



wwPDB EM Validation Summary Report ⓘ

Sep 29, 2025 – 03:58 PM EDT

PDB ID : 9PCX / pdb_00009pcx
EMDB ID : EMD-71521
Title : 22bin20S complex (NSF-alphaSNAP-2:2 syntaxin-1a:SNAP-25), hydrolyzing, class 14
Authors : White, K.I.; Brunger, A.T.
Deposited on : 2025-06-29
Resolution : 4.03 Å(reported)
Based on initial model : 6MDM

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:

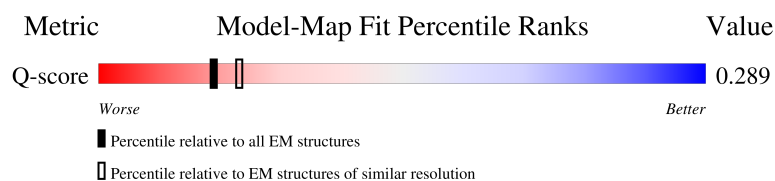
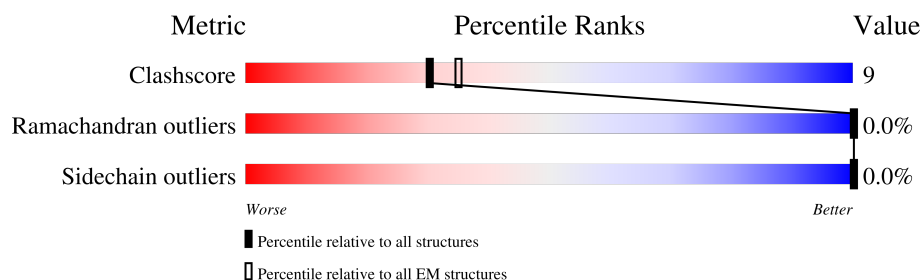
EMDB validation analysis : 0.0.1.dev129
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive 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) : 2.46

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 4.03 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	6618 (3.54 - 4.53)

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	747	
1	B	747	
1	C	747	
1	D	747	

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Mol	Chain	Length	Quality of chain
1	E	747	
1	F	747	
2	G	267	
2	H	267	
3	I	518	
3	J	518	
3	K	518	
3	L	518	
3	M	518	
3	N	518	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 85115 atoms, of which 42740 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 Vesicle-fusing ATPase.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	534	Total	C	H	N	O	S	0	0
			8445	2631	4288	724	779	23		
1	B	721	Total	C	H	N	O	S	0	0
			11358	3551	5746	974	1057	30		
1	C	722	Total	C	H	N	O	S	0	0
			11375	3556	5754	976	1059	30		
1	D	723	Total	C	H	N	O	S	0	0
			11398	3562	5766	980	1060	30		
1	E	722	Total	C	H	N	O	S	0	0
			11374	3556	5753	976	1059	30		
1	F	517	Total	C	H	N	O	S	0	0
			8205	2561	4168	702	752	22		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P18708
A	-1	ALA	-	expression tag	UNP P18708
A	0	HIS	-	expression tag	UNP P18708
B	-2	GLY	-	expression tag	UNP P18708
B	-1	ALA	-	expression tag	UNP P18708
B	0	HIS	-	expression tag	UNP P18708
C	-2	GLY	-	expression tag	UNP P18708
C	-1	ALA	-	expression tag	UNP P18708
C	0	HIS	-	expression tag	UNP P18708
D	-2	GLY	-	expression tag	UNP P18708
D	-1	ALA	-	expression tag	UNP P18708
D	0	HIS	-	expression tag	UNP P18708
E	-2	GLY	-	expression tag	UNP P18708
E	-1	ALA	-	expression tag	UNP P18708
E	0	HIS	-	expression tag	UNP P18708
F	-2	GLY	-	expression tag	UNP P18708
F	-1	ALA	-	expression tag	UNP P18708
F	0	HIS	-	expression tag	UNP P18708

- Molecule 2 is a protein called Syntaxin-1A.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	H	68	Total	C	H	N	O	S	0	0
			1101	345	545	94	112	5		
2	G	80	Total	C	H	N	O	S	0	0
			1263	397	621	108	131	6		

- Molecule 3 is a protein called Synaptosomal-associated protein 25, Synaptosomal-associated protein 25, Alpha-soluble NSF attachment protein chimera.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	I	70	Total	C	H	N	O	S	0	0
			1100	333	547	97	119	4		
3	J	67	Total	C	H	N	O	S	0	0
			1063	319	530	94	116	4		
3	K	289	Total	C	H	N	O	S	0	0
			4501	1435	2229	378	441	18		
3	L	287	Total	C	H	N	O	S	0	0
			4465	1424	2210	375	438	18		
3	M	289	Total	C	H	N	O	S	0	0
			4501	1435	2229	378	441	18		
3	N	287	Total	C	H	N	O	S	0	0
			4465	1424	2210	375	438	18		

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	-15	MET	-	expression tag	UNP P60881
I	-14	GLY	-	expression tag	UNP P60881
I	-13	SER	-	expression tag	UNP P60881
I	-12	SER	-	expression tag	UNP P60881
I	-11	HIS	-	expression tag	UNP P60881
I	-10	HIS	-	expression tag	UNP P60881
I	-9	HIS	-	expression tag	UNP P60881
I	-8	HIS	-	expression tag	UNP P60881
I	-7	HIS	-	expression tag	UNP P60881
I	-6	HIS	-	expression tag	UNP P60881
I	-5	SER	-	expression tag	UNP P60881
I	-4	GLN	-	expression tag	UNP P60881
I	-3	ASP	-	expression tag	UNP P60881
I	-2	PRO	-	expression tag	UNP P60881
I	-1	ASN	-	expression tag	UNP P60881
I	0	SER	-	expression tag	UNP P60881
I	85	ALA	CYS	conflict	UNP P60881

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Chain	Residue	Modelled	Actual	Comment	Reference
I	88	ALA	CYS	conflict	UNP P60881
I	90	ALA	CYS	conflict	UNP P60881
I	92	ALA	CYS	conflict	UNP P60881
I	207	GLY	-	linker	UNP P60881
J	-15	MET	-	expression tag	UNP P60881
J	-14	GLY	-	expression tag	UNP P60881
J	-13	SER	-	expression tag	UNP P60881
J	-12	SER	-	expression tag	UNP P60881
J	-11	HIS	-	expression tag	UNP P60881
J	-10	HIS	-	expression tag	UNP P60881
J	-9	HIS	-	expression tag	UNP P60881
J	-8	HIS	-	expression tag	UNP P60881
J	-7	HIS	-	expression tag	UNP P60881
J	-6	HIS	-	expression tag	UNP P60881
J	-5	SER	-	expression tag	UNP P60881
J	-4	GLN	-	expression tag	UNP P60881
J	-3	ASP	-	expression tag	UNP P60881
J	-2	PRO	-	expression tag	UNP P60881
J	-1	ASN	-	expression tag	UNP P60881
J	0	SER	-	expression tag	UNP P60881
J	85	ALA	CYS	conflict	UNP P60881
J	88	ALA	CYS	conflict	UNP P60881
J	90	ALA	CYS	conflict	UNP P60881
J	92	ALA	CYS	conflict	UNP P60881
J	207	GLY	-	linker	UNP P60881
K	-222	MET	-	expression tag	UNP P60881
K	-221	GLY	-	expression tag	UNP P60881
K	-220	SER	-	expression tag	UNP P60881
K	-219	SER	-	expression tag	UNP P60881
K	-218	HIS	-	expression tag	UNP P60881
K	-217	HIS	-	expression tag	UNP P60881
K	-216	HIS	-	expression tag	UNP P60881
K	-215	HIS	-	expression tag	UNP P60881
K	-214	HIS	-	expression tag	UNP P60881
K	-213	HIS	-	expression tag	UNP P60881
K	-212	SER	-	expression tag	UNP P60881
K	-211	GLN	-	expression tag	UNP P60881
K	-210	ASP	-	expression tag	UNP P60881
K	-209	PRO	-	expression tag	UNP P60881
K	-208	ASN	-	expression tag	UNP P60881
K	-207	SER	-	expression tag	UNP P60881
K	-122	ALA	CYS	conflict	UNP P60881

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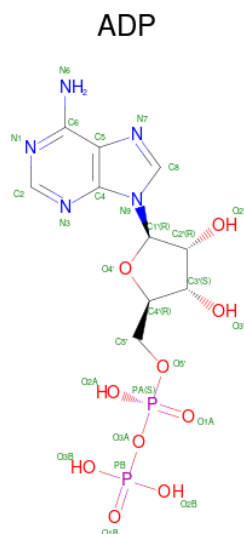
Chain	Residue	Modelled	Actual	Comment	Reference
K	-119	ALA	CYS	conflict	UNP P60881
K	-117	ALA	CYS	conflict	UNP P60881
K	-115	ALA	CYS	conflict	UNP P60881
K	0	GLY	-	linker	UNP P60881
L	-222	MET	-	expression tag	UNP P60881
L	-221	GLY	-	expression tag	UNP P60881
L	-220	SER	-	expression tag	UNP P60881
L	-219	SER	-	expression tag	UNP P60881
L	-218	HIS	-	expression tag	UNP P60881
L	-217	HIS	-	expression tag	UNP P60881
L	-216	HIS	-	expression tag	UNP P60881
L	-215	HIS	-	expression tag	UNP P60881
L	-214	HIS	-	expression tag	UNP P60881
L	-213	HIS	-	expression tag	UNP P60881
L	-212	SER	-	expression tag	UNP P60881
L	-211	GLN	-	expression tag	UNP P60881
L	-210	ASP	-	expression tag	UNP P60881
L	-209	PRO	-	expression tag	UNP P60881
L	-208	ASN	-	expression tag	UNP P60881
L	-207	SER	-	expression tag	UNP P60881
L	-122	ALA	CYS	conflict	UNP P60881
L	-119	ALA	CYS	conflict	UNP P60881
L	-117	ALA	CYS	conflict	UNP P60881
L	-115	ALA	CYS	conflict	UNP P60881
L	0	GLY	-	linker	UNP P60881
M	-222	MET	-	expression tag	UNP P60881
M	-221	GLY	-	expression tag	UNP P60881
M	-220	SER	-	expression tag	UNP P60881
M	-219	SER	-	expression tag	UNP P60881
M	-218	HIS	-	expression tag	UNP P60881
M	-217	HIS	-	expression tag	UNP P60881
M	-216	HIS	-	expression tag	UNP P60881
M	-215	HIS	-	expression tag	UNP P60881
M	-214	HIS	-	expression tag	UNP P60881
M	-213	HIS	-	expression tag	UNP P60881
M	-212	SER	-	expression tag	UNP P60881
M	-211	GLN	-	expression tag	UNP P60881
M	-210	ASP	-	expression tag	UNP P60881
M	-209	PRO	-	expression tag	UNP P60881
M	-208	ASN	-	expression tag	UNP P60881
M	-207	SER	-	expression tag	UNP P60881
M	-122	ALA	CYS	conflict	UNP P60881

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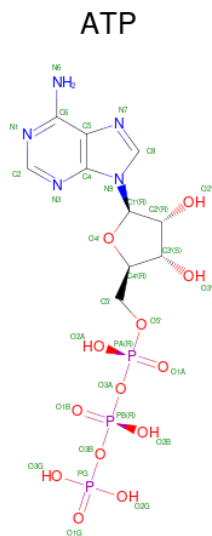
Chain	Residue	Modelled	Actual	Comment	Reference
M	-119	ALA	CYS	conflict	UNP P60881
M	-117	ALA	CYS	conflict	UNP P60881
M	-115	ALA	CYS	conflict	UNP P60881
M	0	GLY	-	linker	UNP P60881
N	-222	MET	-	expression tag	UNP P60881
N	-221	GLY	-	expression tag	UNP P60881
N	-220	SER	-	expression tag	UNP P60881
N	-219	SER	-	expression tag	UNP P60881
N	-218	HIS	-	expression tag	UNP P60881
N	-217	HIS	-	expression tag	UNP P60881
N	-216	HIS	-	expression tag	UNP P60881
N	-215	HIS	-	expression tag	UNP P60881
N	-214	HIS	-	expression tag	UNP P60881
N	-213	HIS	-	expression tag	UNP P60881
N	-212	SER	-	expression tag	UNP P60881
N	-211	GLN	-	expression tag	UNP P60881
N	-210	ASP	-	expression tag	UNP P60881
N	-209	PRO	-	expression tag	UNP P60881
N	-208	ASN	-	expression tag	UNP P60881
N	-207	SER	-	expression tag	UNP P60881
N	-122	ALA	CYS	conflict	UNP P60881
N	-119	ALA	CYS	conflict	UNP P60881
N	-117	ALA	CYS	conflict	UNP P60881
N	-115	ALA	CYS	conflict	UNP P60881
N	0	GLY	-	linker	UNP P60881

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



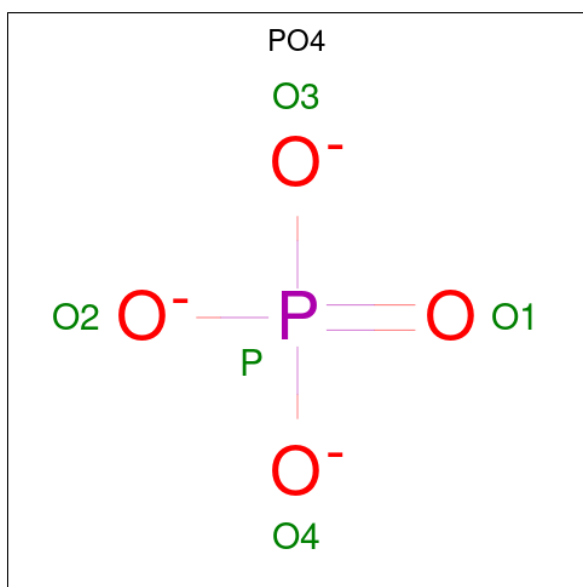
Mol	Chain	Residues	Atoms						AltConf
4	A	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
4	B	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
4	C	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
4	D	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
4	F	1	Total 39	C 10	H 12	N 5	O 10	P 2	0

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$) (labeled as "Ligand of Interest" by depositor).

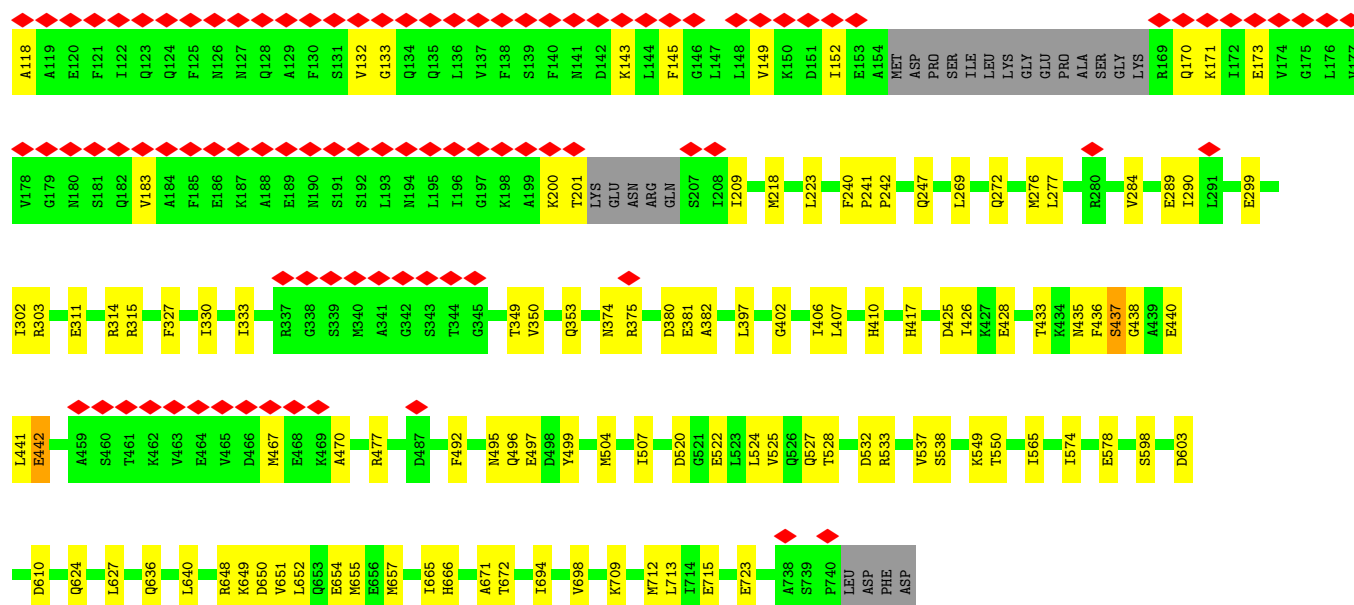


Mol	Chain	Residues	Atoms						AltConf
5	A	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
5	B	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
5	C	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
5	D	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
5	E	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
5	E	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
5	F	1	Total 43	C 10	H 12	N 5	O 13	P 3	0

