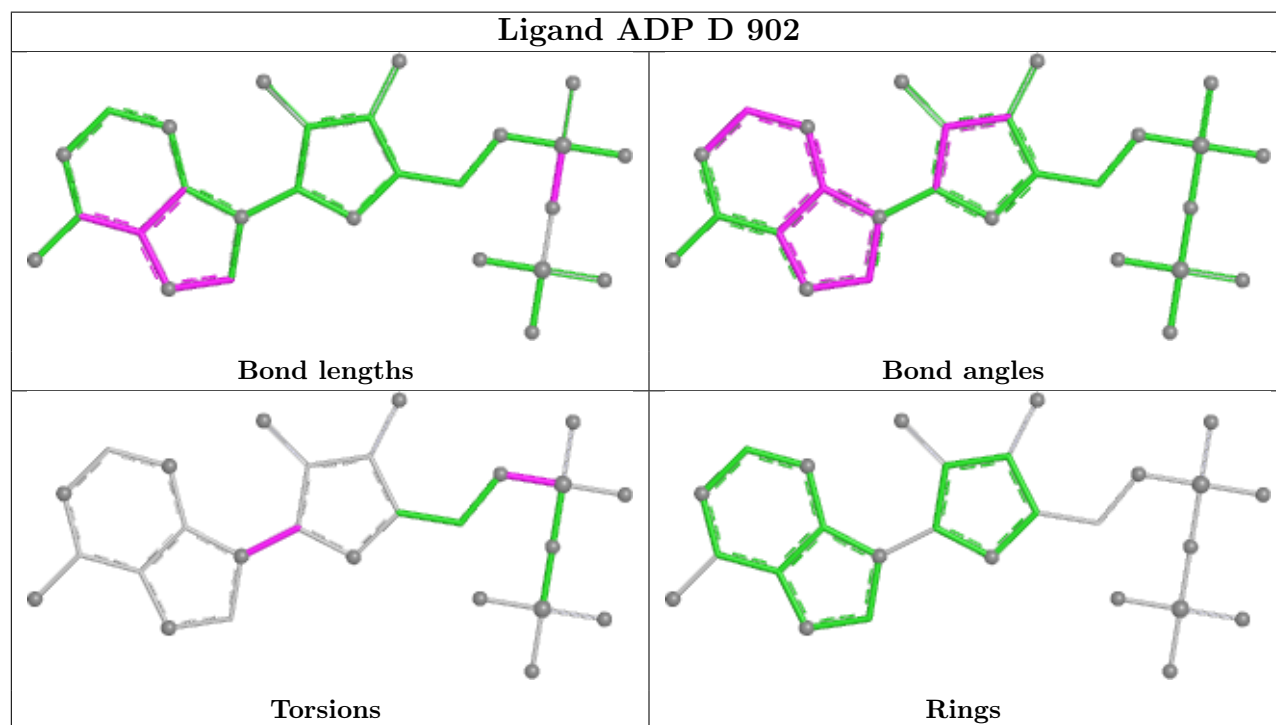
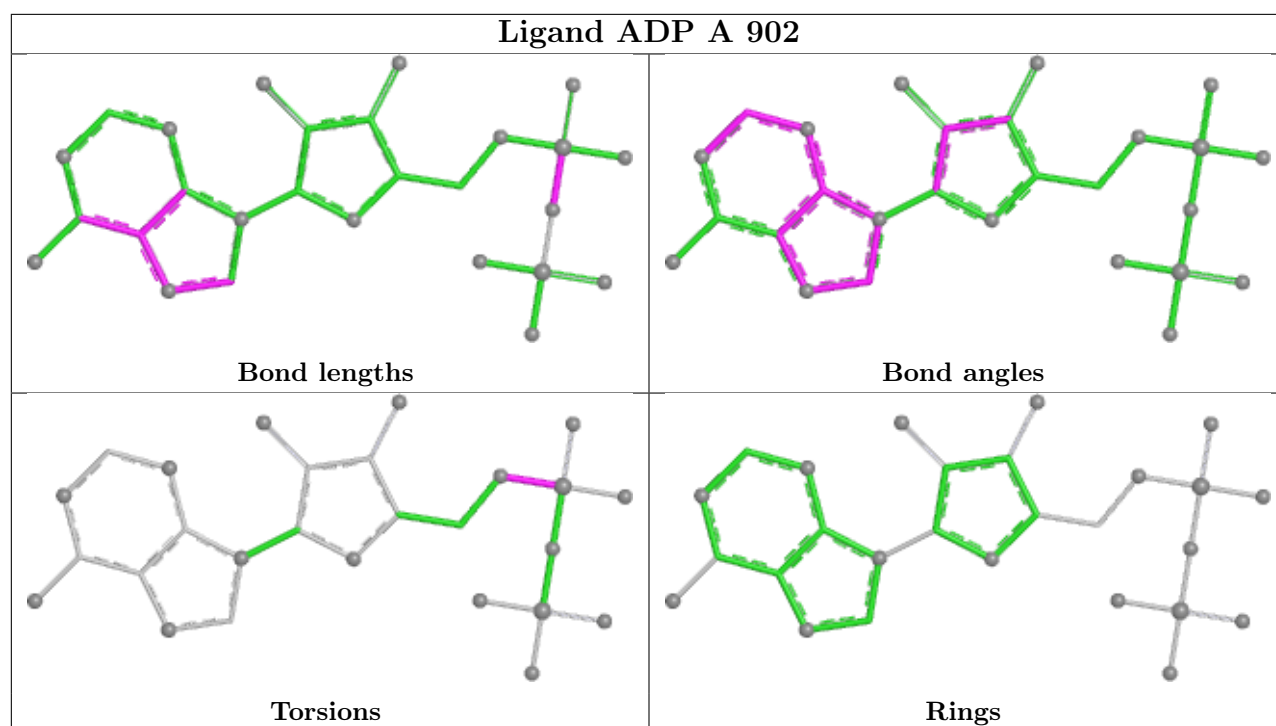
Continued from previous page...

