



wwPDB EM Validation Summary Report ⓘ

Jul 28, 2025 – 04:43 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.dev126
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

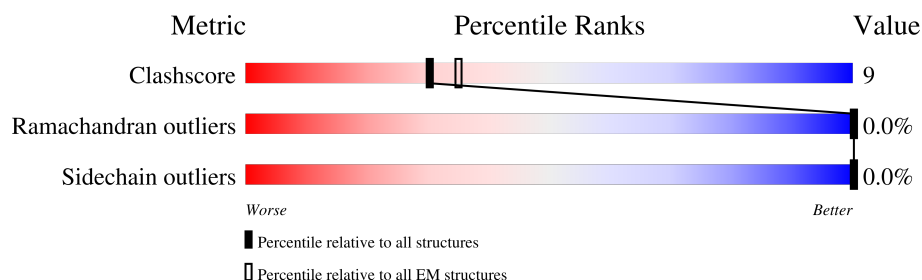
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	747	<div> <div>6%</div> <div>58%</div> <div>13%</div> <div>29%</div> </div>
1	B	747	<div> <div>29%</div> <div>78%</div> <div>18%</div> <div>•</div> </div>
1	C	747	<div> <div>27%</div> <div>80%</div> <div>17%</div> <div>•</div> </div>
1	D	747	<div> <div>27%</div> <div>79%</div> <div>18%</div> <div>•</div> </div>
1	E	747	<div> <div>30%</div> <div>80%</div> <div>16%</div> <div>•</div> </div>
1	F	747	<div> <div>19%</div> <div>55%</div> <div>14%</div> <div>31%</div> </div>
2	G	267	<div> <div>22%</div> <div>22%</div> <div>8%</div> <div>70%</div> </div>
2	H	267	<div> <div>23%</div> <div>17%</div> <div>8%</div> <div>75%</div> </div>

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Mol	Chain	Length	Quality of chain
3	I	518	<div><div><div>11%</div><div>8%</div><div>5%</div></div><div>86%</div></div>
3	J	518	<div><div><div>13%</div><div>9%</div><div></div></div><div>87%</div></div>
3	K	518	<div><div><div>56%</div><div>43%</div><div>12%</div></div><div>44%</div></div>
3	L	518	<div><div><div>55%</div><div>47%</div><div>9%</div></div><div>45%</div></div>
3	M	518	<div><div><div>56%</div><div>46%</div><div>10%</div></div><div>44%</div></div>
3	N	518	<div><div><div>55%</div><div>45%</div><div>10%</div></div><div>45%</div></div>

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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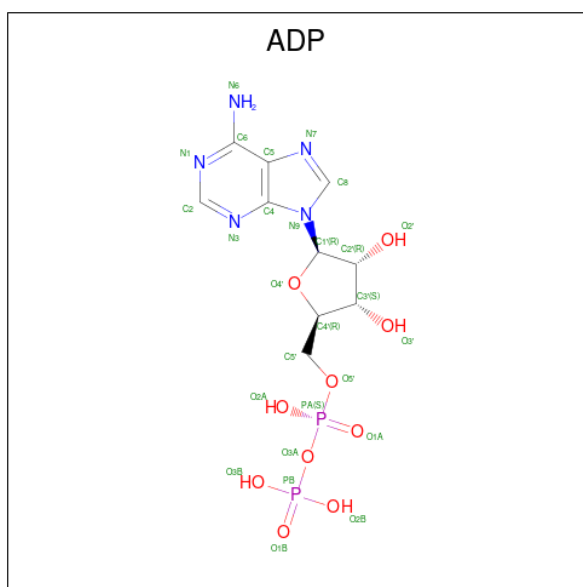
Chain	Residue	Modelled	Actual	Comment	Reference
K	-119	ALA	CYS	conflict	UNP P60881
K	-117	ALA	CYS	conflict	UNP P60881
K	-115	ALA	CYS	conflict	UNP P60881
K	0	GLY	-	linker	UNP P60881
L	-222	MET	-	expression tag	UNP P60881
L	-221	GLY	-	expression tag	UNP P60881
L	-220	SER	-	expression tag	UNP P60881
L	-219	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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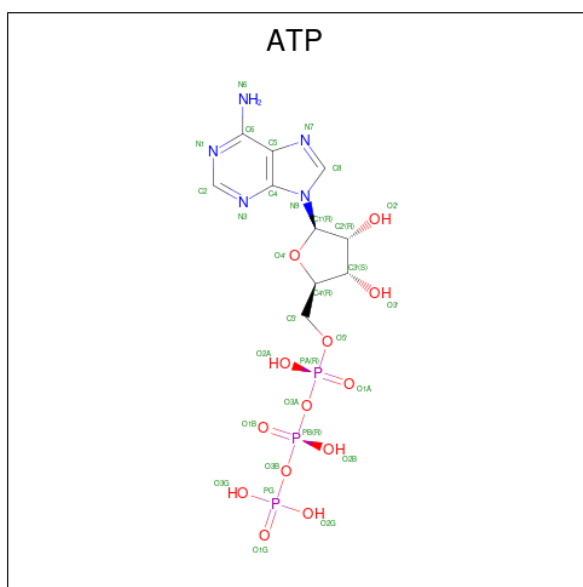
Chain	Residue	Modelled	Actual	Comment	Reference
M	-119	ALA	CYS	conflict	UNP P60881
M	-117	ALA	CYS	conflict	UNP P60881
M	-115	ALA	CYS	conflict	UNP P60881
M	0	GLY	-	linker	UNP P60881
N	-222	MET	-	expression tag	UNP P60881
N	-221	GLY	-	expression tag	UNP P60881
N	-220	SER	-	expression tag	UNP P60881
N	-219	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).