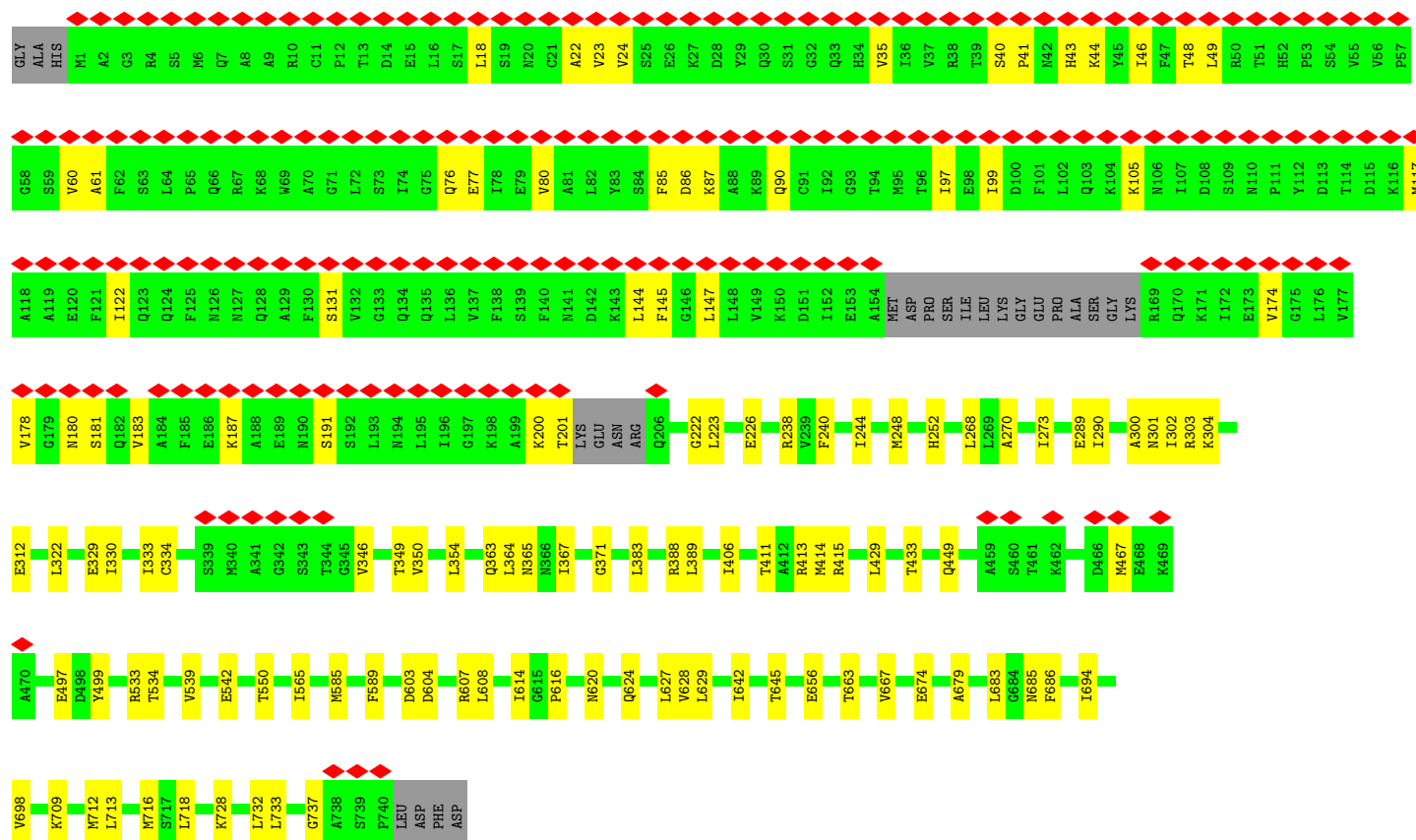
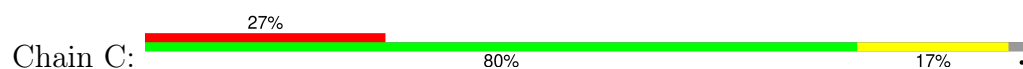
- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P) (labeled as "Ligand of Interest" by depositor).



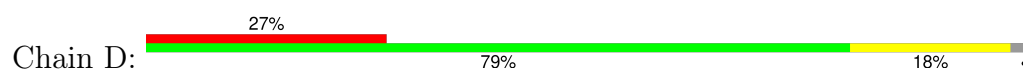
Mol	Chain	Residues	Atoms			AltConf
			Total	O	P	
6	C	1	5	4	1	0

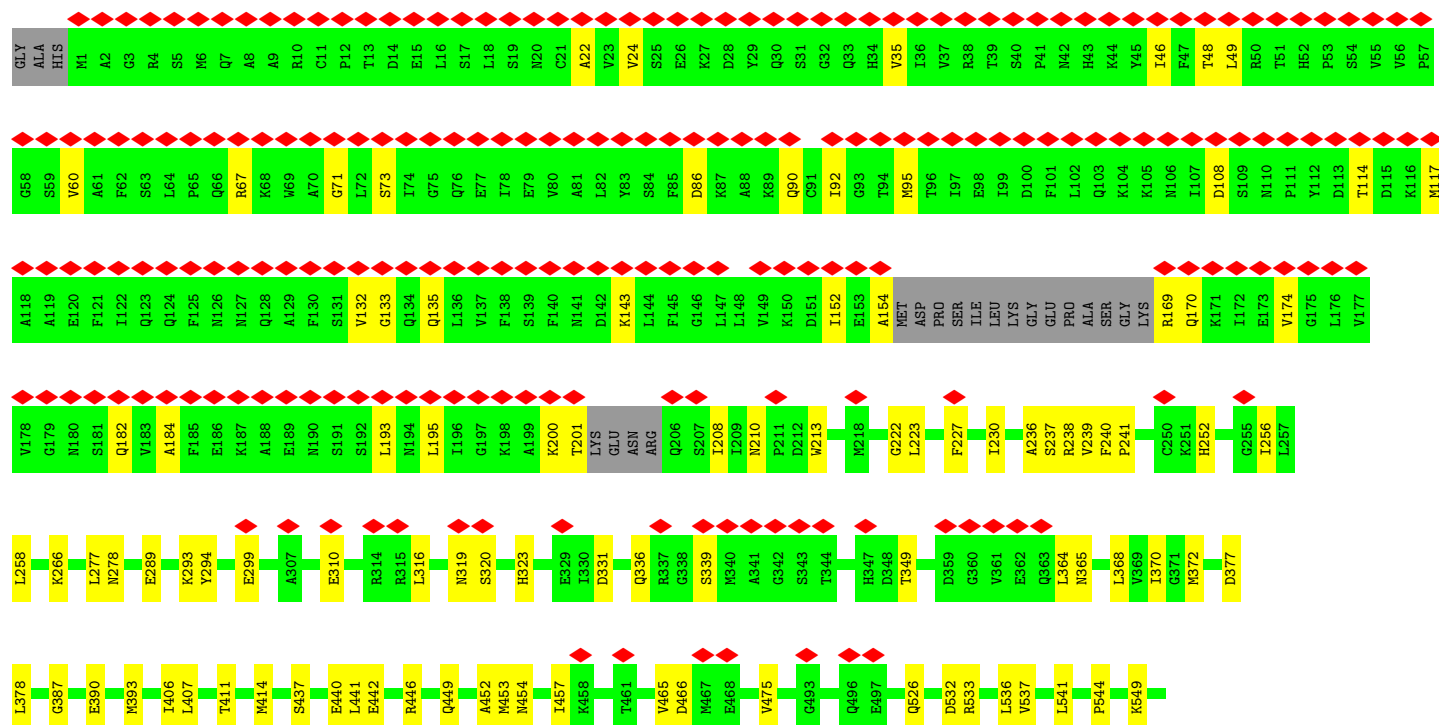


• Molecule 1: Vesicle-fusing ATPase



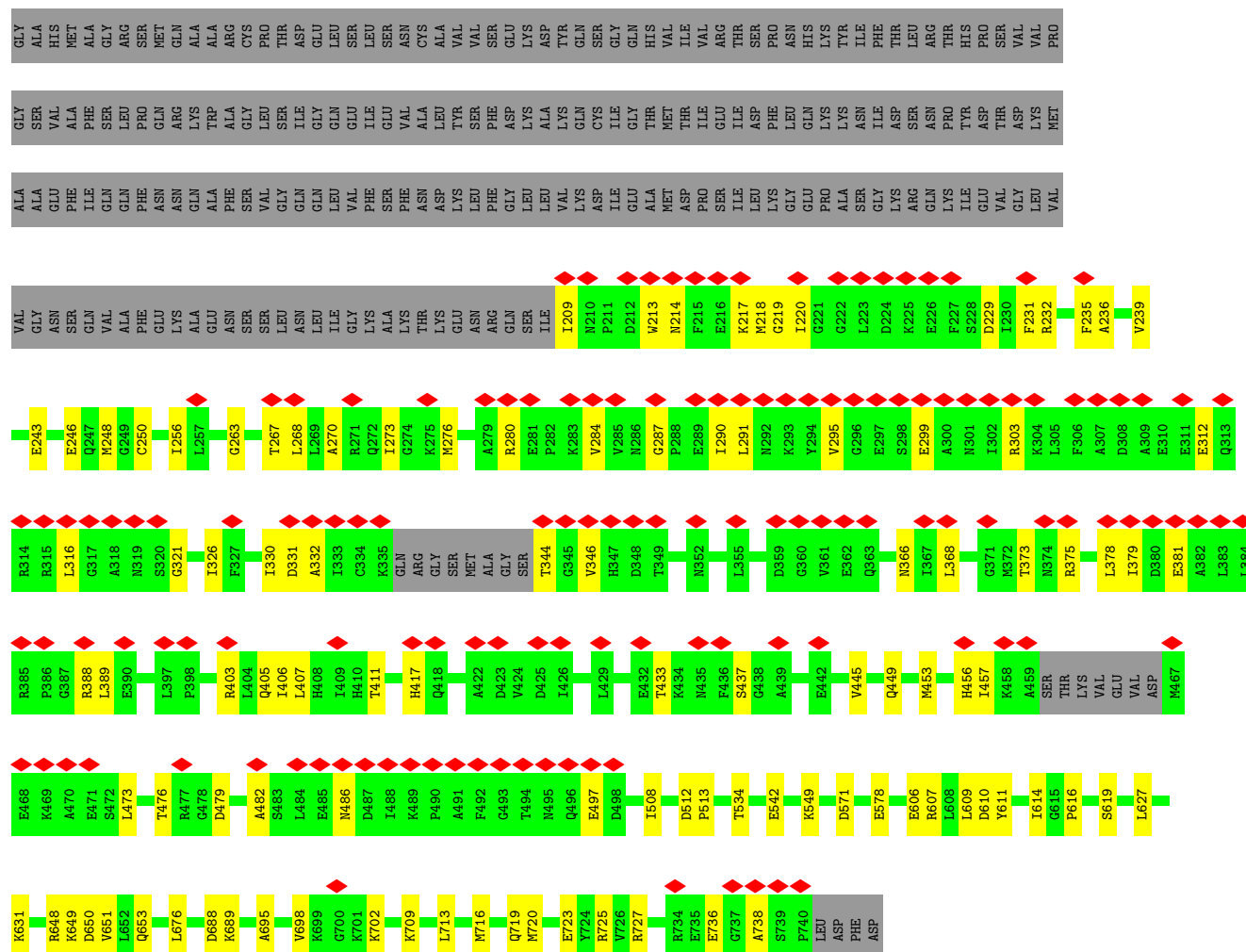
• Molecule 1: Vesicle-fusing ATPase



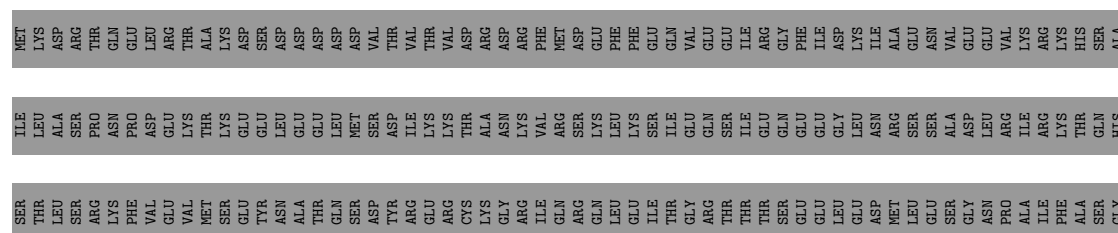


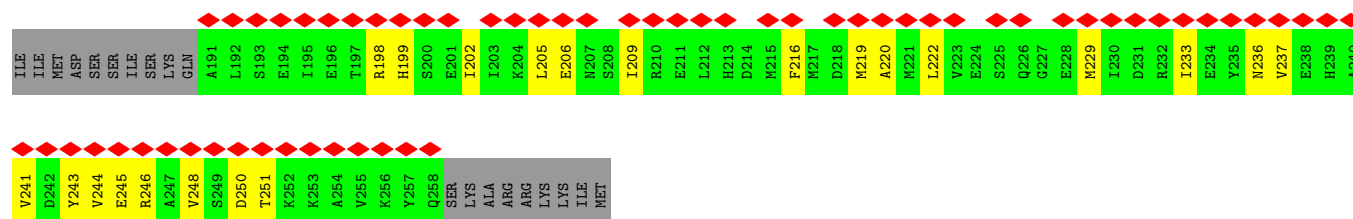


• Molecule 1: Vesicle-fusing ATPase

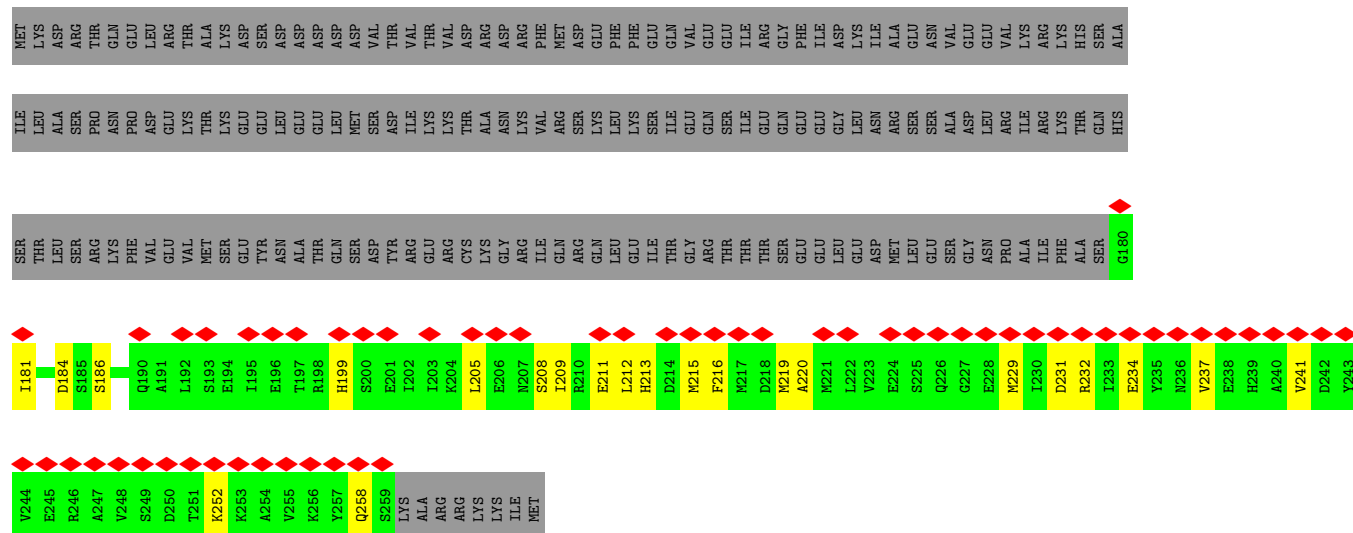


• Molecule 2: Syntaxin-1A

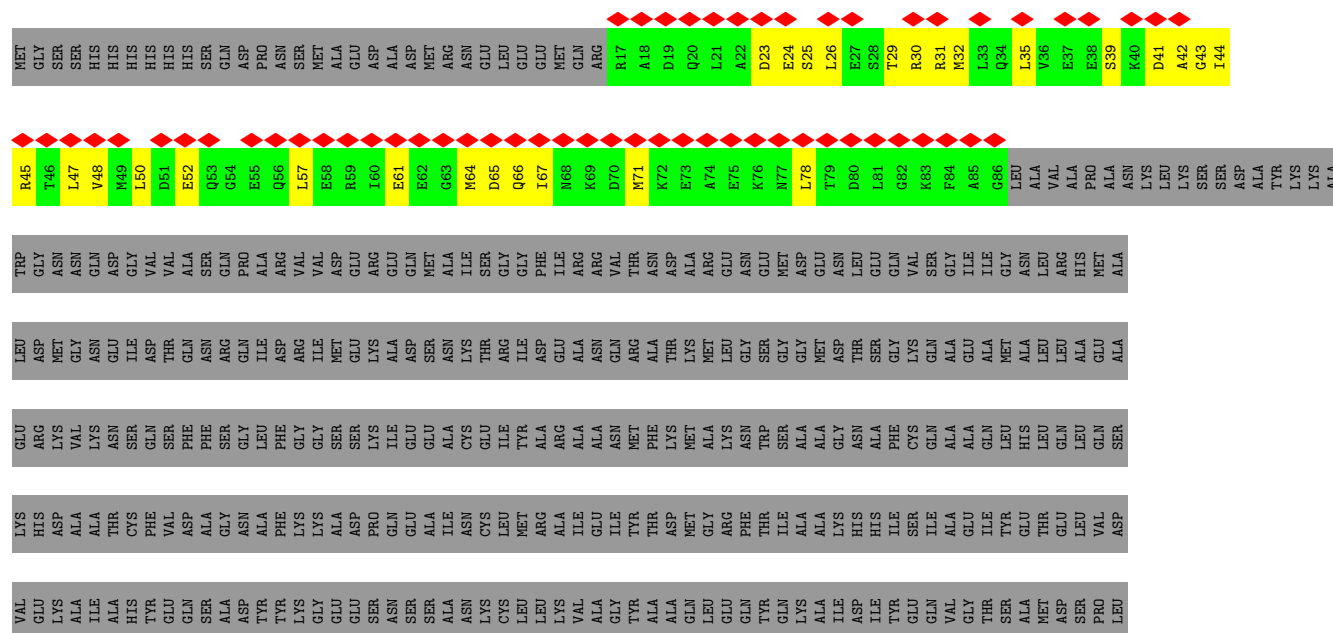




• Molecule 2: Syntaxin-1A



• Molecule 3: Synaptosomal-associated protein 25, Synaptosomal-associated protein 25, Alpha-soluble NSF attachment protein chimera