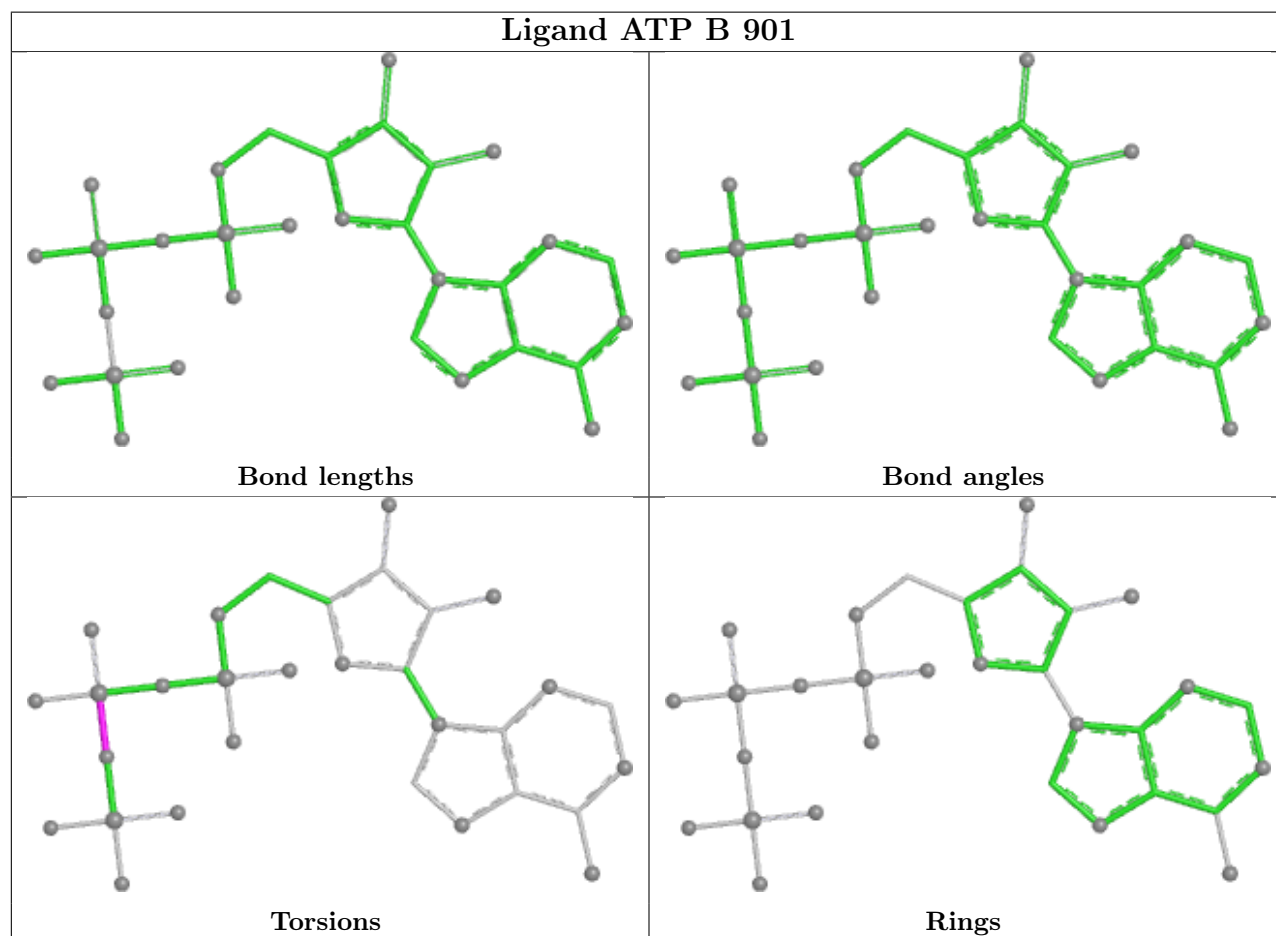
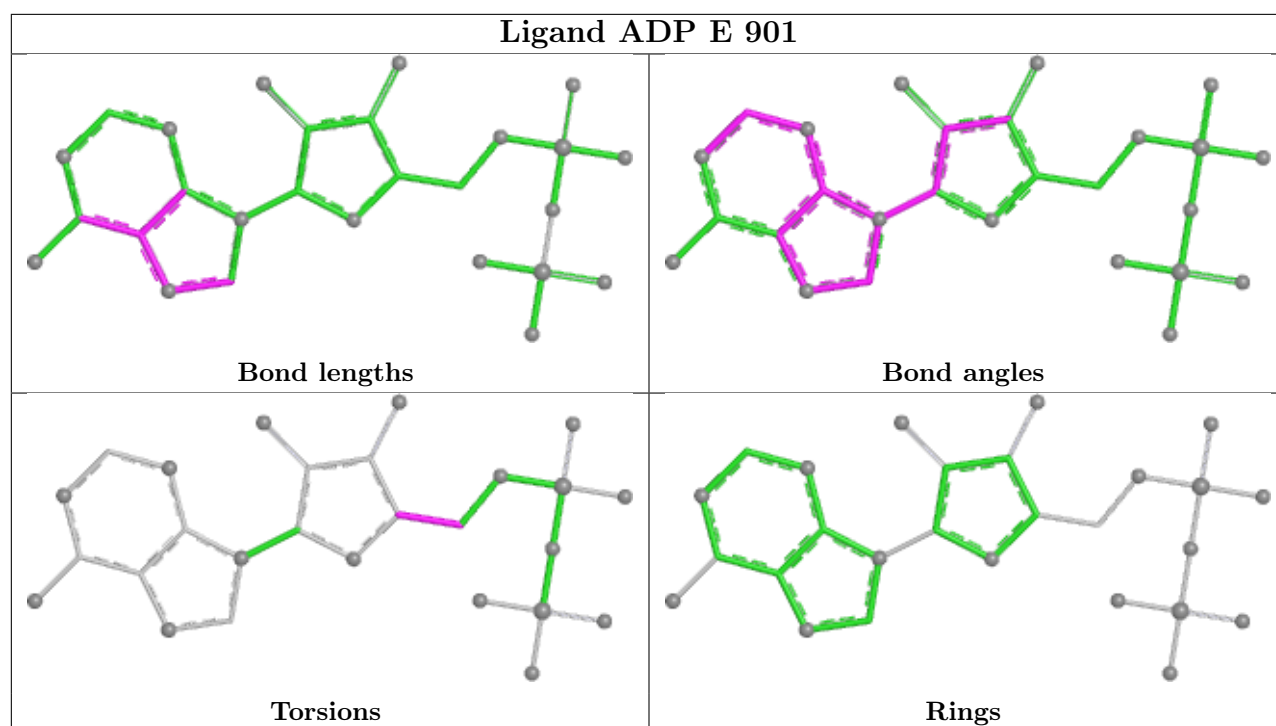
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	901	ADP	3	0
7	C	902	ADP	3	0
7	B	902	ADP	3	0
7	F	902	ADP	1	0
6	C	901	ATP	2	0

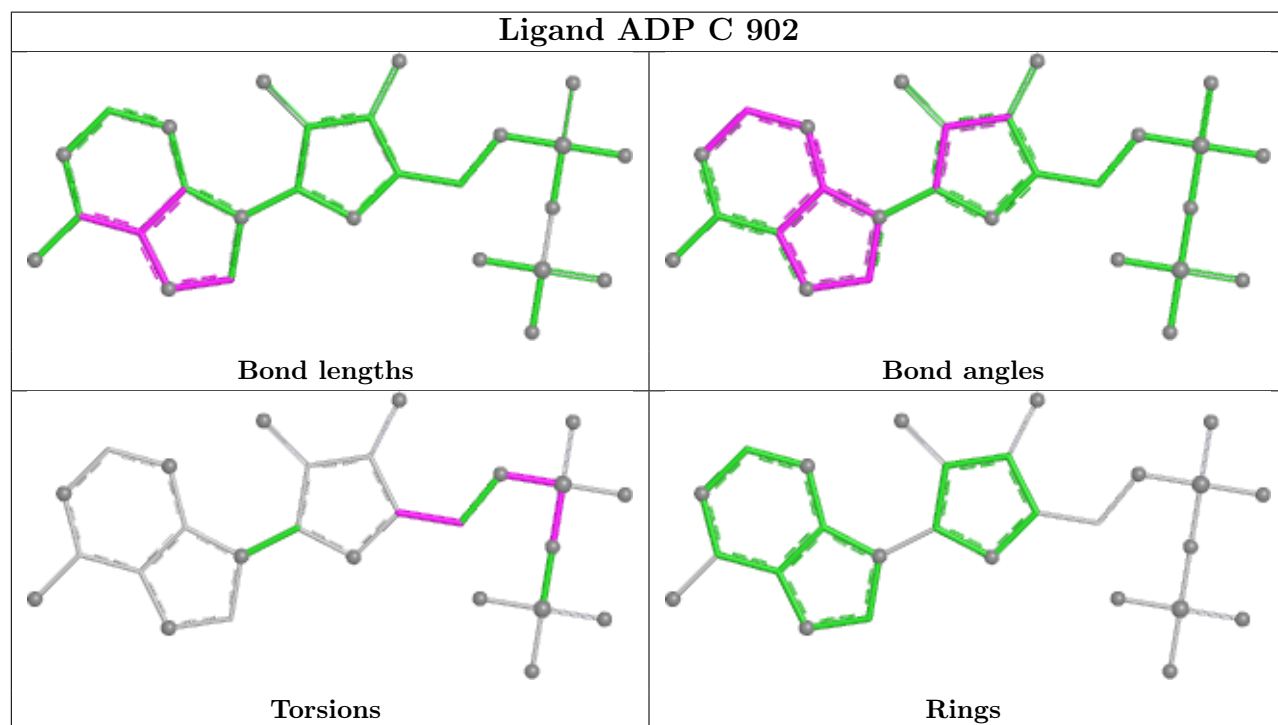
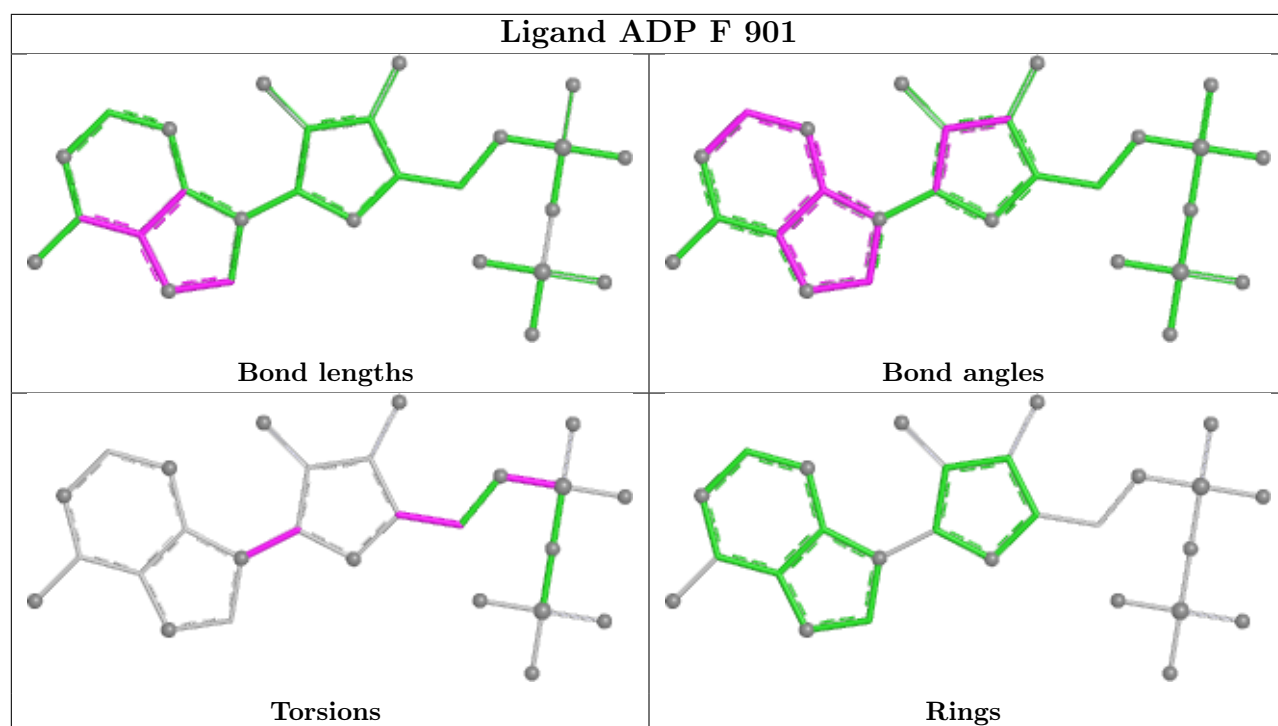
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