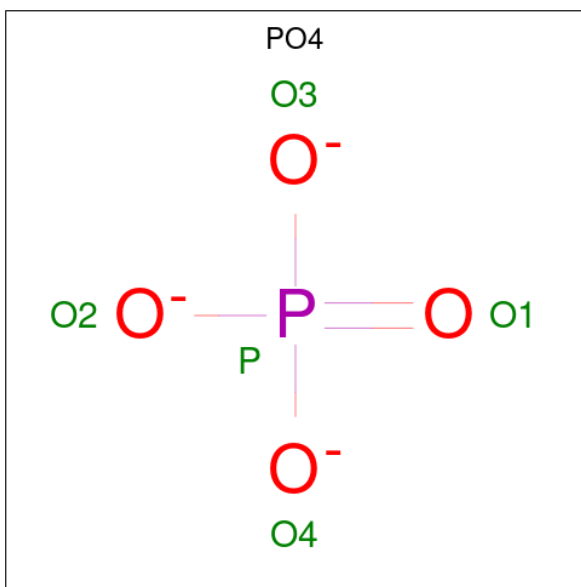
Mol	Chain	Residues	Atoms						AltConf
4	A	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
4	B	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
4	C	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
4	D	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
4	F	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	

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

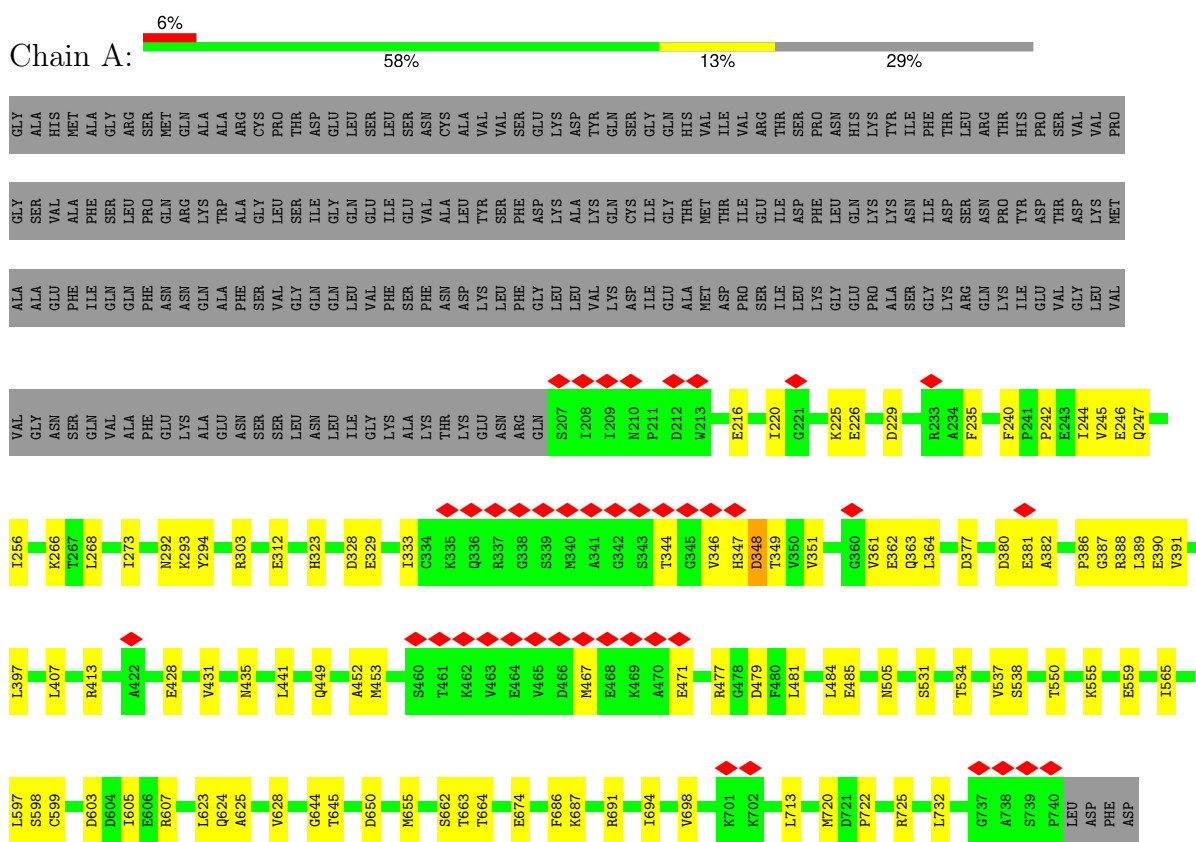


Mol	Chain	Residues	Atoms			AltConf
			Total	O	P	
6	C	1	5	4	1	0

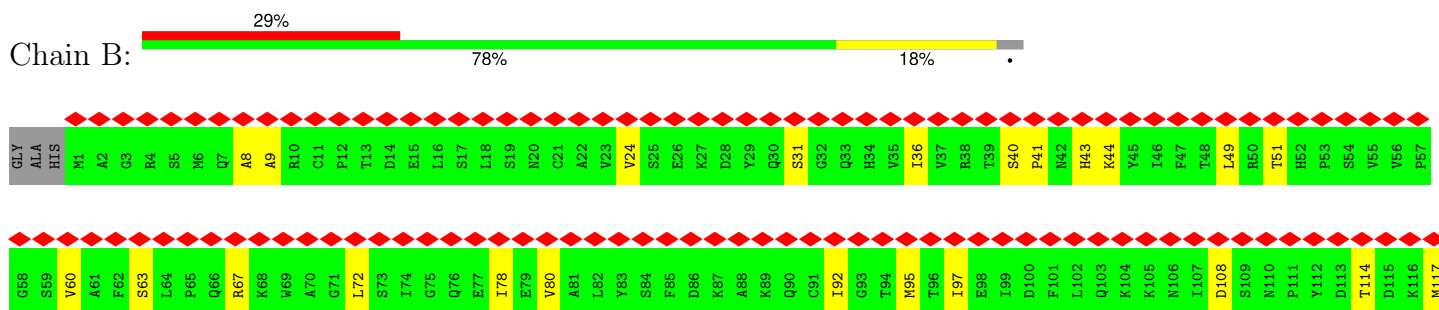
3 Residue-property plots

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.