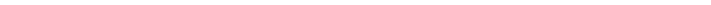
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- Molecule 3: Synaptosomal-associated protein 25, Synaptosomal-associated protein 25, Alpha-soluble NSF attachment protein chimera

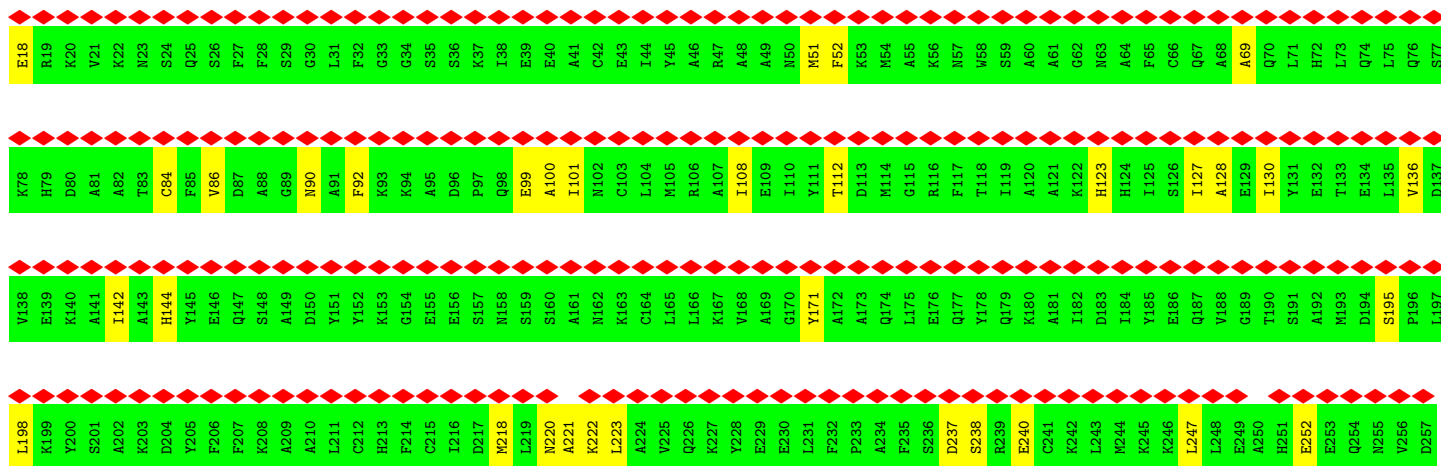
Chain J:  13% 9% 87%

[illegible]

- Molecule 3: Synaptosomal-associated protein 25, Synaptosomal-associated protein 25, Alpha-soluble NSF attachment protein chimera

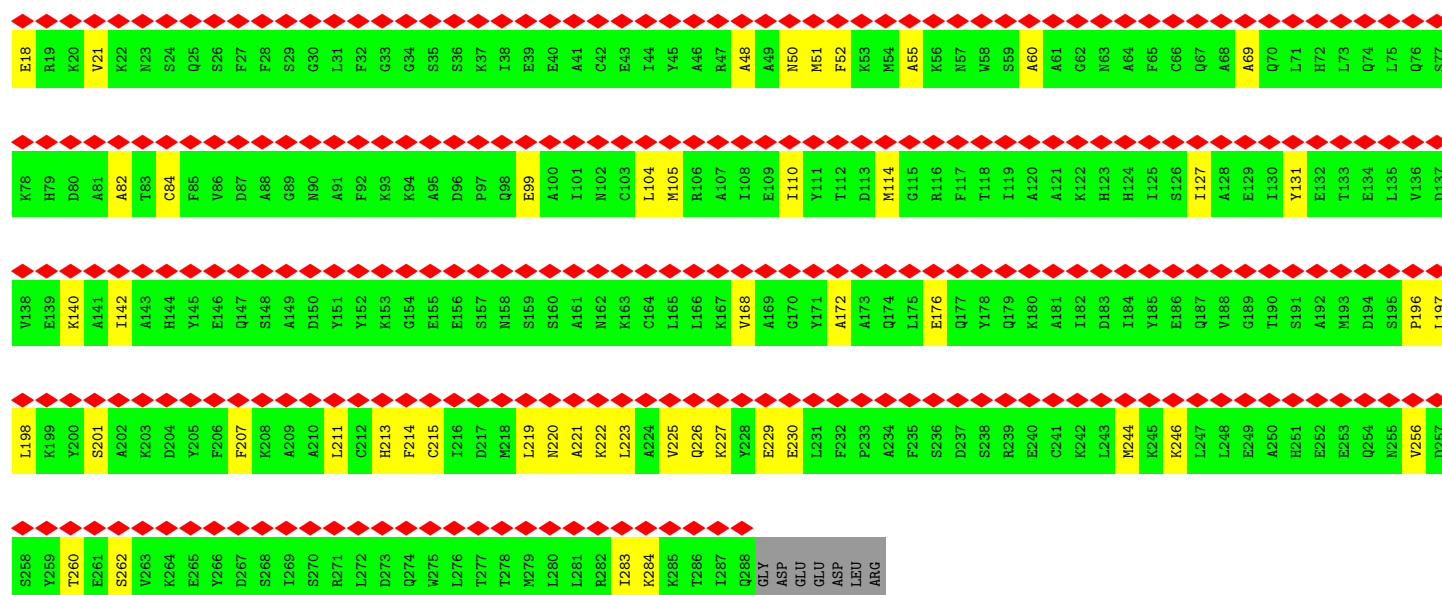
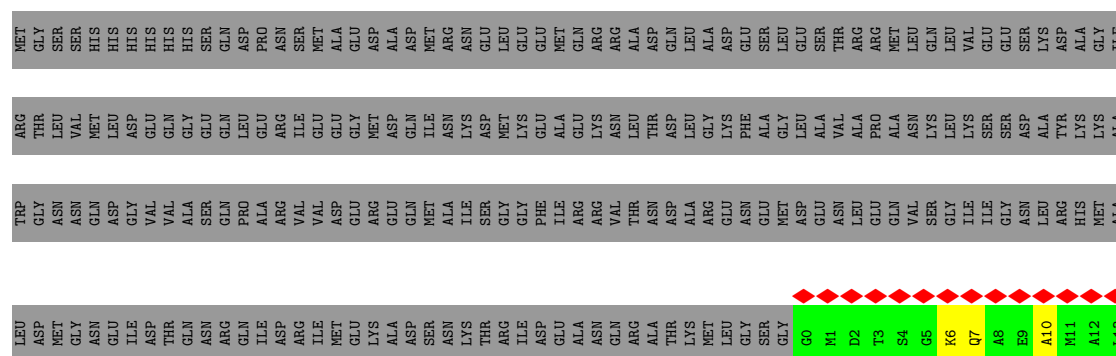
Chain K: 

[illegible]

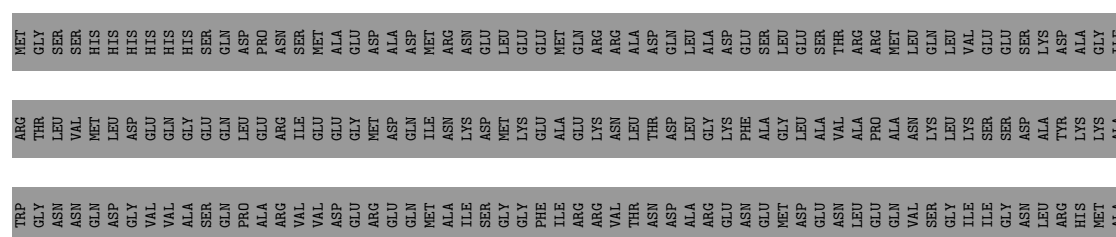




- Molecule 3: Synaptosomal-associated protein 25, Synaptosomal-associated protein 25, Alpha-soluble NSF attachment protein chimera



- Molecule 3: Synaptosomal-associated protein 25, Synaptosomal-associated protein 25, Alpha-soluble NSF attachment protein chimera



S258	L198	V138	K78	E18	LEU
S259	K199	E139	H79	R19	ASP
T260	Y200	K140	D80	K20	MET
E261	S201	A141	A81	V21	GLY
S262	A202	I142			ASN
S263	K203	A143	T83	K22	GLU
K264	D204	H144	C84	N23	ILE
E265	Y205	E145	F85	S24	ASP
Y266	F206	E146	V86	Q25	THR
D267	F207	Q147	D87	S26	GLN
S268	K208	S148	A88	F27	ARG
L269	A209	A149	G89	S28	ASP
S270	A210	D150	N90	S29	ARG
K271	L211	Y151	A91	G30	ILE
L272	C212	Y152	F92	L31	MET
D273	H213	K153	K93	F32	GLY
Q274	F214	G154	K94	G33	ALA
W275	C215	E155	A95	G34	ALA
L276	I216	E156	D96	S35	ASP
T277	D217	S157	P97	S36	SER
T278	M218	N158	Q98	K37	ASN
M279	L219	S159	E99	I38	LYS
L280	N220	S160	A100	I39	ASN
L281	A221	A161	I101	E40	GLN
R282	K222	N162	N102	A41	ARG
L283	L223	K163	C103	E42	ALA
K284	A224	C164	L104	E43	ALA
K285	V225	L165	M105	I44	ALA
T286	Q226	L166	Y45	Y46	THR
ILE	K227	K167	R106	A47	LYS
GLN	Y228	V168	A107	R47	LYS
GLY	E229	A169	I108	A48	MET
ASP	E230	G170	E109	A49	LEU
GLU	L231	Y171	Y111	N50	GLY
ASP	F232	A172	T112	M51	SER
LEU	P233	A173	D113	F52	GLY
ARG	A234	Q174	M114	K53	
	F235	L175	G115	M54	
	S236	E176	R116	A55	
	D237	Q177	F117	K56	
	S238	Y178	T118	N57	
	R239	Q179	I119	W58	
	E240	K180	A120	S59	
	C241	A181	A121	A60	
	K242	I182	K122	A61	
	L243	D183	H123	G62	
	M244	I184	H124	N63	
	K245	Y185	I125	A64	
	K246	E186	S126	F65	
	L247	Q187	I127	C66	
	L248	V188	A128	Q67	
	E249	G189	E129	A68	
	A250	T190	I130	A69	
	H251	S191	Y131	Q70	
	E252	A192	E132	L71	
	E253	M193	T133	H72	
	Q254	D194	E134	L73	
	M255	S195	L135	Q74	
	V256	P196	V136	L75	
	P257	L197	D137	Q76	
				S77	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50776	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 ($e^-/\text{\AA}^2$)	33.960	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	22500	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.643	Depositor
Minimum map value	-0.917	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.054	Depositor
Recommended contour level	0.3	Depositor
Map size (\AA)	322.224, 322.224, 322.224	wwPDB
Map dimensions	294, 294, 294	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.096, 1.096, 1.096	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, PO4, 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	0.14	0/4220	0.31	0/5687
1	B	0.20	2/5699 (0.0%)	0.33	0/7680
1	C	0.19	1/5708 (0.0%)	0.31	0/7692
1	D	0.14	0/5719	0.31	0/7706
1	E	0.13	0/5708	0.30	0/7692
1	F	0.14	0/4098	0.32	0/5521
2	G	0.15	0/648	0.34	0/867
2	H	0.17	0/562	0.39	0/753
3	I	0.17	0/553	0.37	0/735
3	J	0.16	0/532	0.33	0/707
3	K	0.19	0/2312	0.31	0/3107
3	L	0.11	0/2295	0.23	0/3084
3	M	0.12	0/2312	0.28	0/3107
3	N	0.16	0/2295	0.36	0/3084
All	All	0.16	3/42661 (0.0%)	0.31	0/57422

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	87	LYS	C-N	8.32	1.45	1.34
1	B	442	GLU	C-N	5.69	1.41	1.33
1	B	435	ASN	C-N	5.25	1.40	1.33

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	4157	4288	4288	76	0
1	B	5612	5746	5746	98	0
1	C	5621	5754	5754	99	0
1	D	5632	5766	5767	105	0
1	E	5621	5753	5754	93	0
1	F	4037	4168	4166	84	0
2	G	642	621	634	26	0
2	H	556	545	544	22	0
3	I	553	547	546	34	0
3	J	533	530	529	23	0
3	K	2272	2229	2231	52	0
3	L	2255	2210	2212	39	0
3	M	2272	2229	2231	38	0
3	N	2255	2210	2212	44	0
4	A	27	12	12	1	0
4	B	27	12	12	0	0
4	C	27	12	12	1	0
4	D	27	12	12	0	0
4	F	27	12	12	1	0
5	A	31	12	12	1	0
5	B	31	12	12	1	0
5	C	31	12	12	0	0
5	D	31	12	12	0	0
5	E	62	24	24	1	0
5	F	31	12	12	2	0
6	C	5	0	0	0	0
All	All	42375	42740	42758	746	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 746 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)
3:I:67:ILE:HG22	3:I:71:MET:HE1	1.42	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:220:ALA:HB1	3:M:197:LEU:HD12	1.56	0.87
1:E:46:ILE:HD12	1:E:174:VAL:HG21	1.60	0.83
1:E:237:SER:HG	1:E:252:HIS:HD1	1.19	0.83
2:H:229:MET:HE2	3:I:57:LEU:HD23	1.62	0.81

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	532/747 (71%)	500 (94%)	31 (6%)	1 (0%)	44	76
1	B	715/747 (96%)	674 (94%)	41 (6%)	0	100	100
1	C	716/747 (96%)	681 (95%)	35 (5%)	0	100	100
1	D	717/747 (96%)	688 (96%)	28 (4%)	1 (0%)	48	81
1	E	716/747 (96%)	672 (94%)	44 (6%)	0	100	100
1	F	511/747 (68%)	484 (95%)	27 (5%)	0	100	100
2	G	78/267 (29%)	76 (97%)	2 (3%)	0	100	100
2	H	66/267 (25%)	66 (100%)	0	0	100	100
3	I	68/518 (13%)	68 (100%)	0	0	100	100
3	J	65/518 (12%)	65 (100%)	0	0	100	100
3	K	287/518 (55%)	279 (97%)	8 (3%)	0	100	100
3	L	285/518 (55%)	277 (97%)	8 (3%)	0	100	100
3	M	287/518 (55%)	280 (98%)	7 (2%)	0	100	100
3	N	285/518 (55%)	281 (99%)	4 (1%)	0	100	100
All	All	5328/8124 (66%)	5091 (96%)	235 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	723	GLU
1	A	348	ASP

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	456/638 (72%)	456 (100%)	0	100	100
1	B	617/638 (97%)	616 (100%)	1 (0%)	92	94
1	C	618/638 (97%)	618 (100%)	0	100	100
1	D	619/638 (97%)	619 (100%)	0	100	100
1	E	618/638 (97%)	618 (100%)	0	100	100
1	F	442/638 (69%)	442 (100%)	0	100	100
2	G	73/245 (30%)	73 (100%)	0	100	100
2	H	62/245 (25%)	62 (100%)	0	100	100
3	I	60/430 (14%)	60 (100%)	0	100	100
3	J	59/430 (14%)	59 (100%)	0	100	100
3	K	237/430 (55%)	237 (100%)	0	100	100
3	L	235/430 (55%)	235 (100%)	0	100	100
3	M	237/430 (55%)	237 (100%)	0	100	100
3	N	235/430 (55%)	234 (100%)	1 (0%)	89	91
All	All	4568/6898 (66%)	4566 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	437	SER
3	N	3	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	454	ASN
3	M	288	GLN
1	F	408	HIS
3	N	255	ASN
3	K	123	HIS

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 [i](#)

13 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ADP	B	802	-	24,29,29	0.83	0	29,45,45	1.25	2 (6%)
5	ATP	D	801	-	28,33,33	0.79	0	34,52,52	0.89	2 (5%)
4	ADP	D	802	-	24,29,29	0.84	0	29,45,45	1.26	2 (6%)
4	ADP	A	801	-	24,29,29	0.88	0	29,45,45	1.25	2 (6%)
5	ATP	C	801	-	28,33,33	0.81	0	34,52,52	0.89	1 (2%)
5	ATP	E	802	-	28,33,33	0.75	0	34,52,52	0.96	2 (5%)
5	ATP	E	801	-	28,33,33	0.69	0	34,52,52	0.94	1 (2%)
5	ATP	B	801	-	28,33,33	0.78	0	34,52,52	0.88	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ADP	F	802	-	24,29,29	0.89	0	29,45,45	1.26	2 (6%)
6	PO4	C	803	-	4,4,4	1.00	0	6,6,6	0.46	0
4	ADP	C	802	-	24,29,29	0.85	0	29,45,45	1.26	2 (6%)
5	ATP	F	801	-	28,33,33	0.71	0	34,52,52	0.88	1 (2%)
5	ATP	A	802	-	28,33,33	0.72	0	34,52,52	0.88	1 (2%)

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	B	802	-	-	3/12/32/32	0/3/3/3
5	ATP	D	801	-	-	8/18/38/38	0/3/3/3
4	ADP	D	802	-	-	5/12/32/32	0/3/3/3
4	ADP	A	801	-	-	2/12/32/32	0/3/3/3
5	ATP	C	801	-	-	7/18/38/38	0/3/3/3
5	ATP	E	802	-	-	7/18/38/38	0/3/3/3
5	ATP	E	801	-	-	3/18/38/38	0/3/3/3
5	ATP	B	801	-	-	6/18/38/38	0/3/3/3
4	ADP	F	802	-	-	0/12/32/32	0/3/3/3
4	ADP	C	802	-	-	2/12/32/32	0/3/3/3
5	ATP	F	801	-	-	4/18/38/38	0/3/3/3
5	ATP	A	802	-	-	4/18/38/38	0/3/3/3

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	802	ADP	N3-C2-N1	-4.23	122.93	128.67
4	B	802	ADP	N3-C2-N1	-4.23	122.93	128.67
4	D	802	ADP	N3-C2-N1	-4.12	123.08	128.67
4	C	802	ADP	N3-C2-N1	-4.07	123.15	128.67
4	A	801	ADP	N3-C2-N1	-4.05	123.17	128.67

There are no chirality outliers.