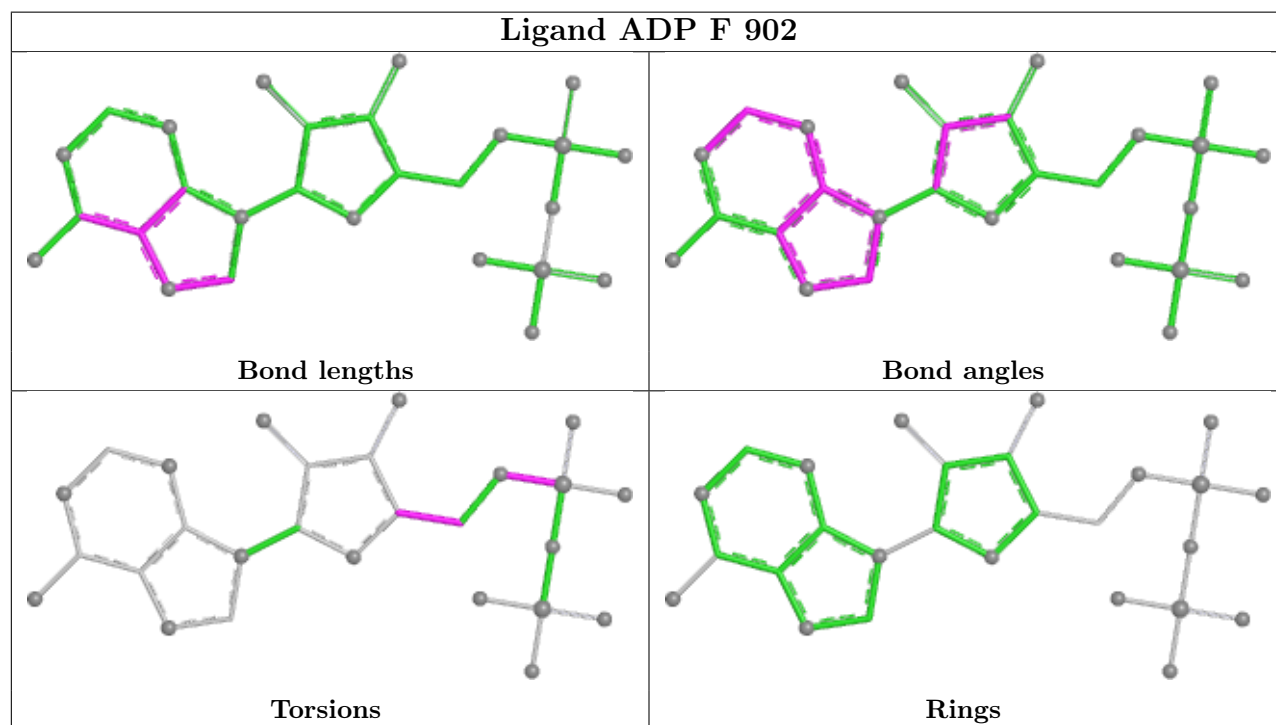
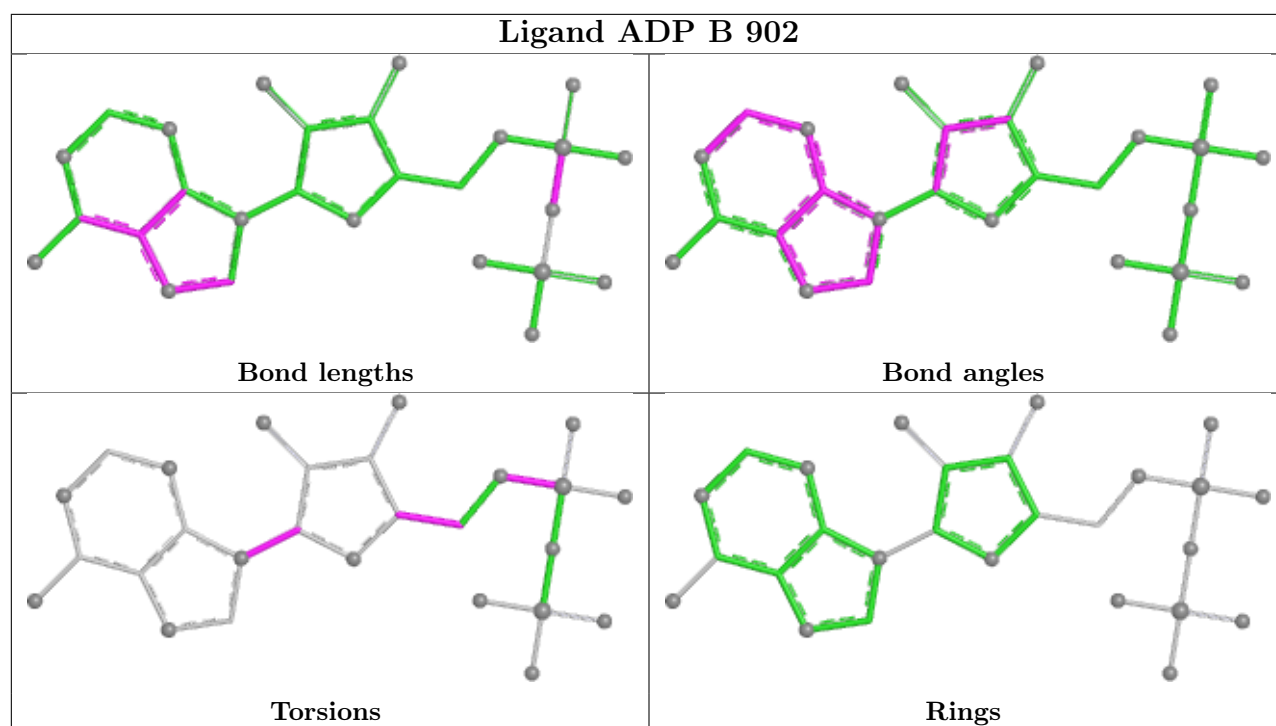