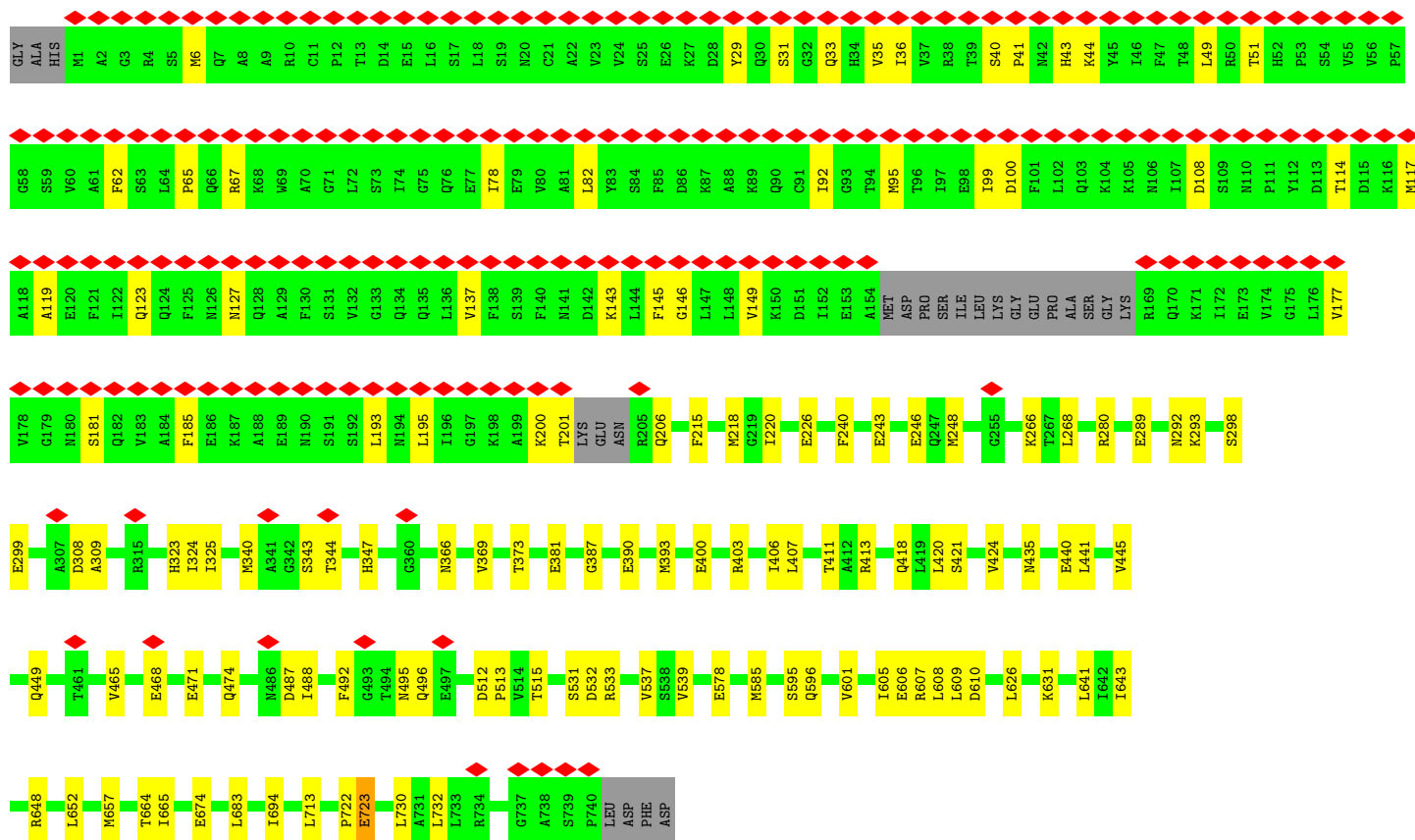
• Molecule 1: Vesicle-fusing ATPase



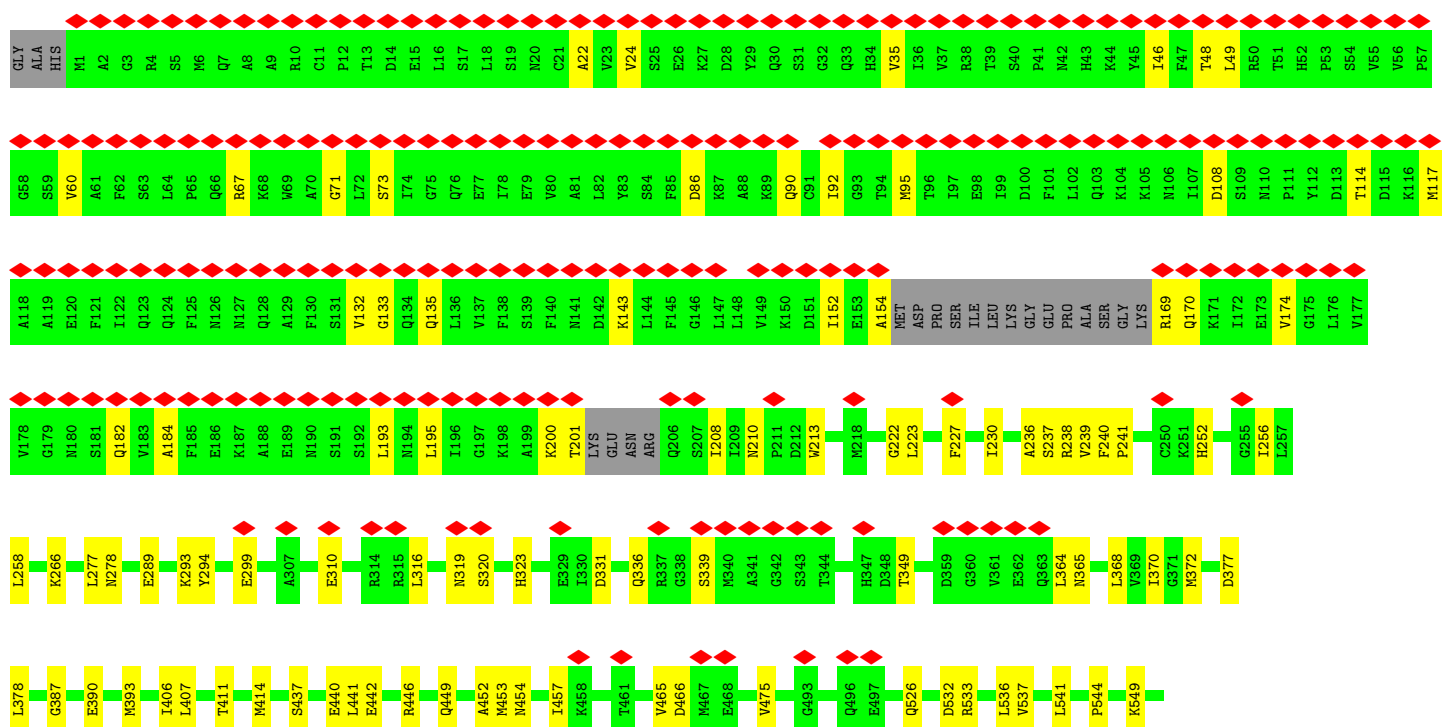
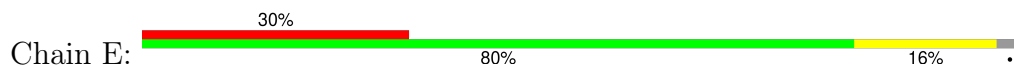
• Molecule 1: Vesicle-fusing ATPase