5 of 51 torsion outliers are listed below:

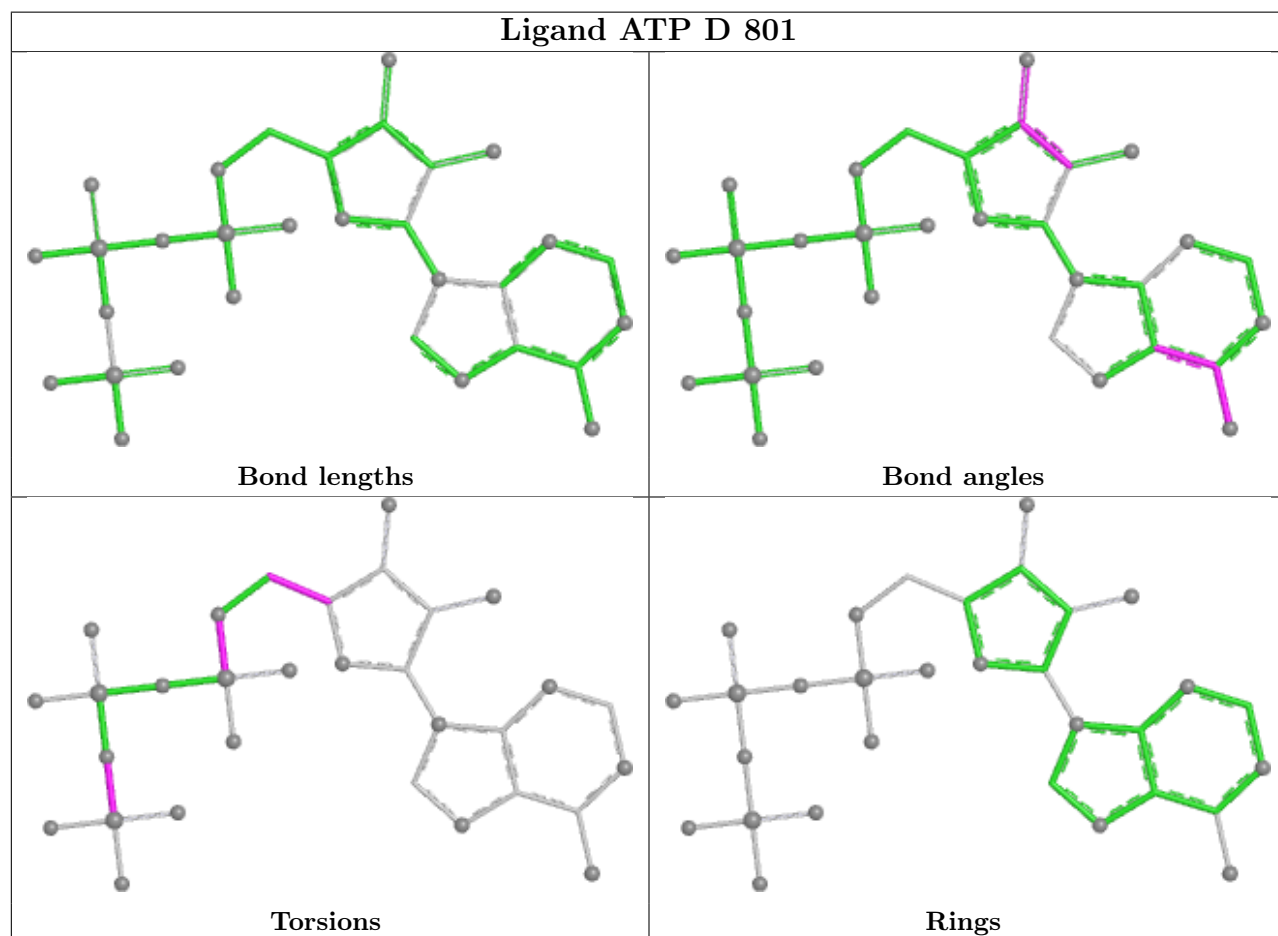
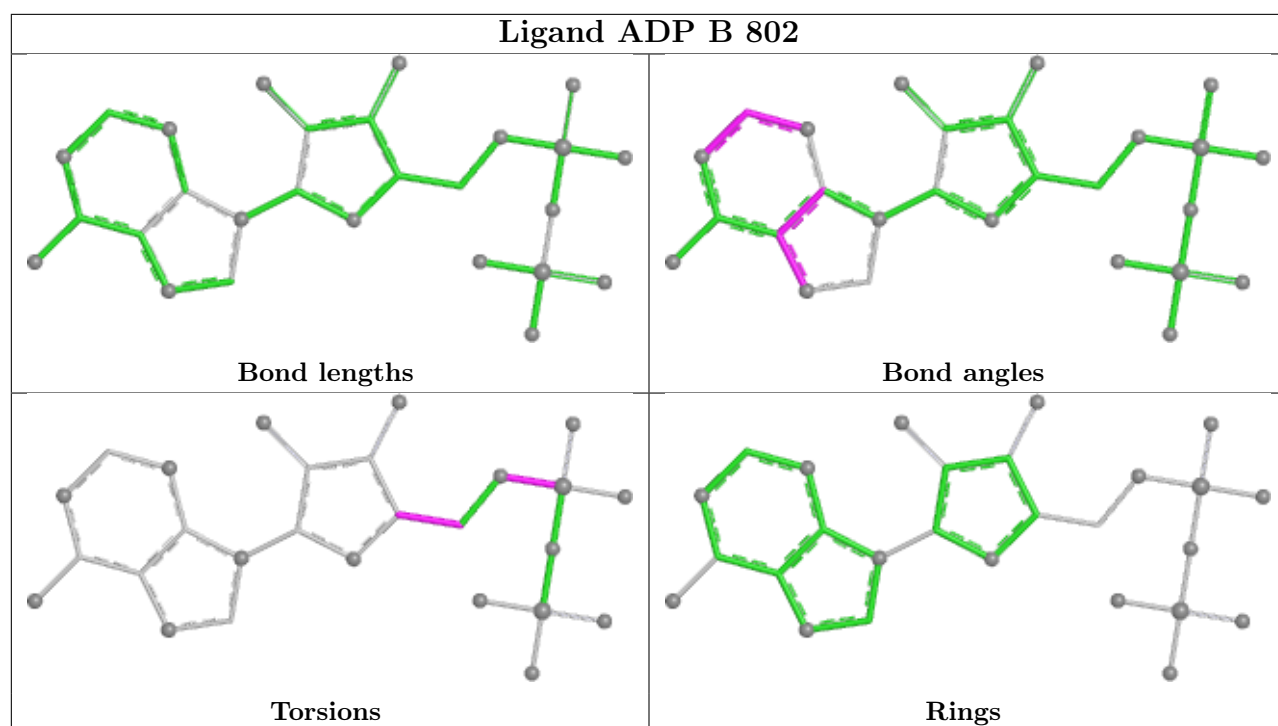
Mol	Chain	Res	Type	Atoms
4	B	802	ADP	C5'-O5'-PA-O1A
4	C	802	ADP	C5'-O5'-PA-O3A
4	D	802	ADP	C5'-O5'-PA-O1A
4	D	802	ADP	C5'-O5'-PA-O3A
5	A	802	ATP	PB-O3B-PG-O2G

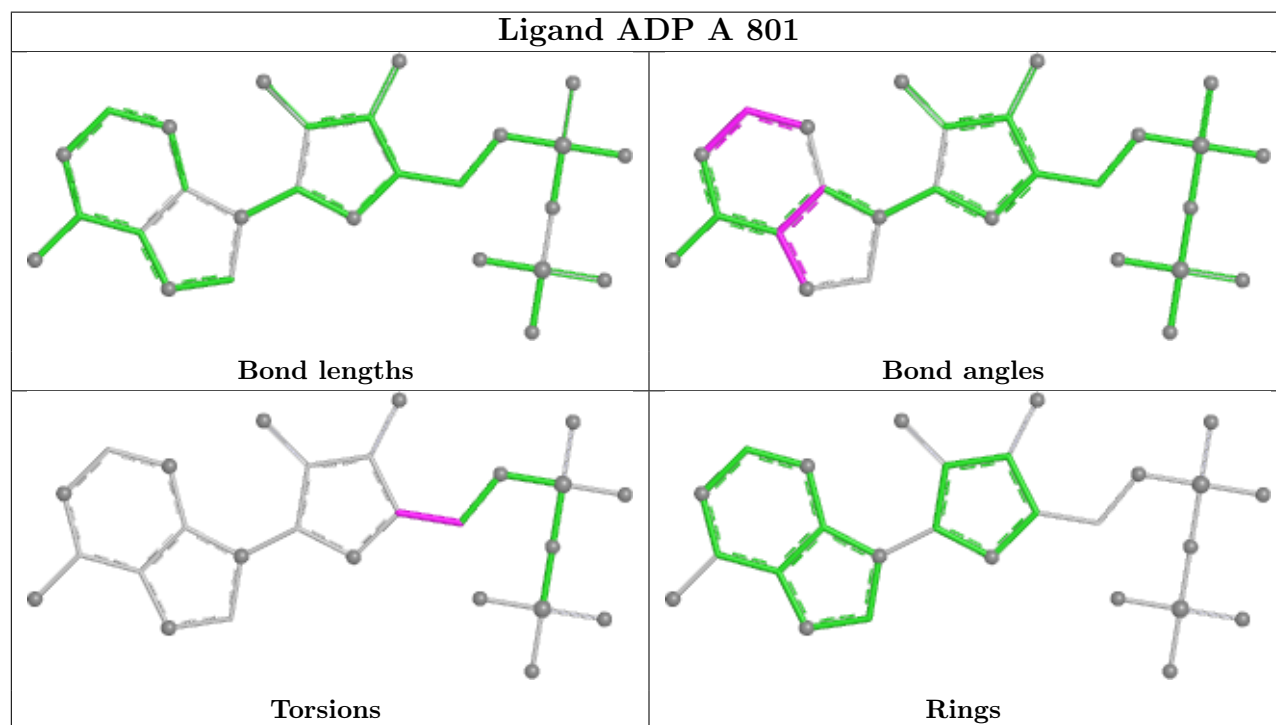
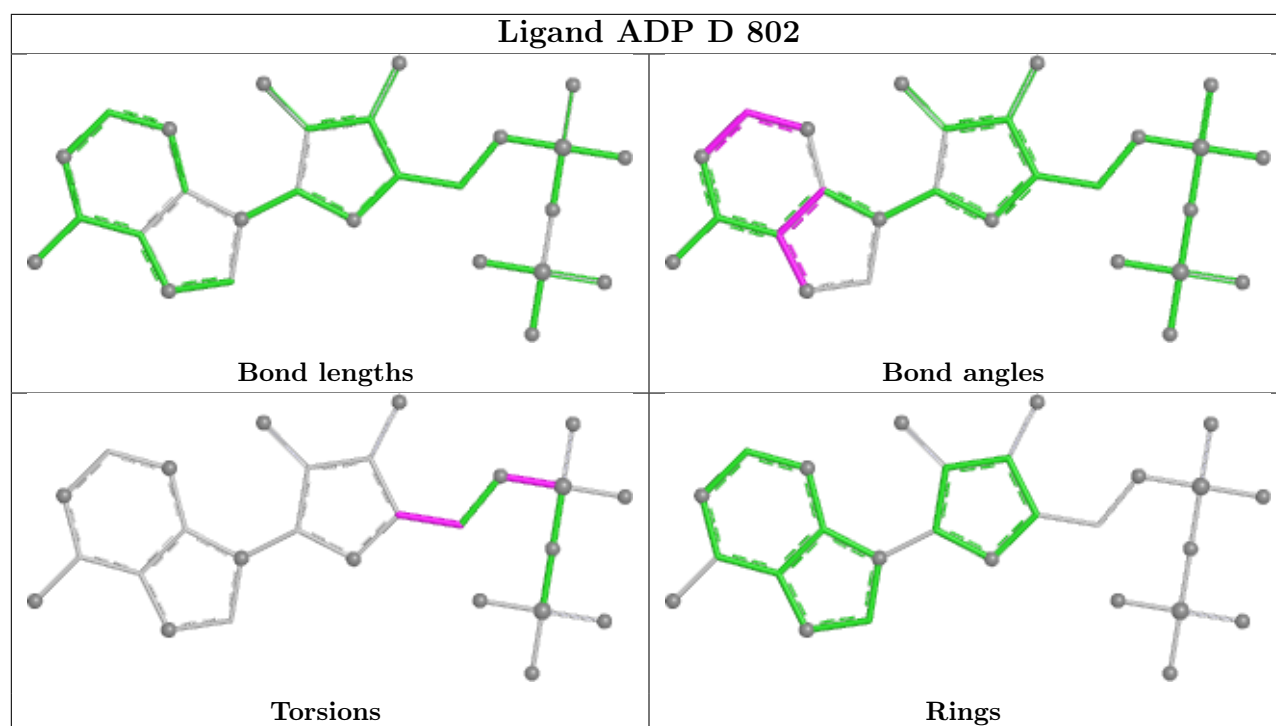
There are no ring outliers.

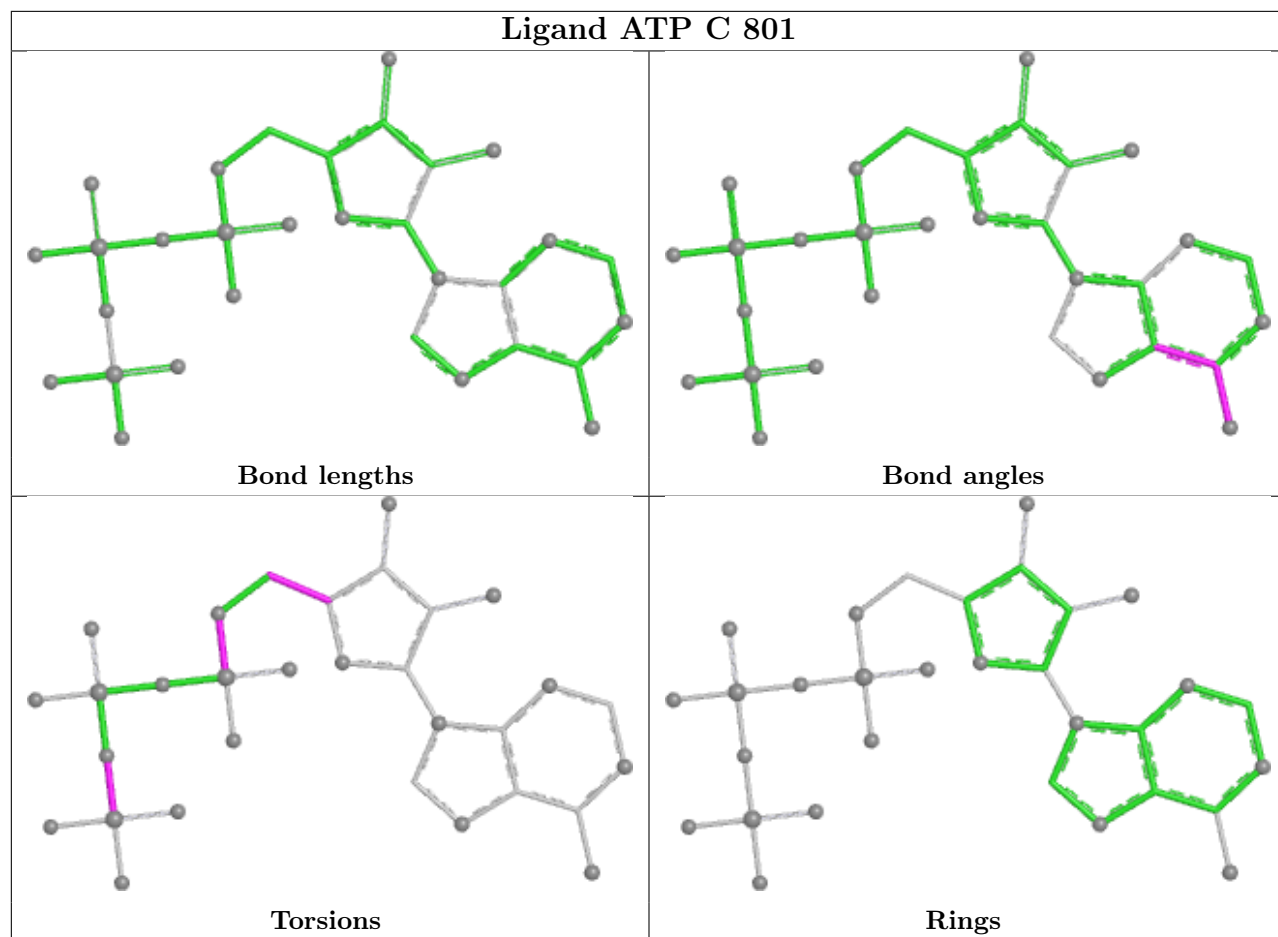
7 monomers are involved in 8 short contacts:

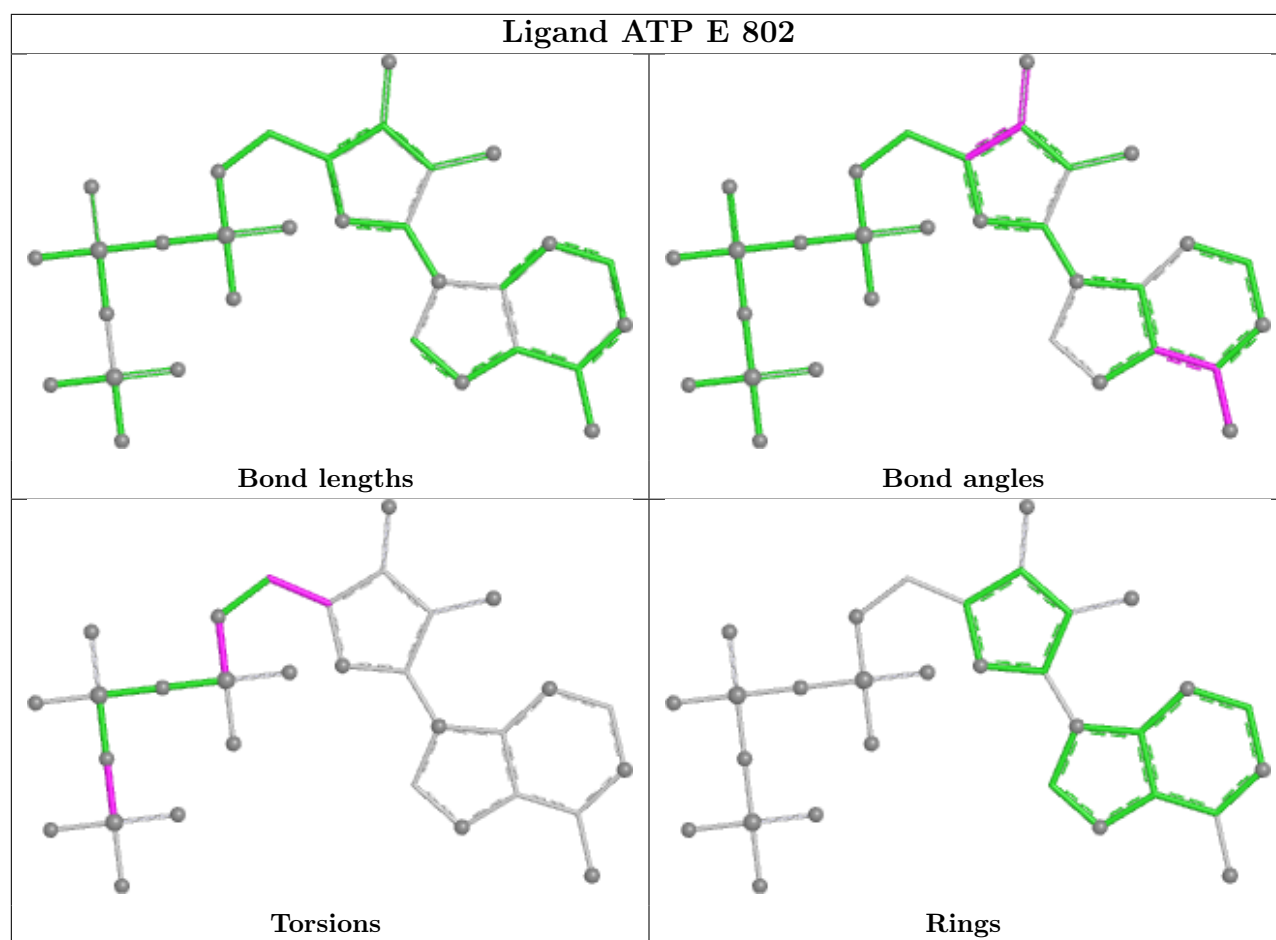
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	801	ADP	1	0
5	E	802	ATP	1	0
5	B	801	ATP	1	0
4	F	802	ADP	1	0
4	C	802	ADP	1	0
5	F	801	ATP	2	0
5	A	802	ATP	1	0

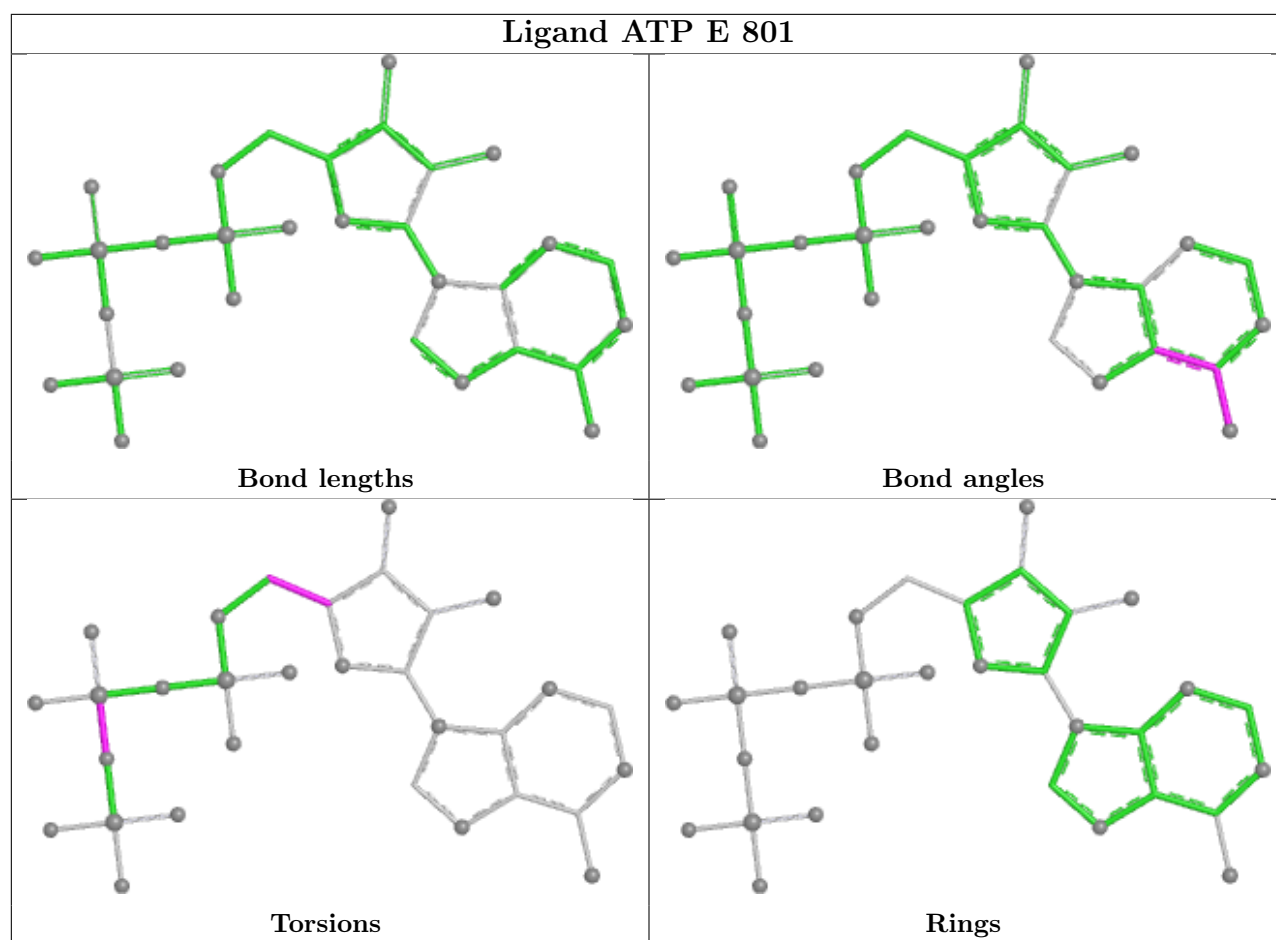
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