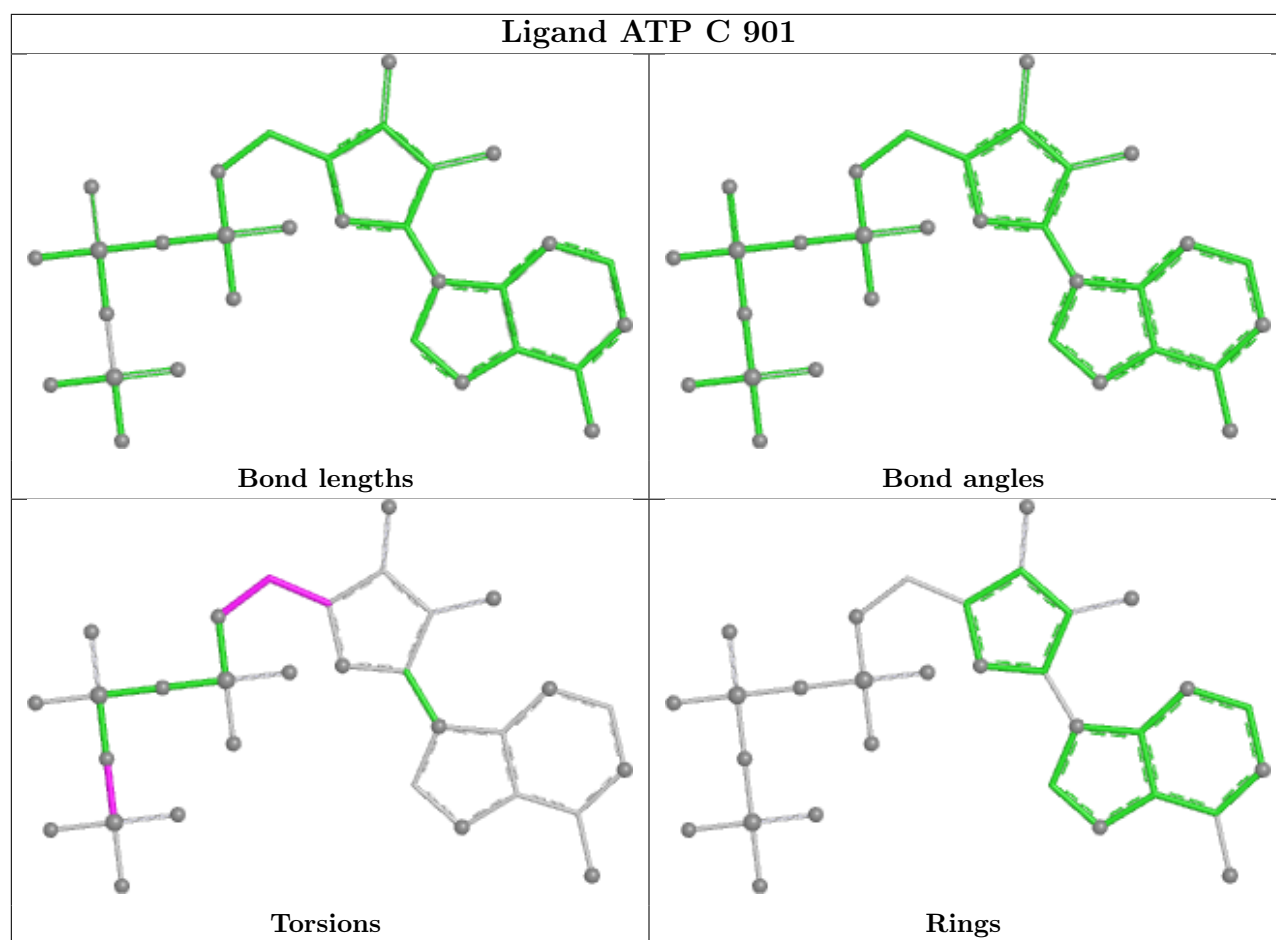












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

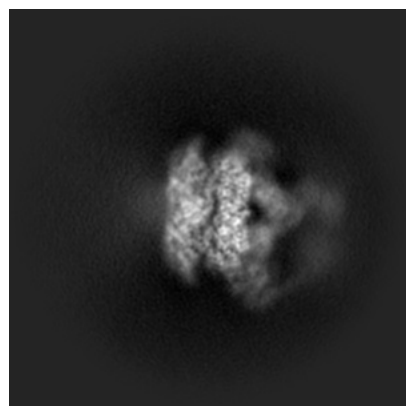
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-76074. These allow visual inspection of the internal detail of the map and identification of artifacts.

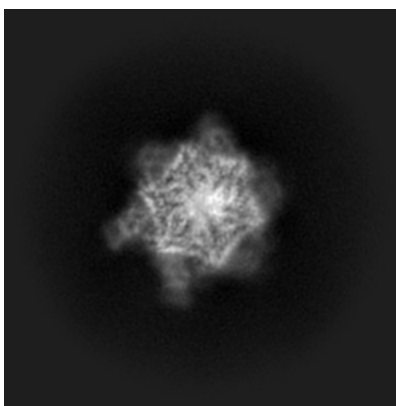
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

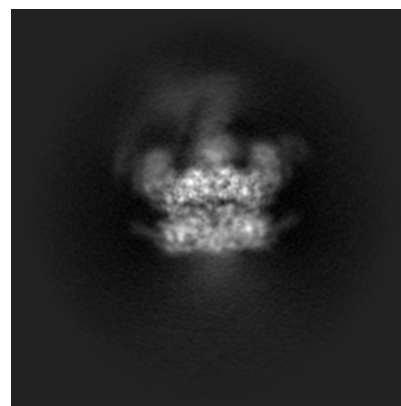
6.1.1 Primary map



X

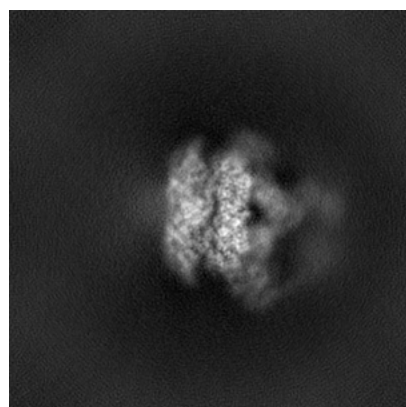


Y

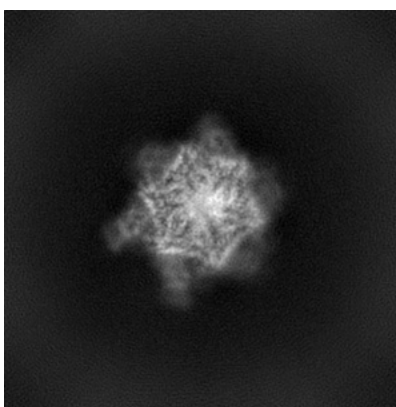


Z

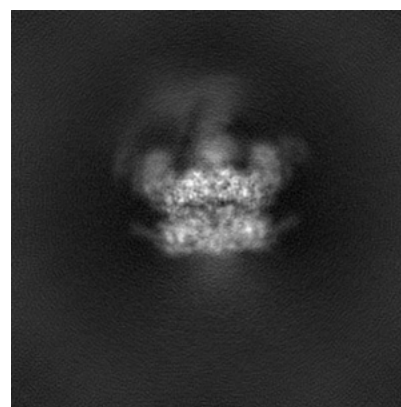
6.1.2 Raw map



X



Y

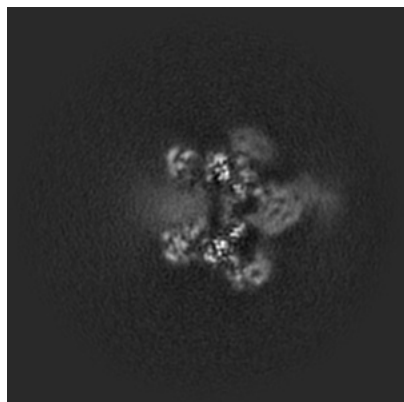


Z

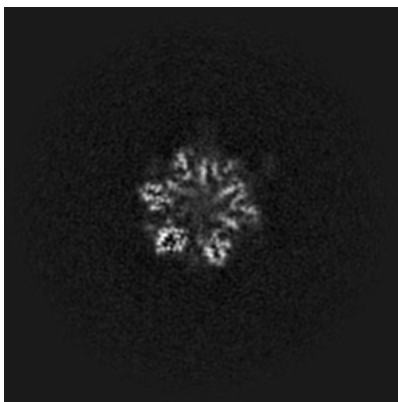
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

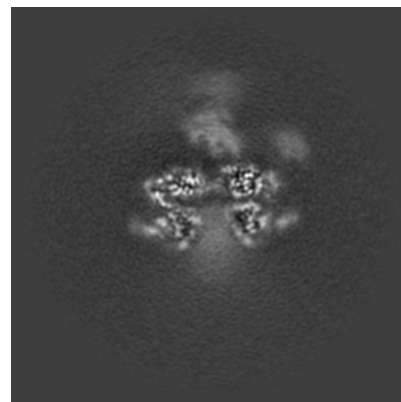
6.2.1 Primary map



X Index: 128

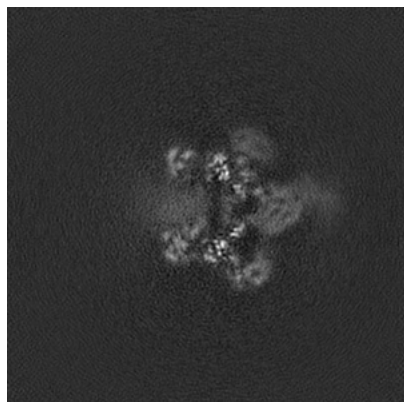


Y Index: 128

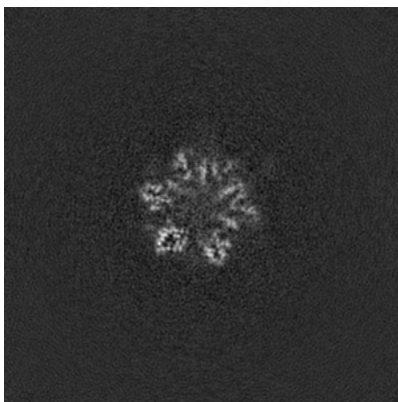


Z Index: 128

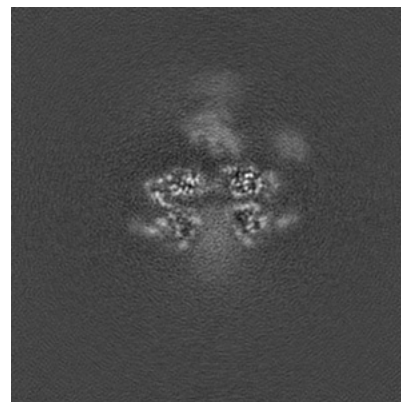
6.2.2 Raw map



X Index: 128



Y Index: 128

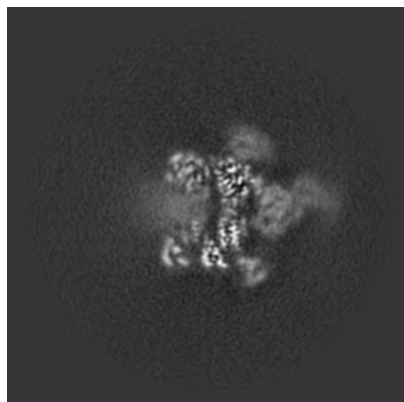


Z Index: 128

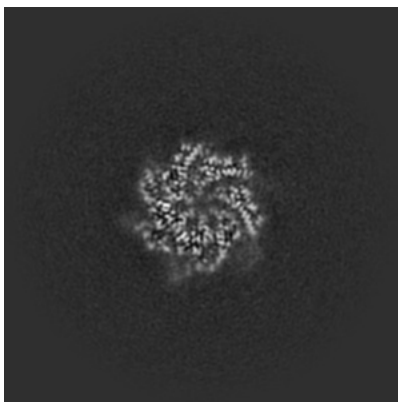
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

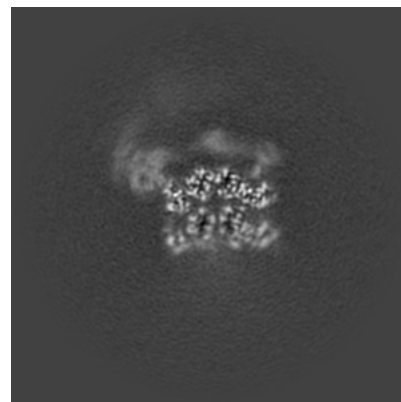
6.3.1 Primary map



X Index: 133

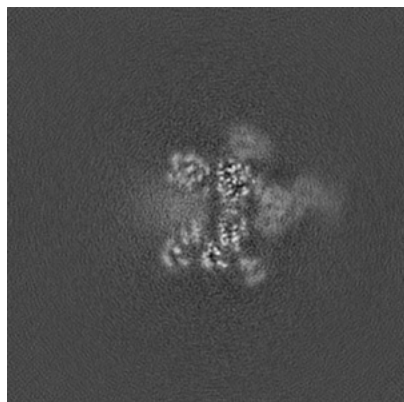


Y Index: 137

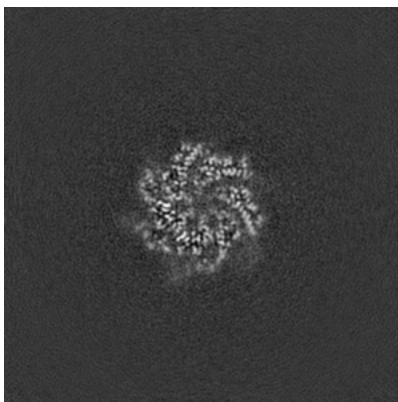


Z Index: 112

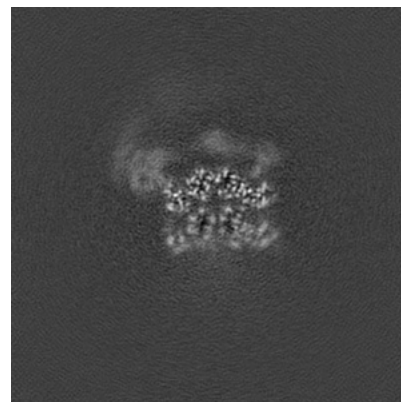
6.3.2 Raw map



X Index: 134



Y Index: 137

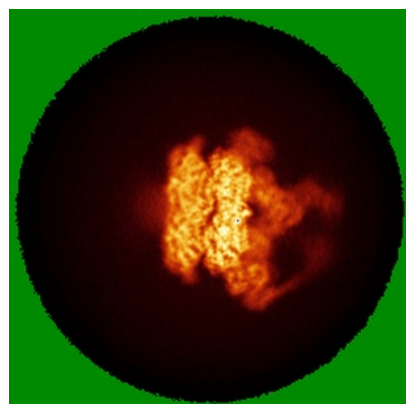


Z Index: 112

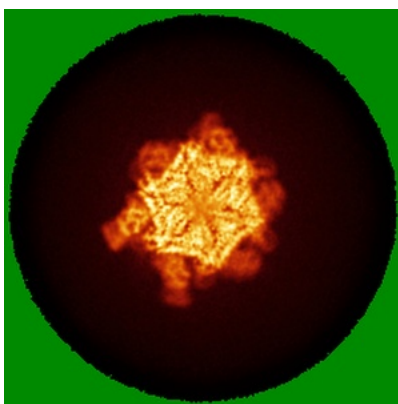
The images above show the largest variance slices of the map in three orthogonal directions.

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

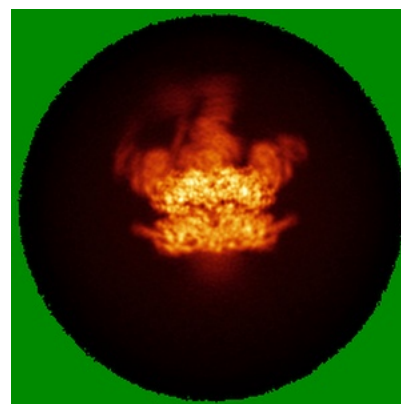
6.4.1 Primary map



X

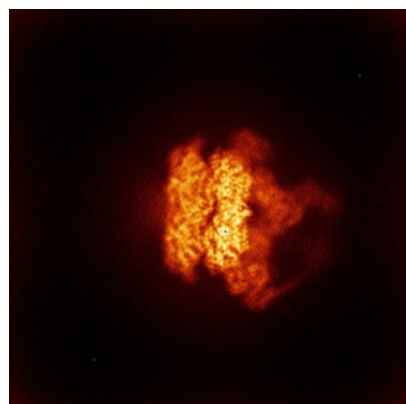


Y

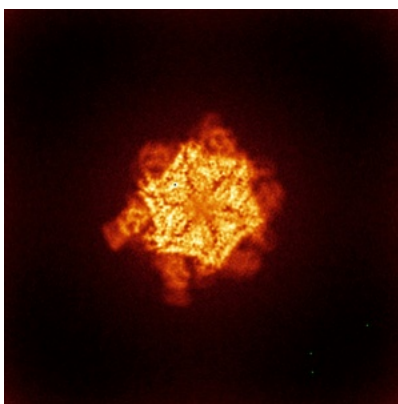


Z

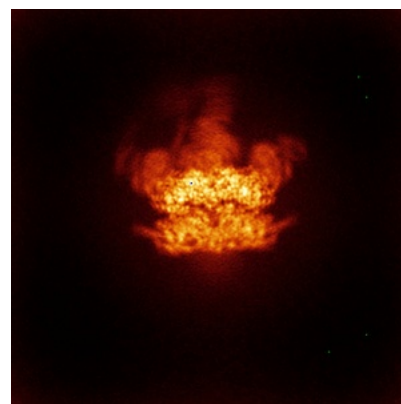
6.4.2 Raw map



X



Y

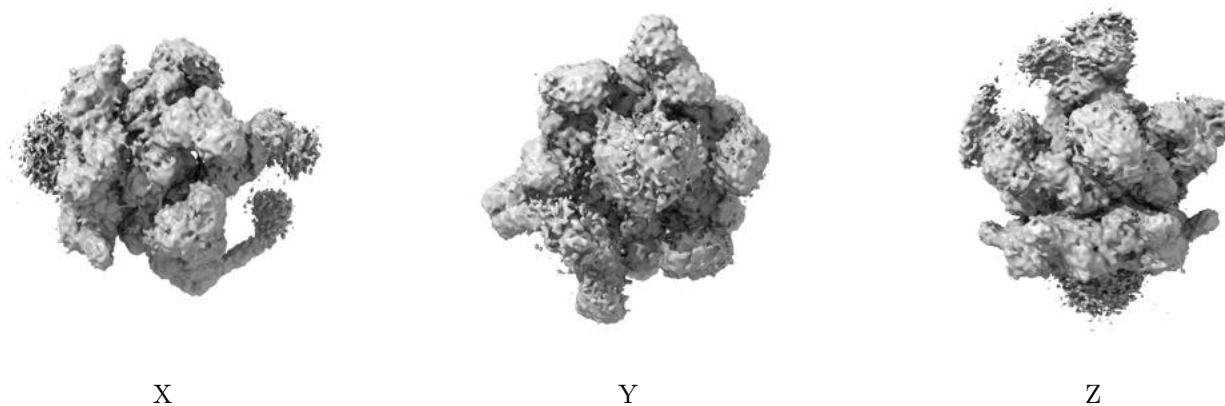


Z

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.