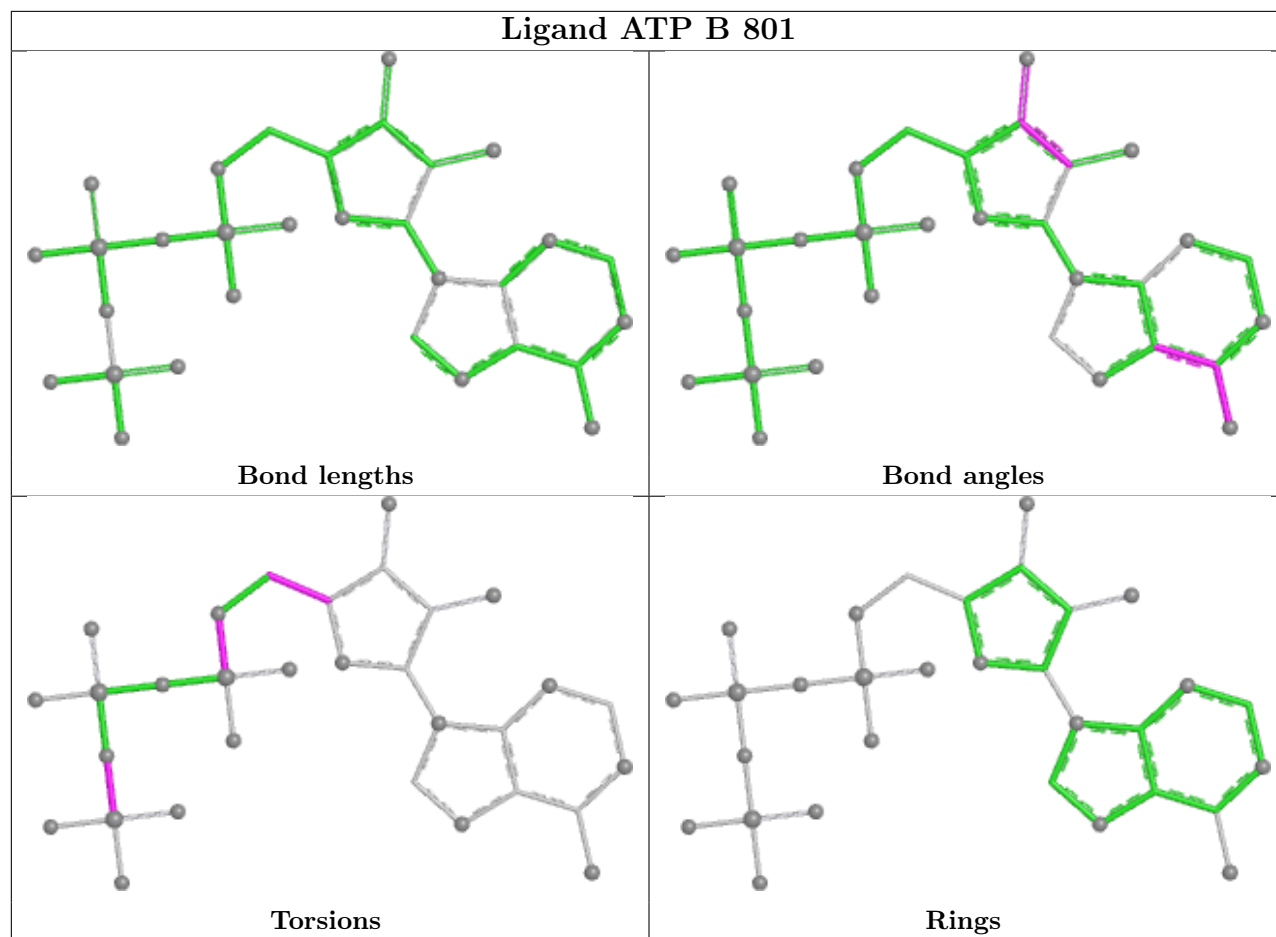




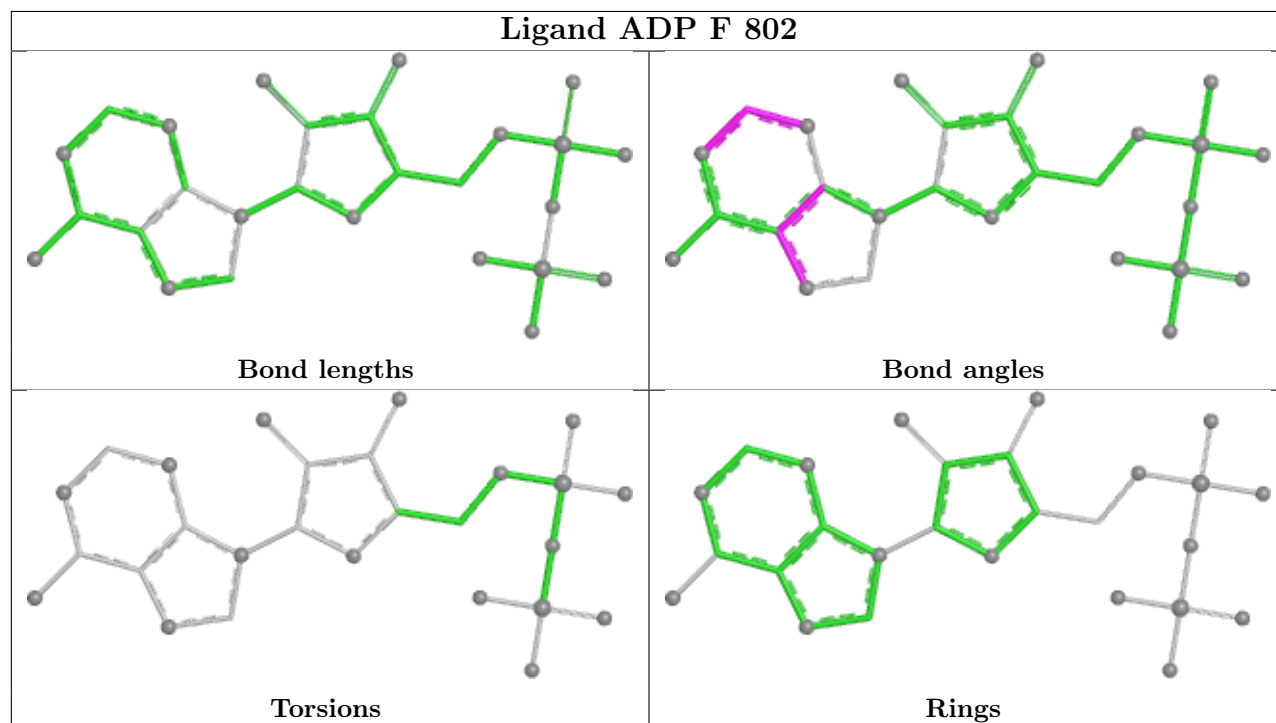


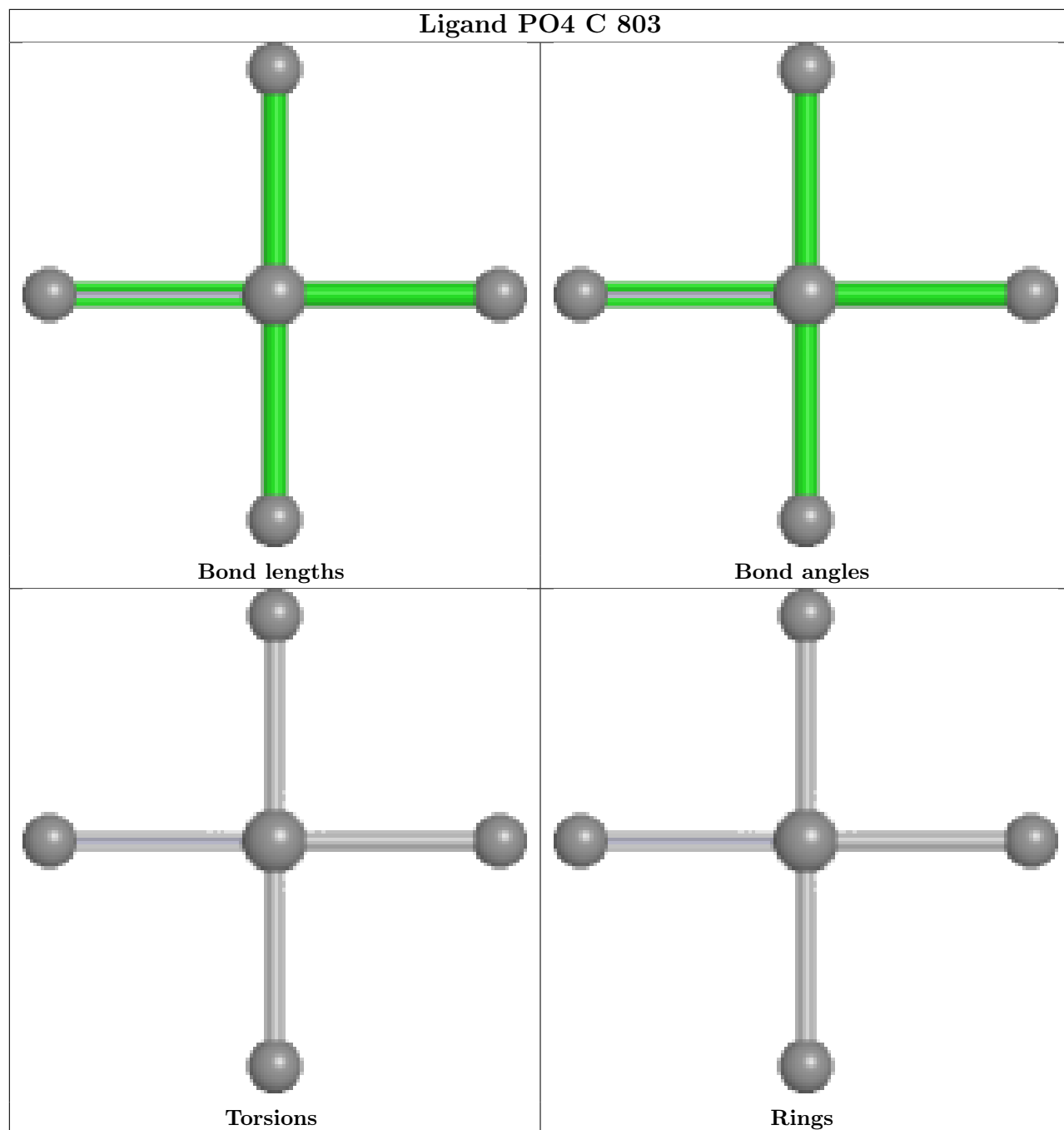


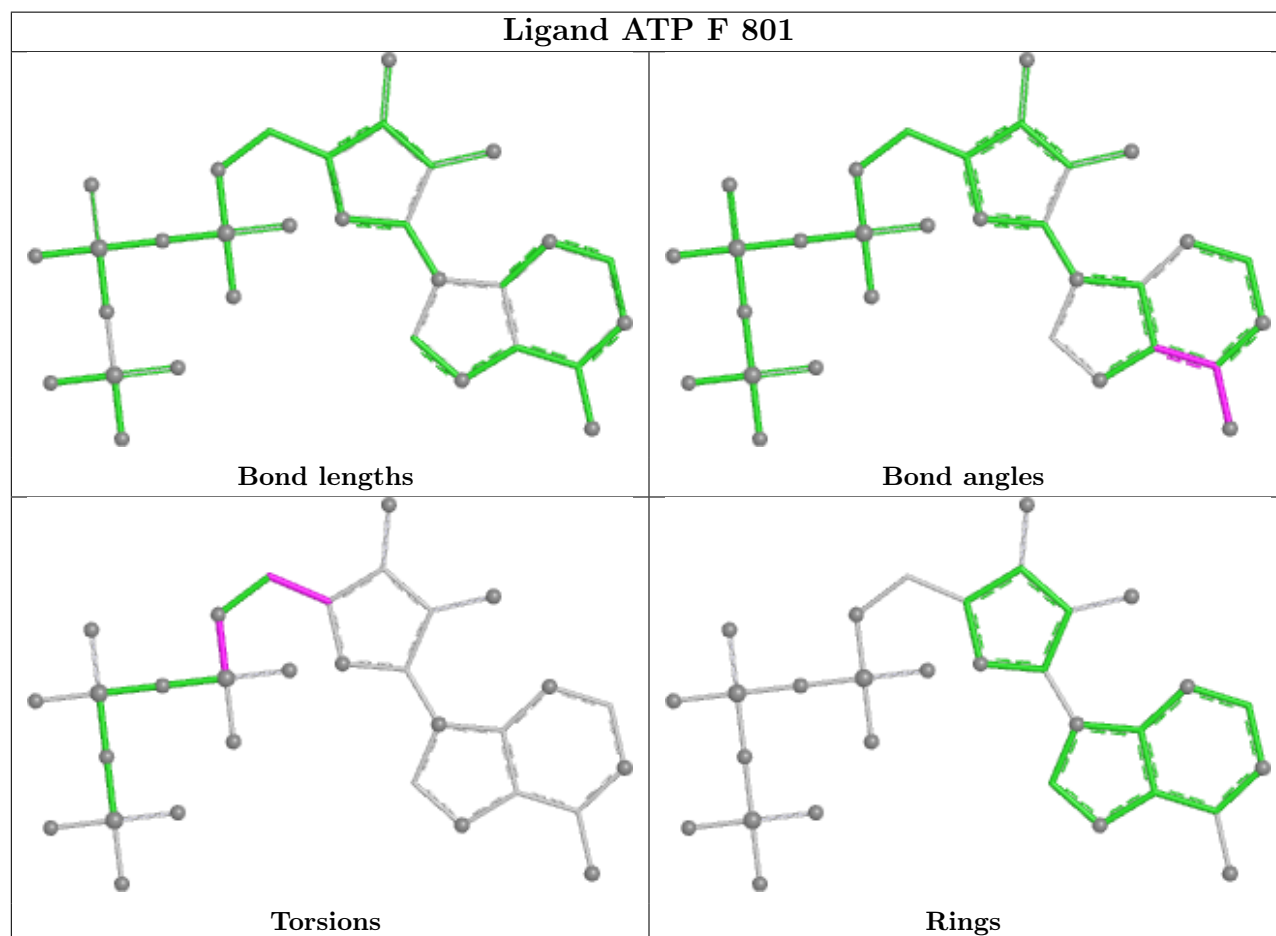
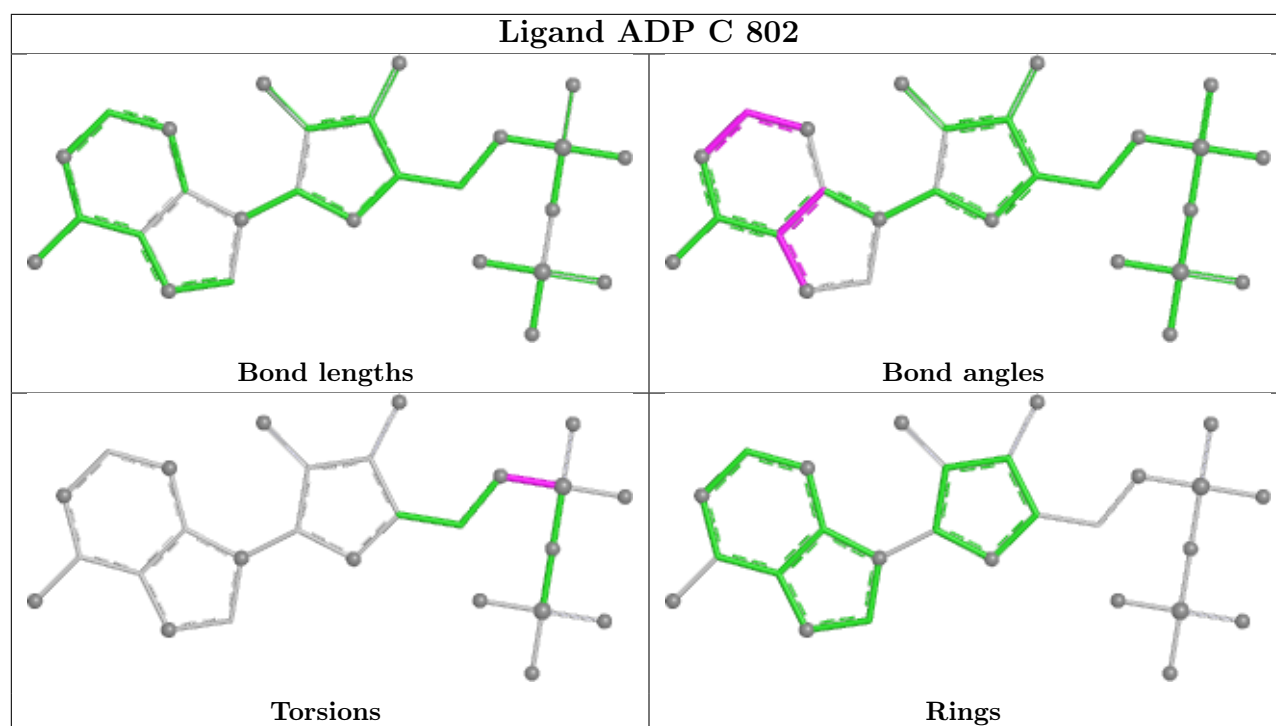
Ligand ATP B 801

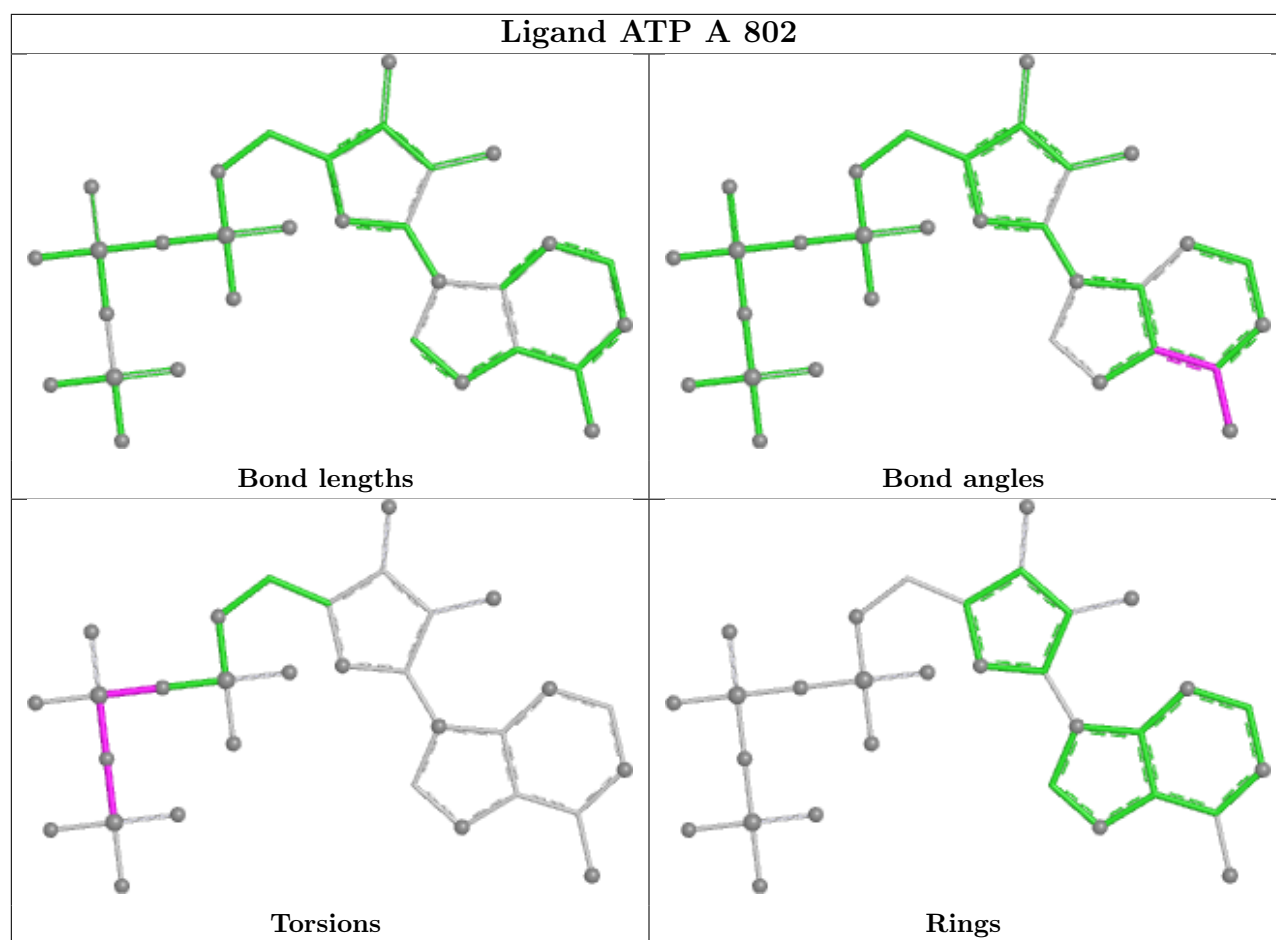


Ligand ADP F 802









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.

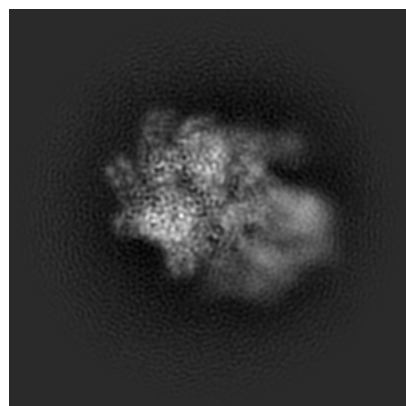
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71521. These allow visual inspection of the internal detail of the map and identification of artifacts.

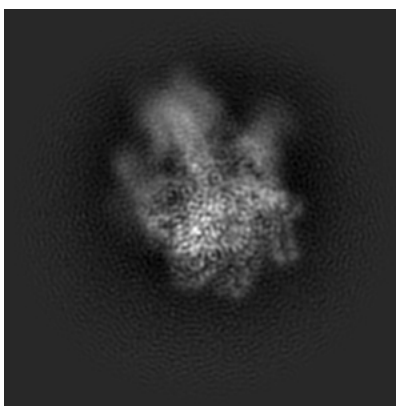
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

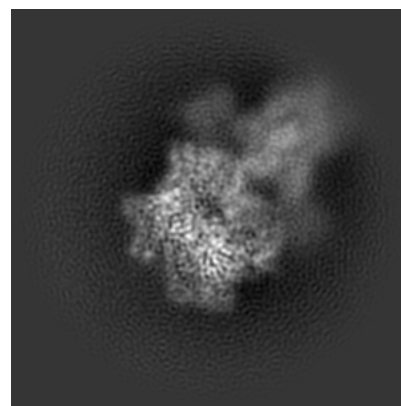
6.1.1 Primary map



X

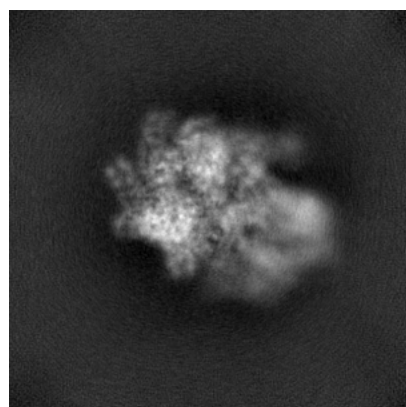


Y

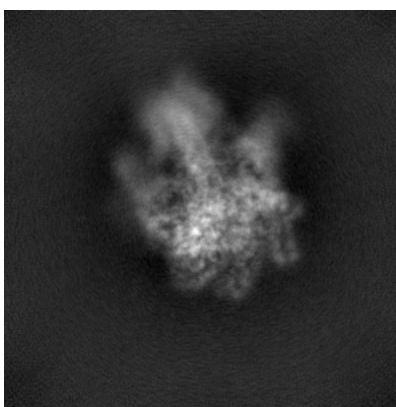


Z

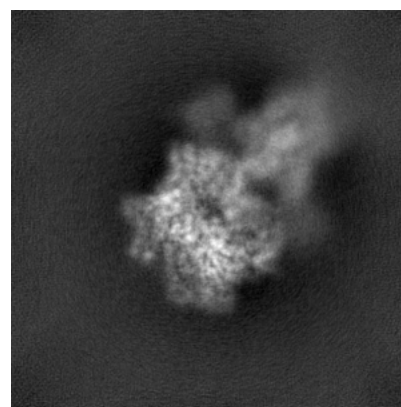
6.1.2 Raw map



X



Y

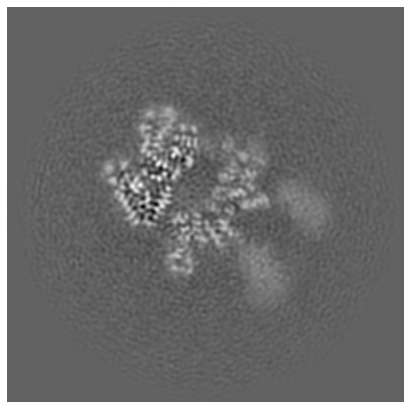


Z

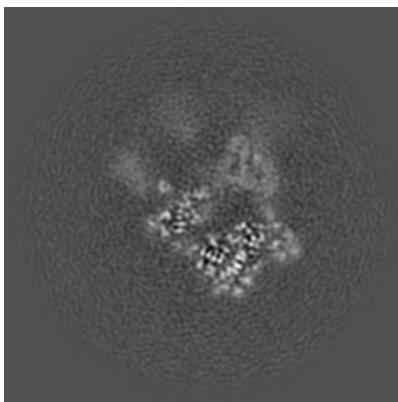
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