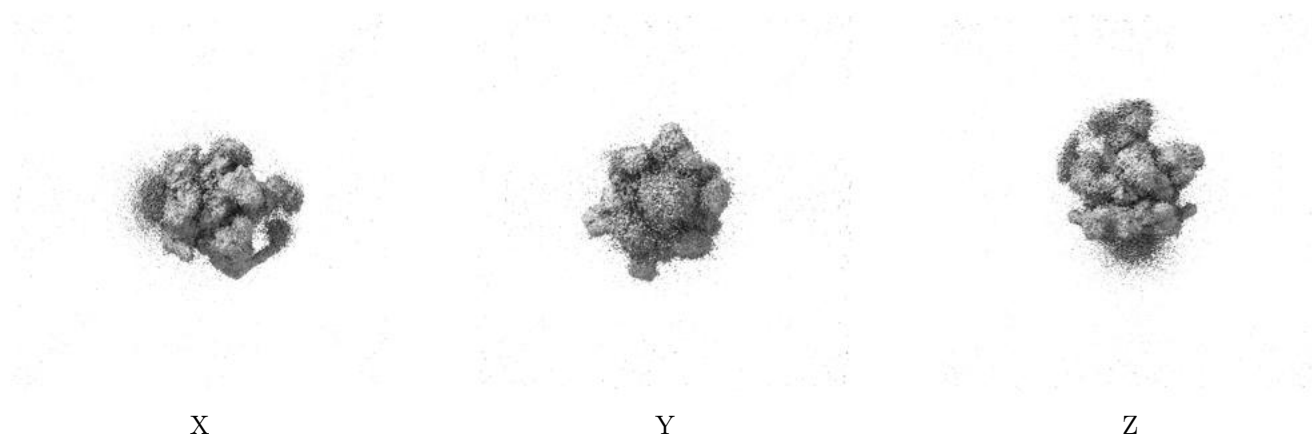
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0682. 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.

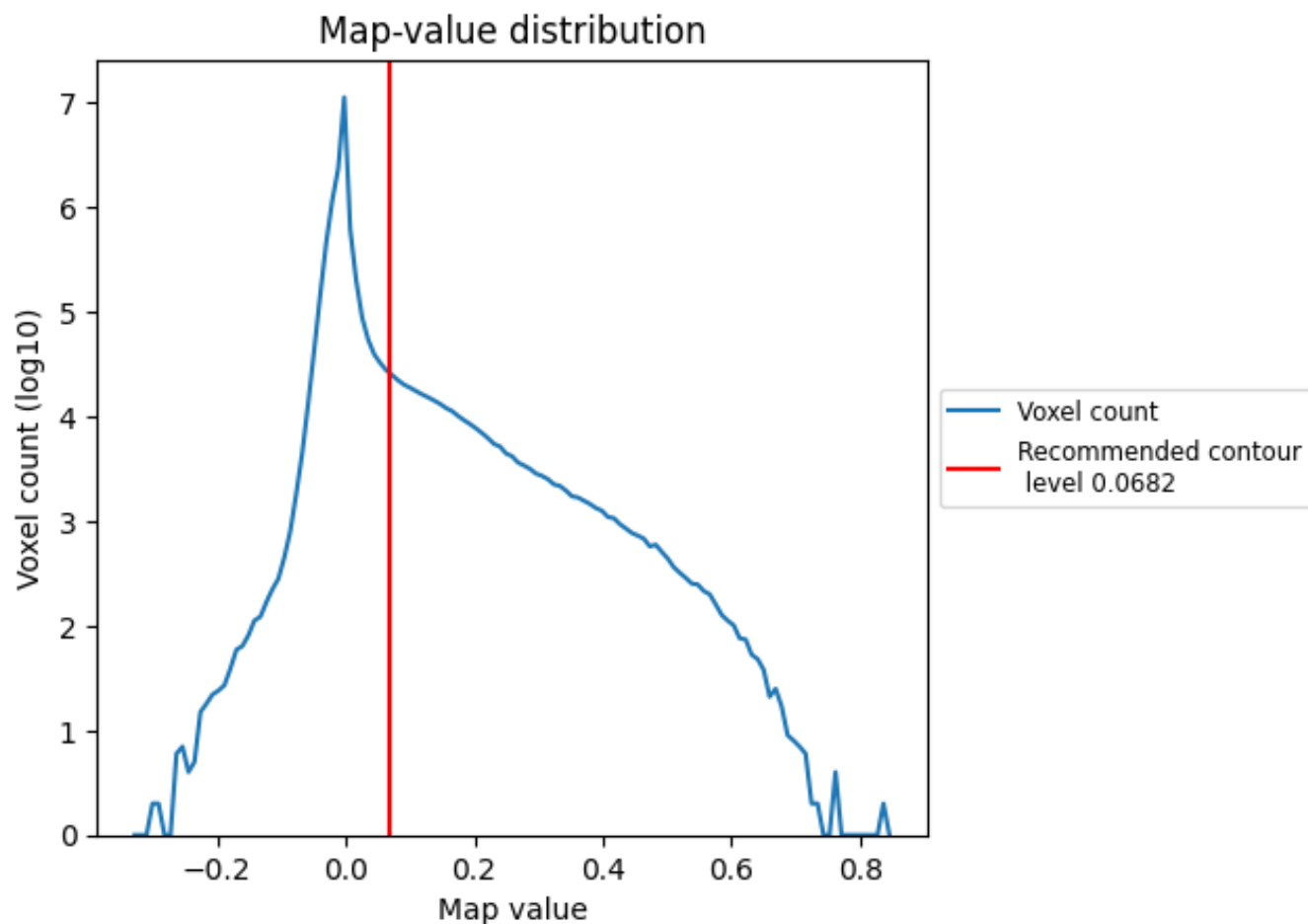
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

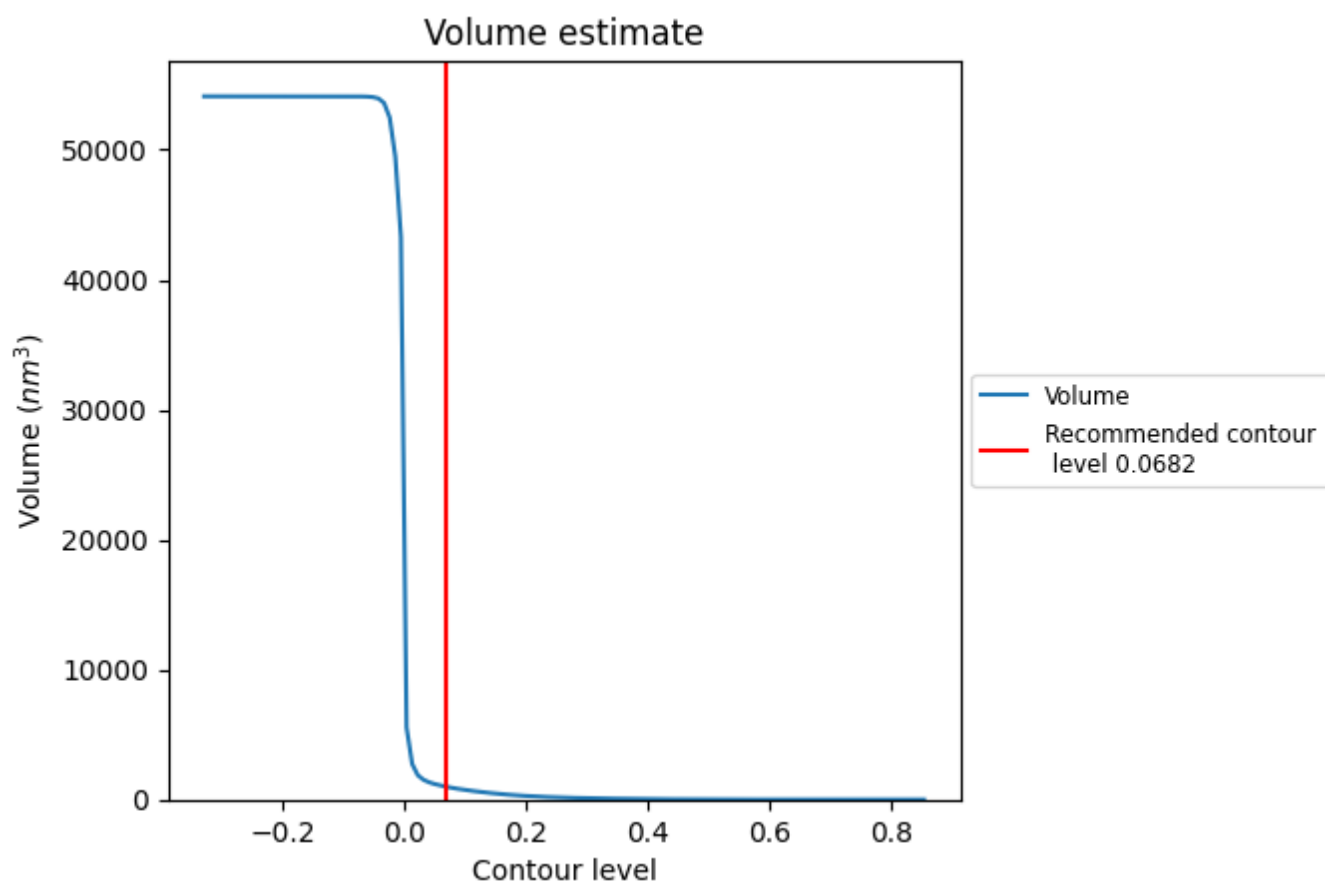
This section contains the results of statistical analysis of the map.

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.

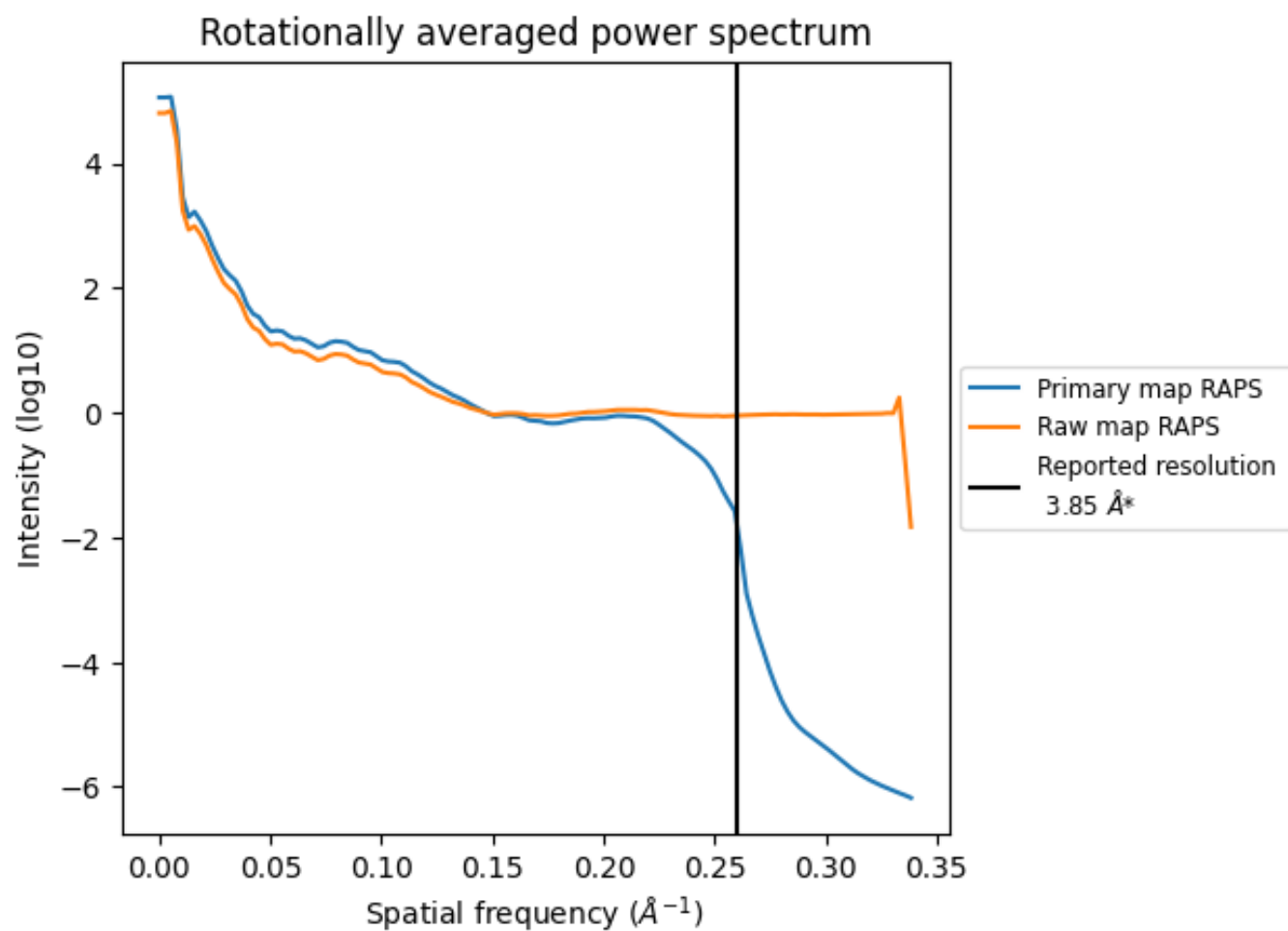
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1001 nm³; this corresponds to an approximate mass of 904 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 ⓘ

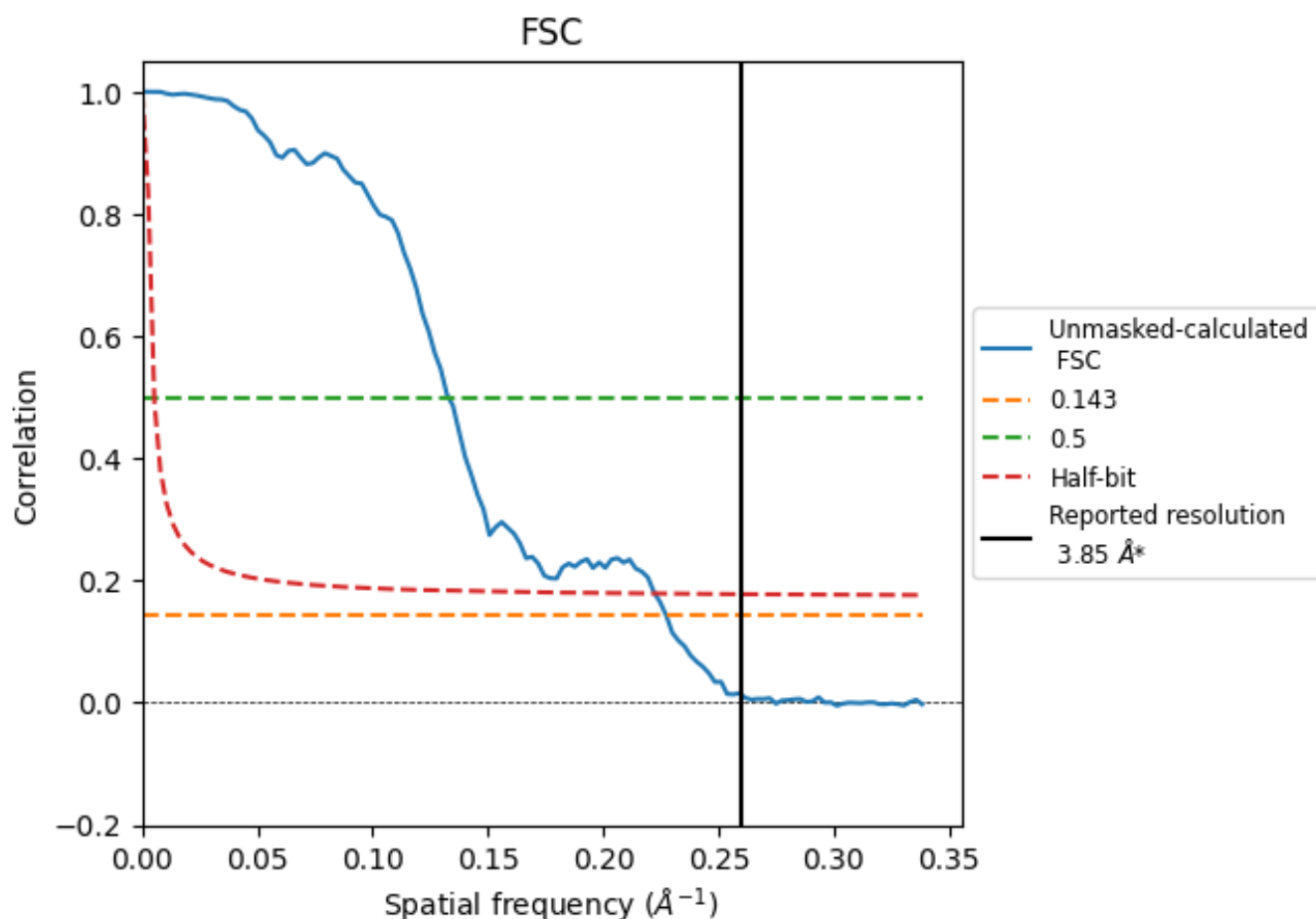


*Reported resolution corresponds to spatial frequency of 0.260 \AA^{-1}

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 0.260 Å⁻¹

8.2 Resolution estimates [i](#)

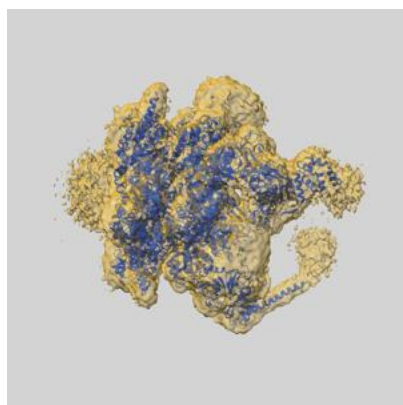
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.85	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.40	7.52	4.50