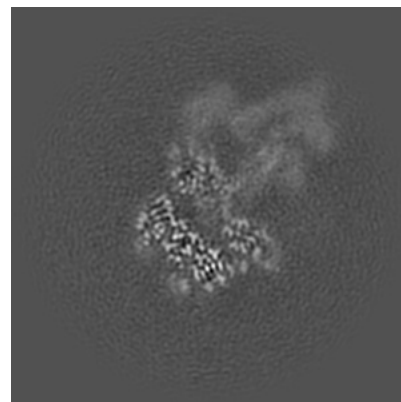
6.2.1 Primary map



X Index: 147

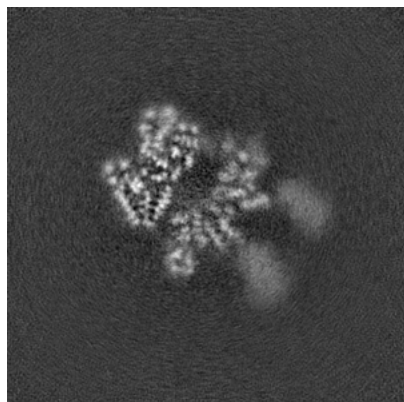


Y Index: 147

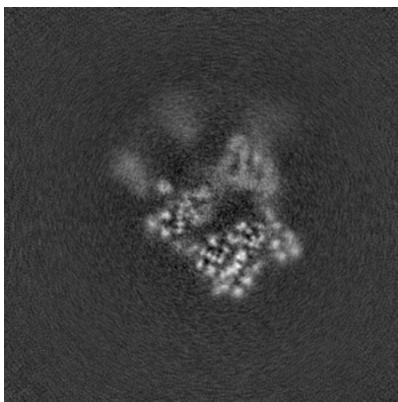


Z Index: 147

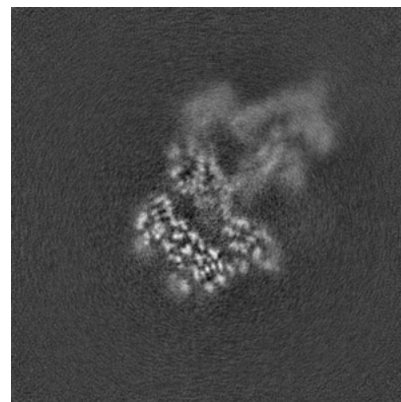
6.2.2 Raw map



X Index: 147



Y Index: 147

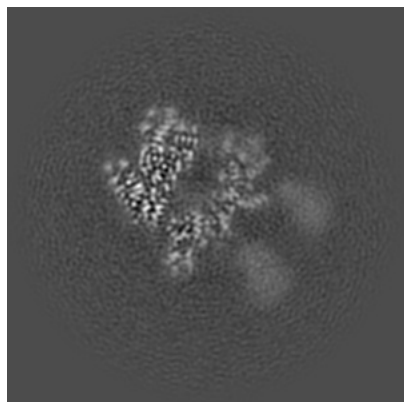


Z Index: 147

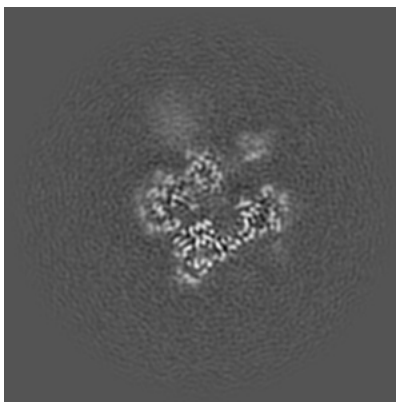
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

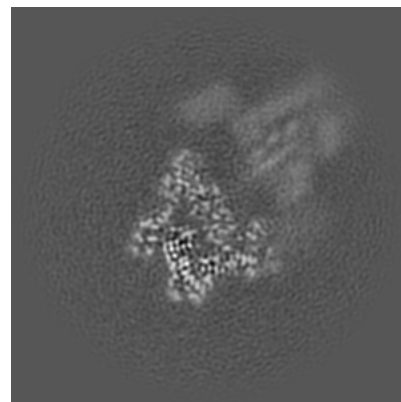
6.3.1 Primary map



X Index: 149

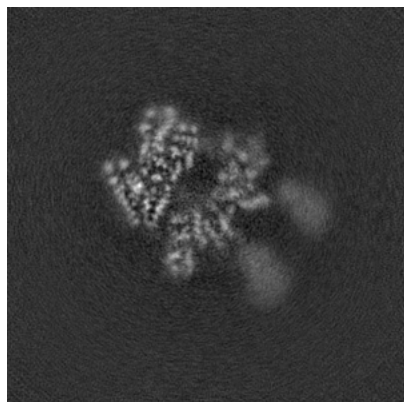


Y Index: 126

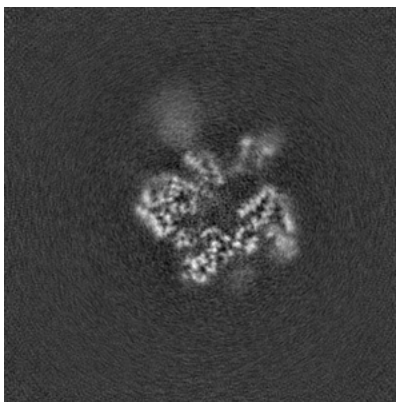


Z Index: 138

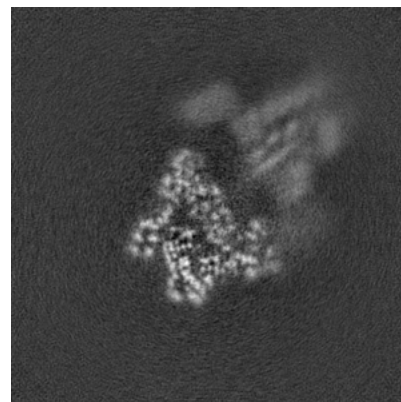
6.3.2 Raw map



X Index: 148



Y Index: 132

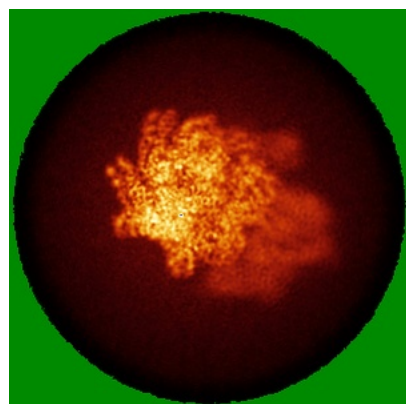


Z Index: 138

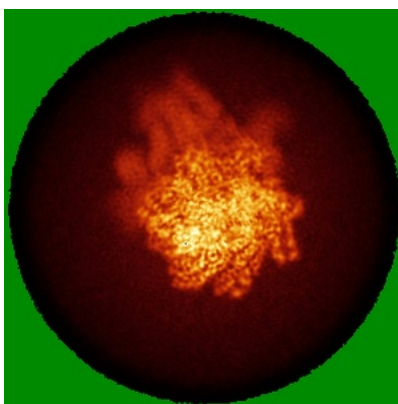
The images above show the largest variance slices of the map in three orthogonal directions.

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

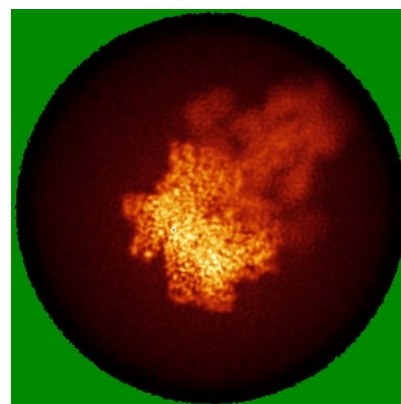
6.4.1 Primary map



X

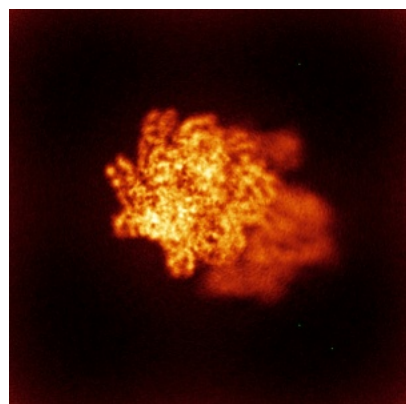


Y

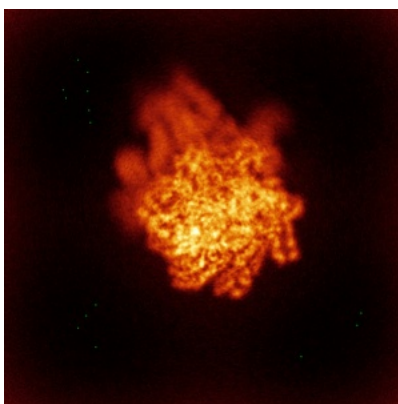


Z

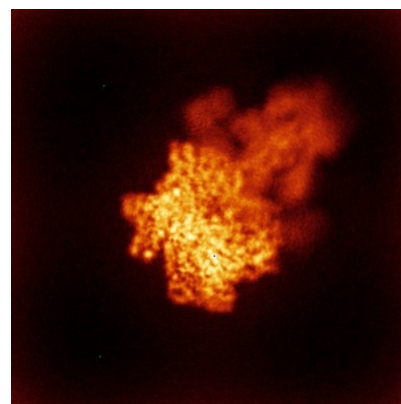
6.4.2 Raw map



X



Y

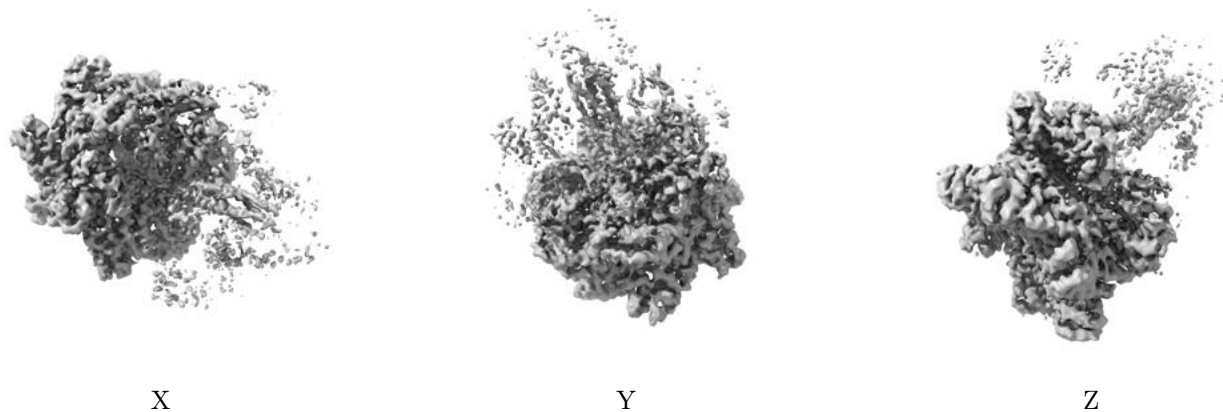


Z

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 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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.

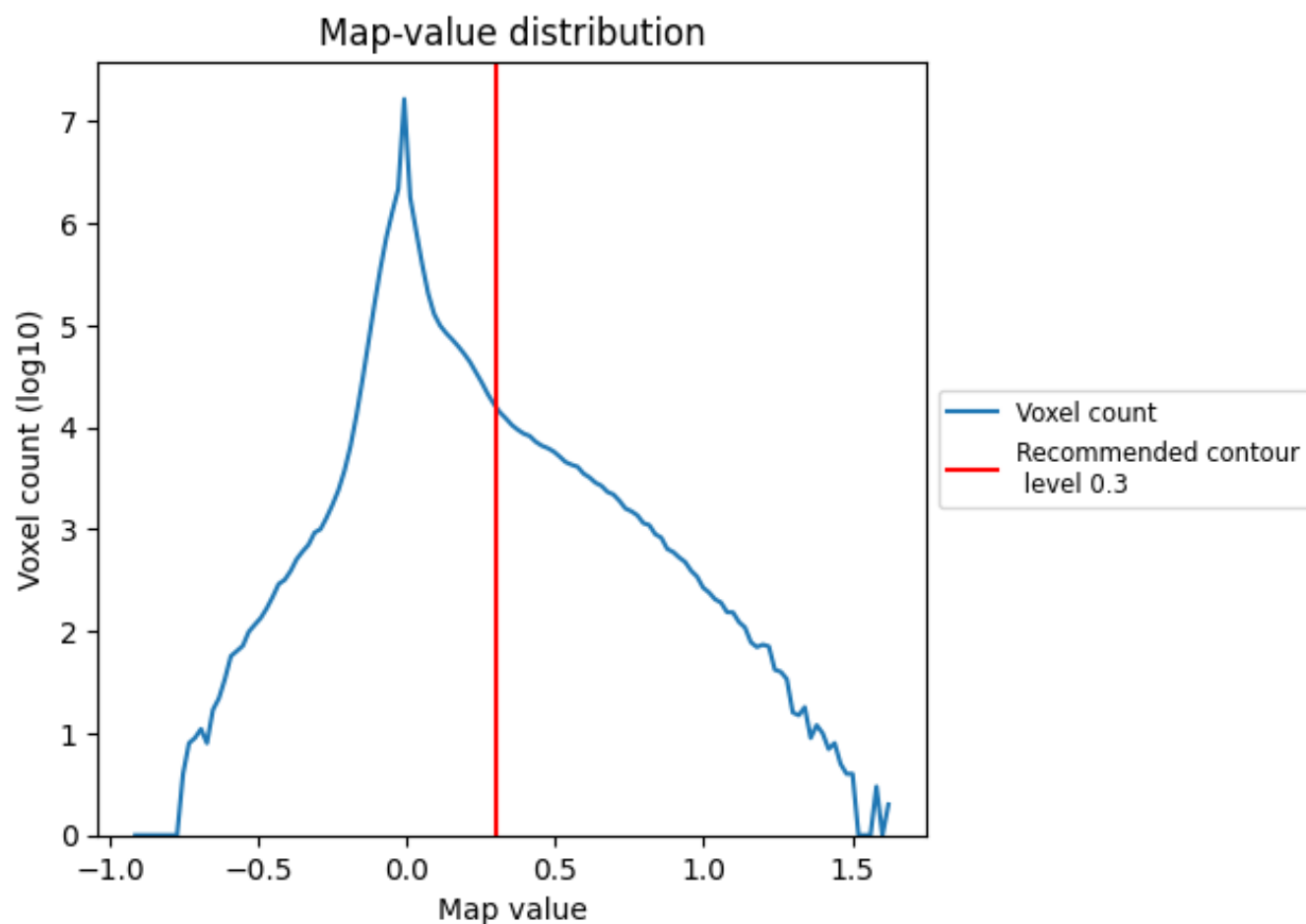
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

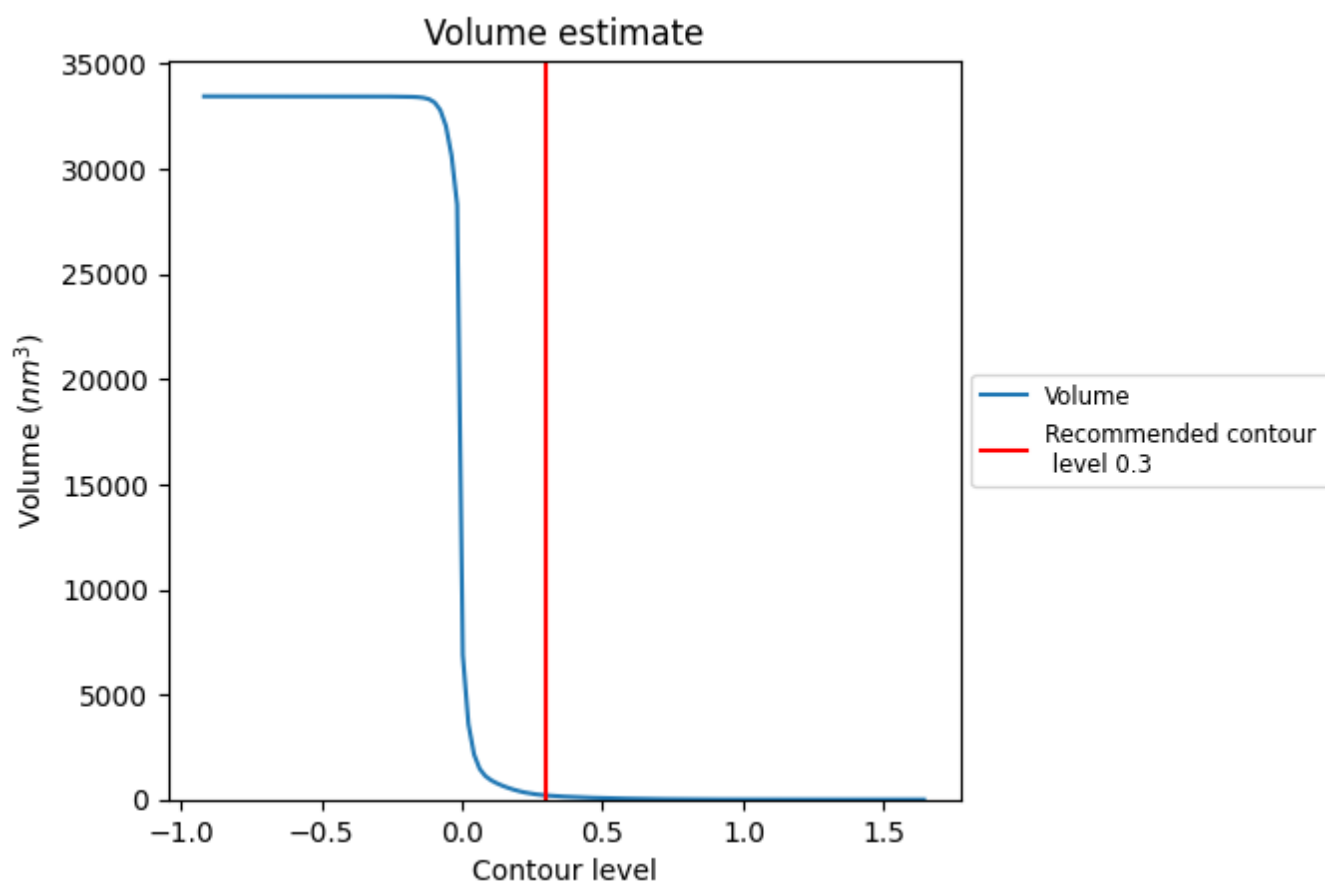
This section contains the results of statistical analysis of the map.

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.