*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 4.40 differs from the reported value 3.85 by more than 10 %

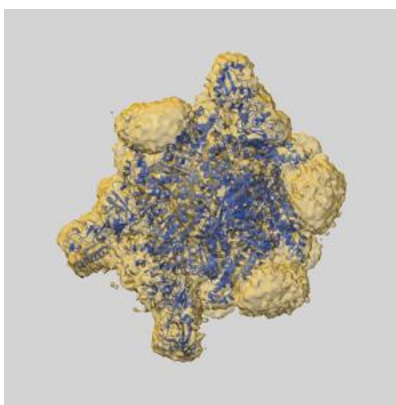
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-76074 and PDB model 11VE. Per-residue inclusion information can be found in section [3](#) on page [10](#).

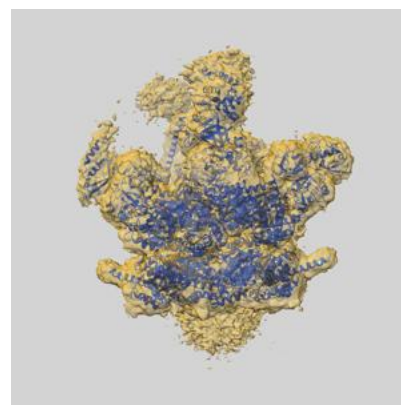
9.1 Map-model overlay [i](#)



X



Y



Z

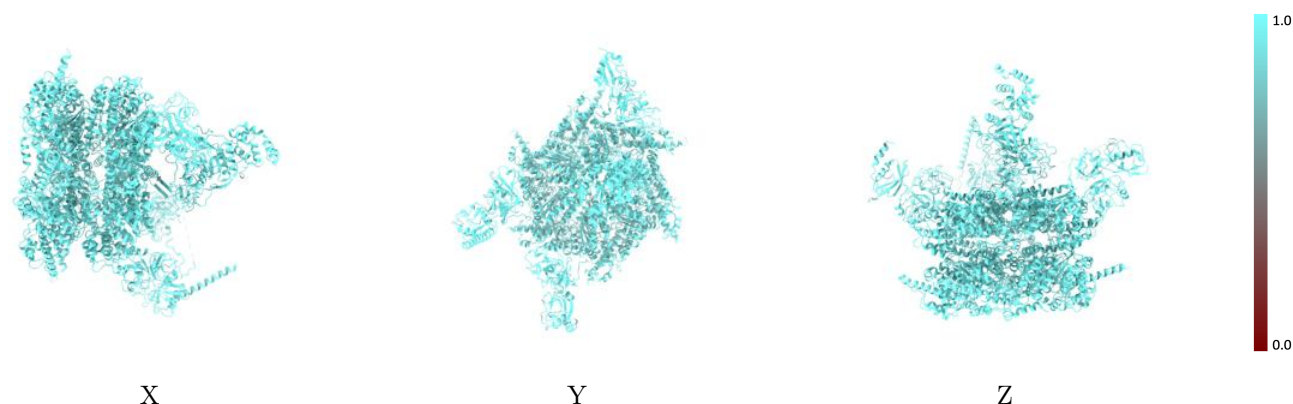
The images above show the 3D surface view of the map at the recommended contour level 0.0682 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



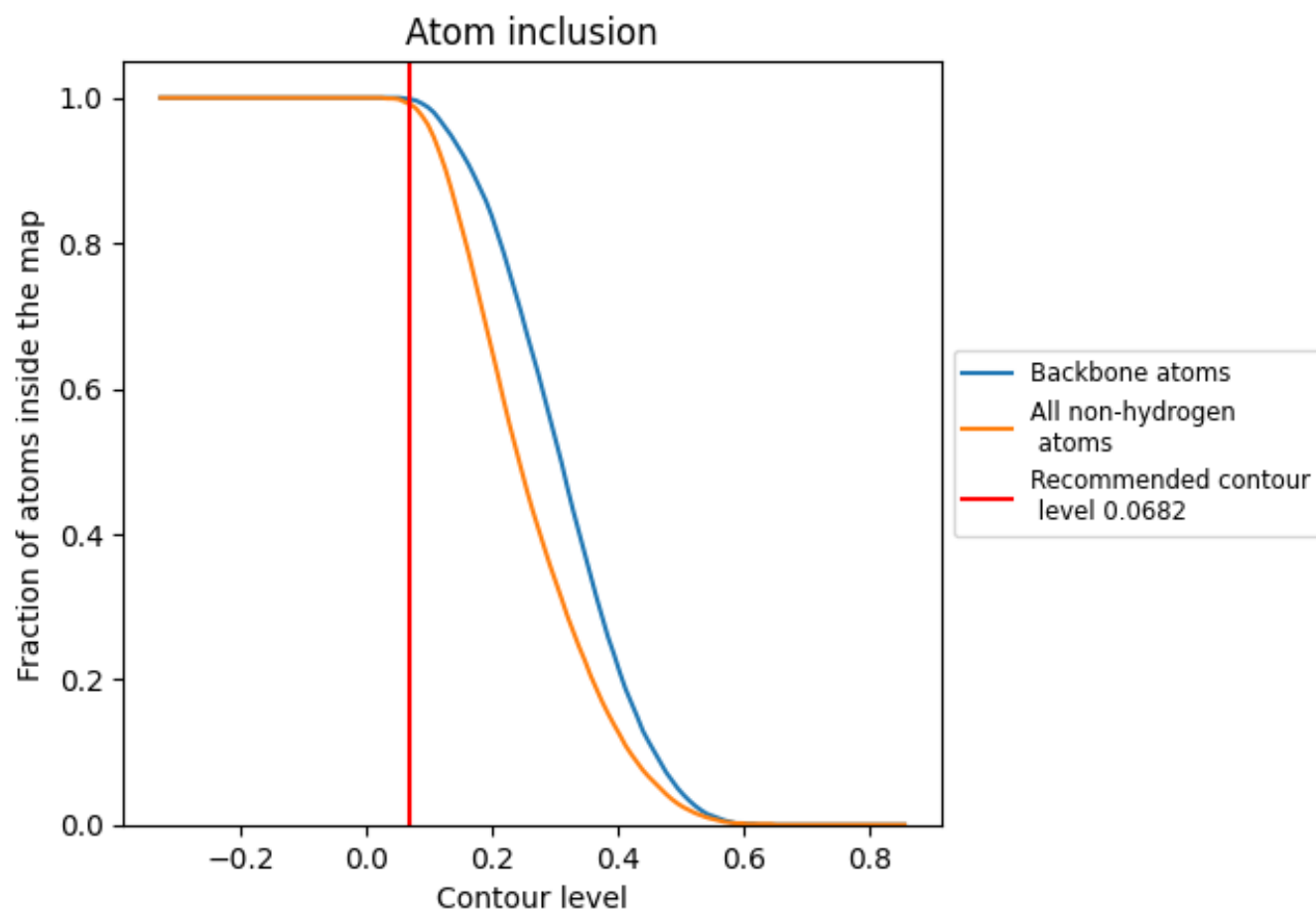
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0682).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 99% 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 (0.0682) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9910	<div><div></div></div> 0.3140
A	<div><div></div></div> 0.9970	<div><div></div></div> 0.3560
B	<div><div></div></div> 0.9930	<div><div></div></div> 0.3520
C	<div><div></div></div> 0.9940	<div><div></div></div> 0.3370
D	<div><div></div></div> 0.9950	<div><div></div></div> 0.3380
E	<div><div></div></div> 0.9930	<div><div></div></div> 0.3350
F	<div><div></div></div> 0.9940	<div><div></div></div> 0.3390
G	<div><div></div></div> 0.9780	<div><div></div></div> 0.1830
M	<div><div></div></div> 0.9860	<div><div></div></div> 0.2170
O	<div><div></div></div> 0.9450	<div><div></div></div> 0.1780
P	<div><div></div></div> 0.9930	<div><div></div></div> 0.1950

1.0

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