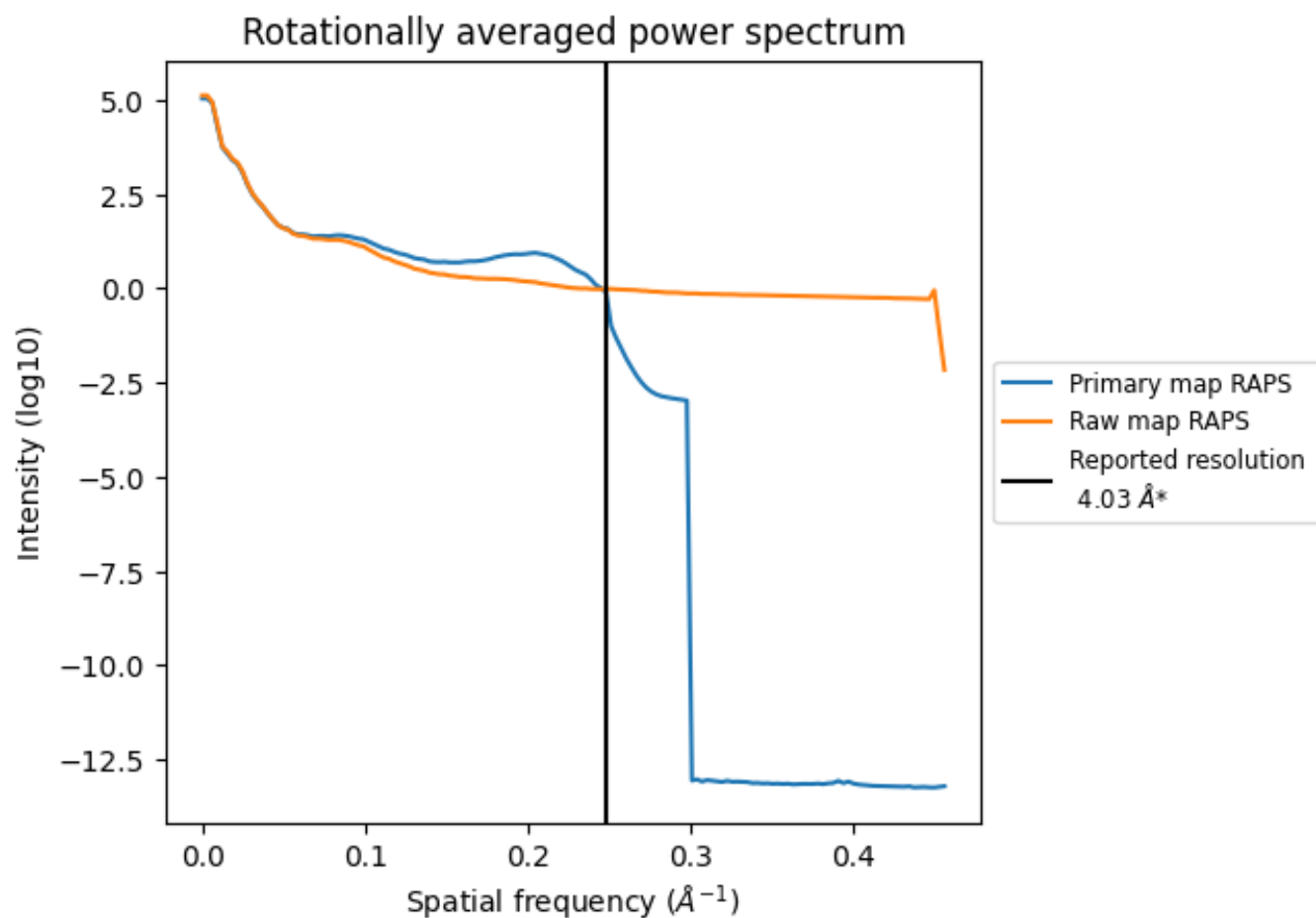
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 197 nm³; this corresponds to an approximate mass of 178 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 ⓘ

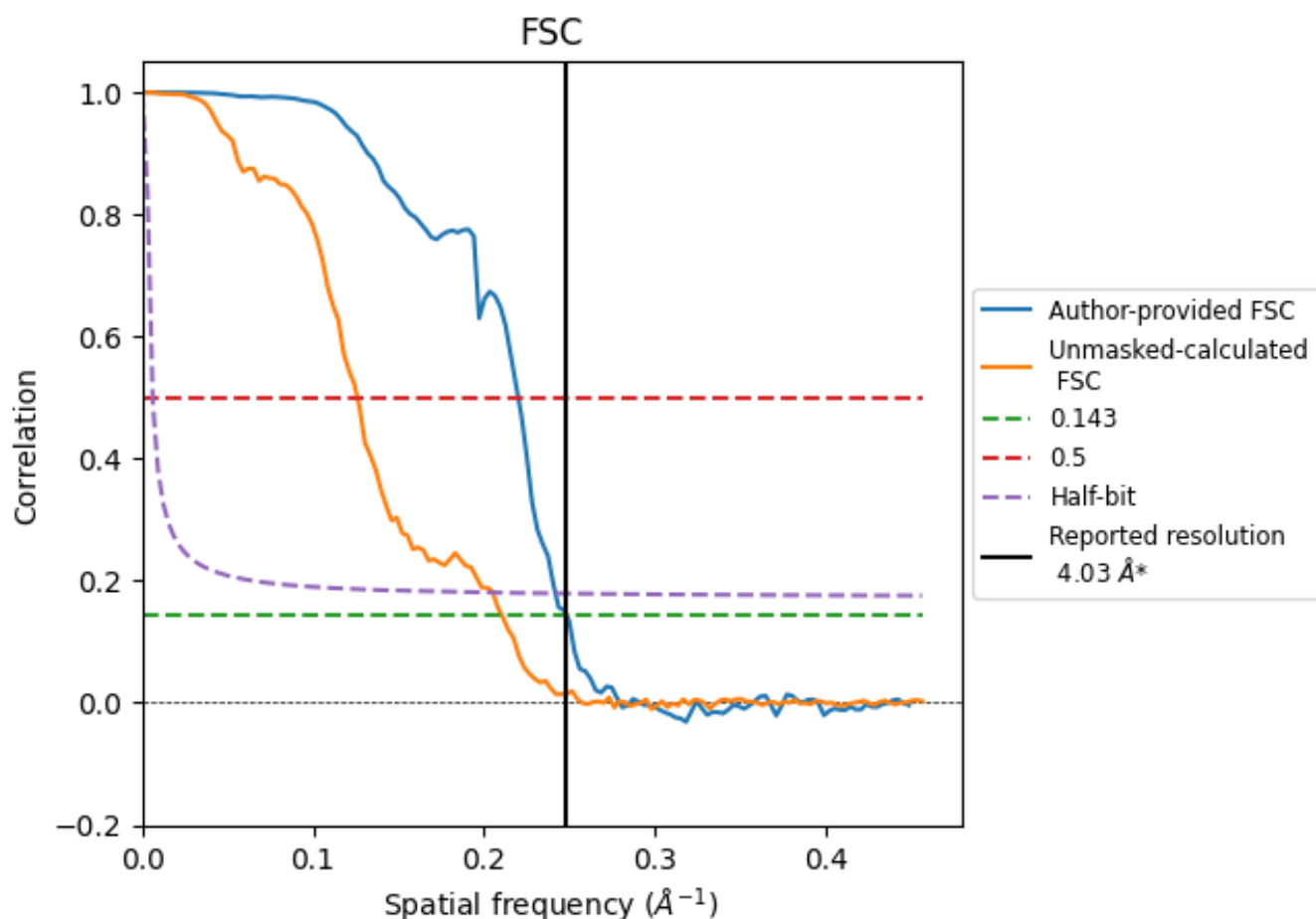


*Reported resolution corresponds to spatial frequency of 0.248 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.248 \AA^{-1}

8.2 Resolution estimates [i](#)

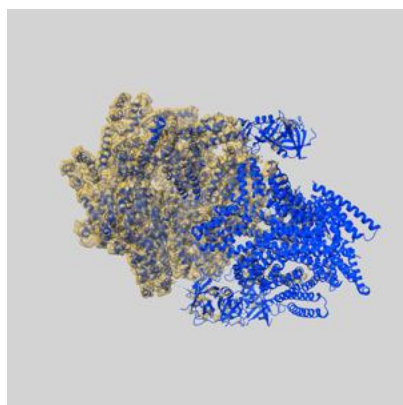
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.03	-	-
Author-provided FSC curve	4.03	4.55	4.14
Unmasked-calculated*	4.75	7.94	4.88

*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 4.75 differs from the reported value 4.03 by more than 10 %

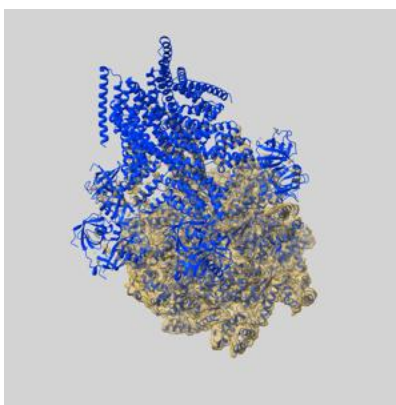
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-71521 and PDB model 9PCX. Per-residue inclusion information can be found in section 3 on page 12.

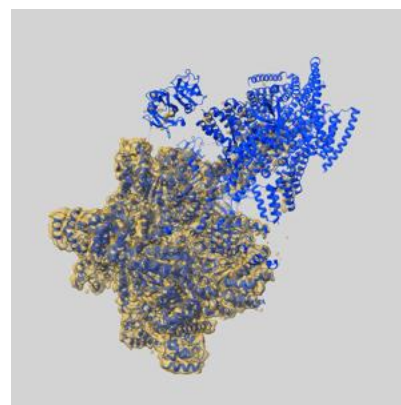
9.1 Map-model overlay [i](#)



X



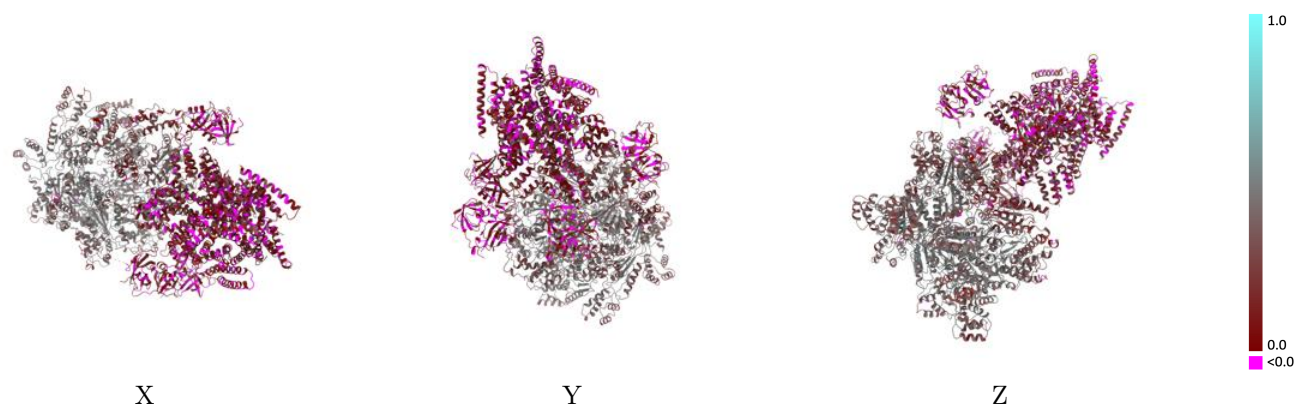
Y



Z

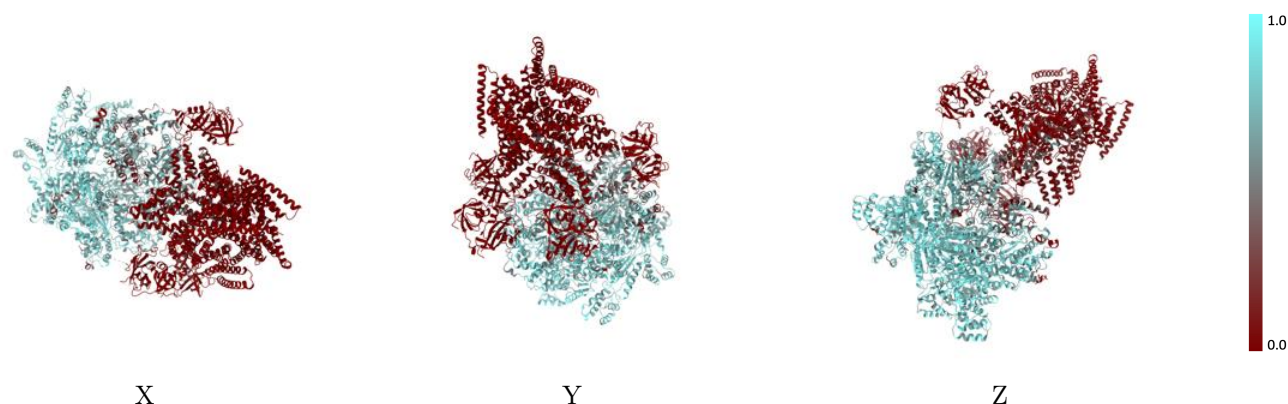
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



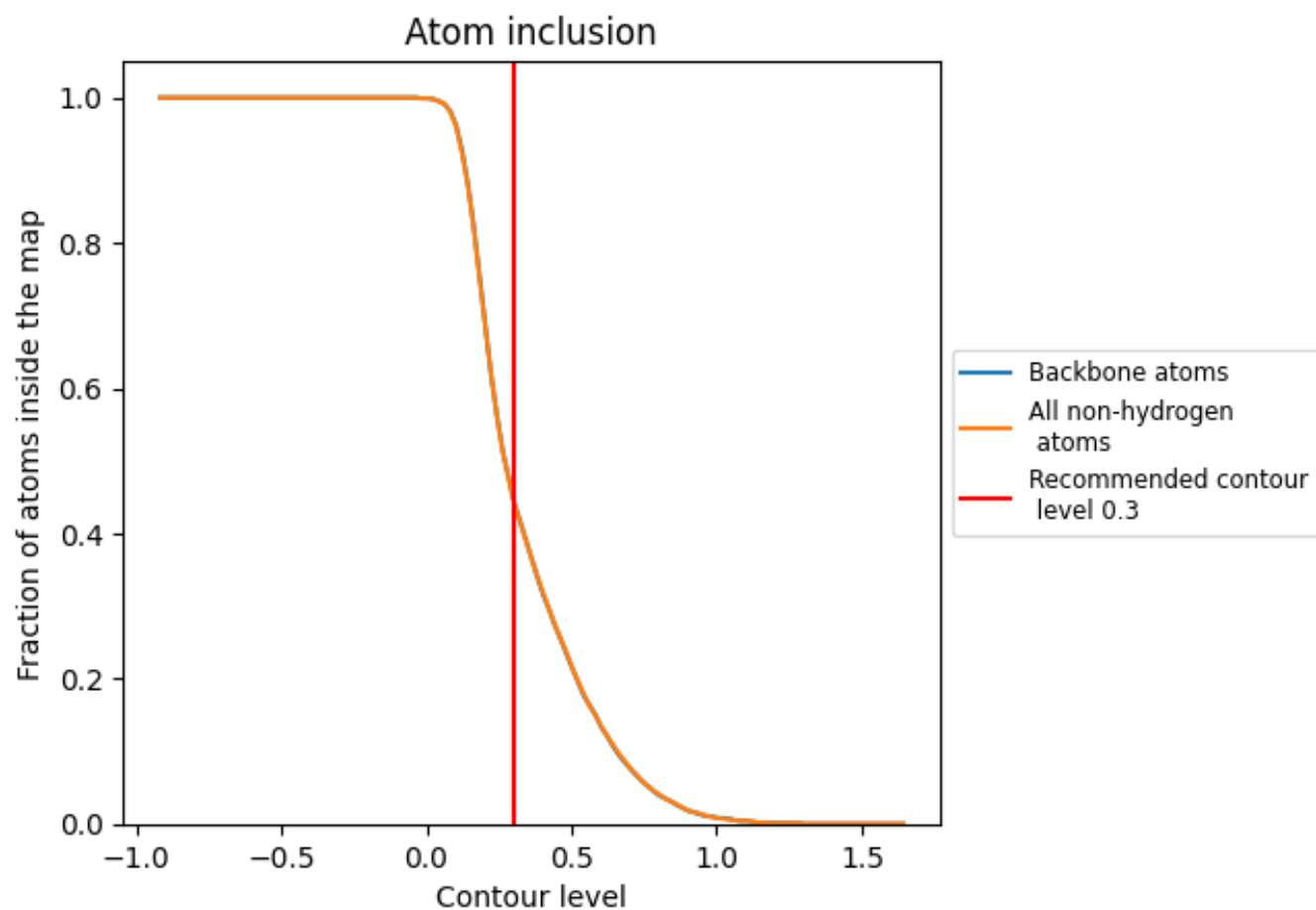
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 45% of all backbone atoms, 45% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4460	<div></div> 0.2890
A	<div></div> 0.7420	<div></div> 0.4080
B	<div></div> 0.5870	<div></div> 0.3470
C	<div></div> 0.6000	<div></div> 0.3440
D	<div></div> 0.5870	<div></div> 0.3370
E	<div></div> 0.5310	<div></div> 0.3200
F	<div></div> 0.5880	<div></div> 0.3350
G	<div></div> 0.2040	<div></div> 0.2070
H	<div></div> 0.1270	<div></div> 0.1580
I	<div></div> 0.1200	<div></div> 0.1580
J	<div></div> 0.0820	<div></div> 0.1260
K	<div></div> 0.0130	<div></div> 0.1270
L	<div></div> 0.0270	<div></div> 0.1310
M	<div></div> 0.0250	<div></div> 0.1240
N	<div></div> 0.0240	<div></div> 0.1200

1.0

0.0

<0.0