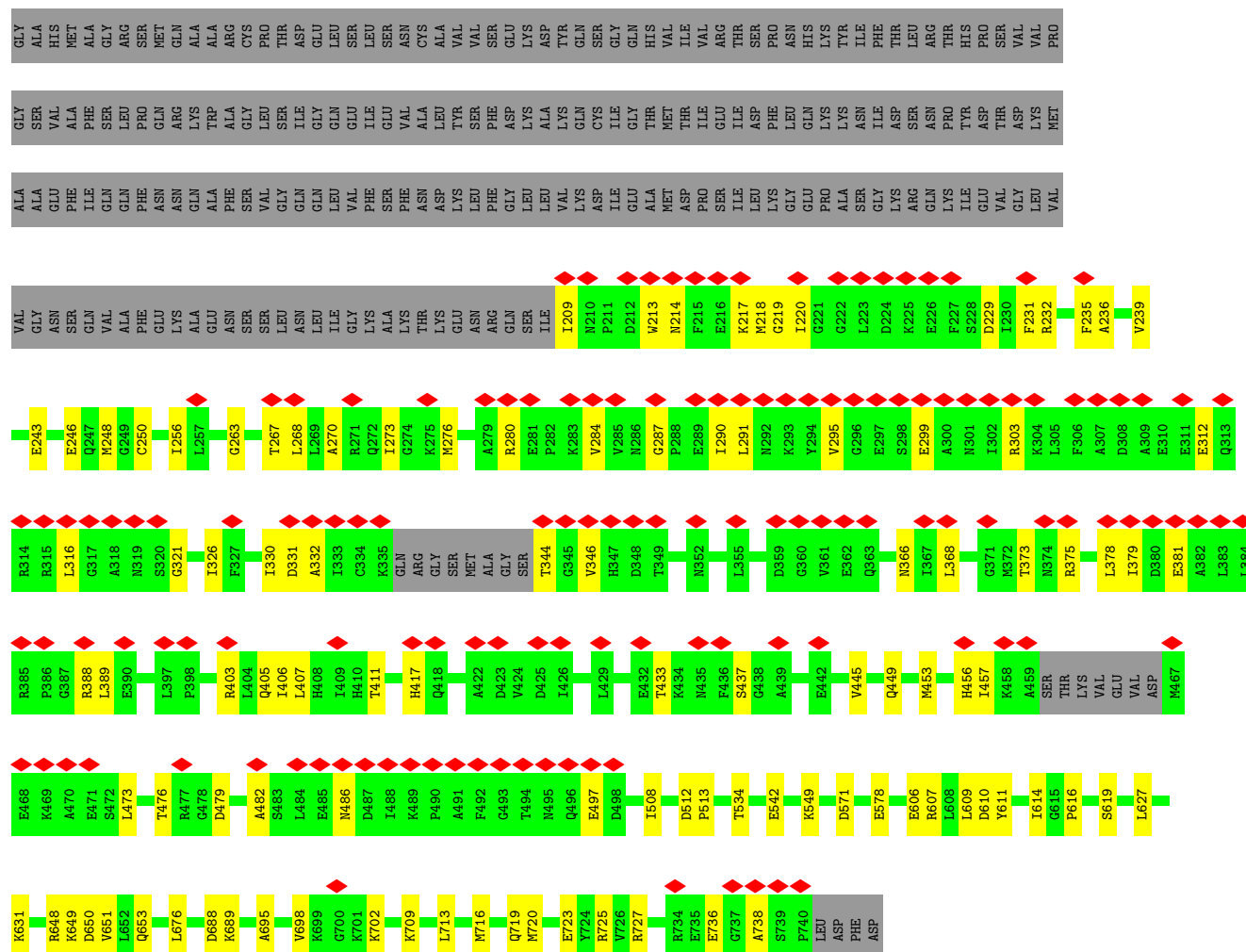


• Molecule 1: Vesicle-fusing ATPase

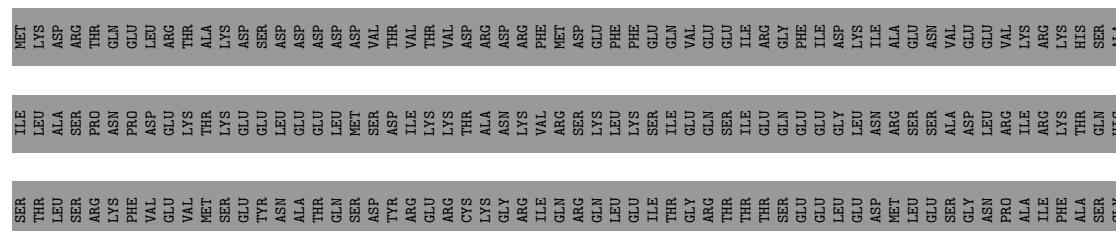


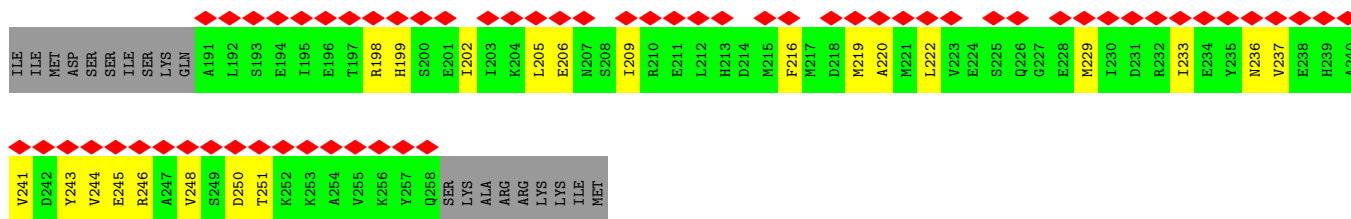


• Molecule 1: Vesicle-fusing ATPase

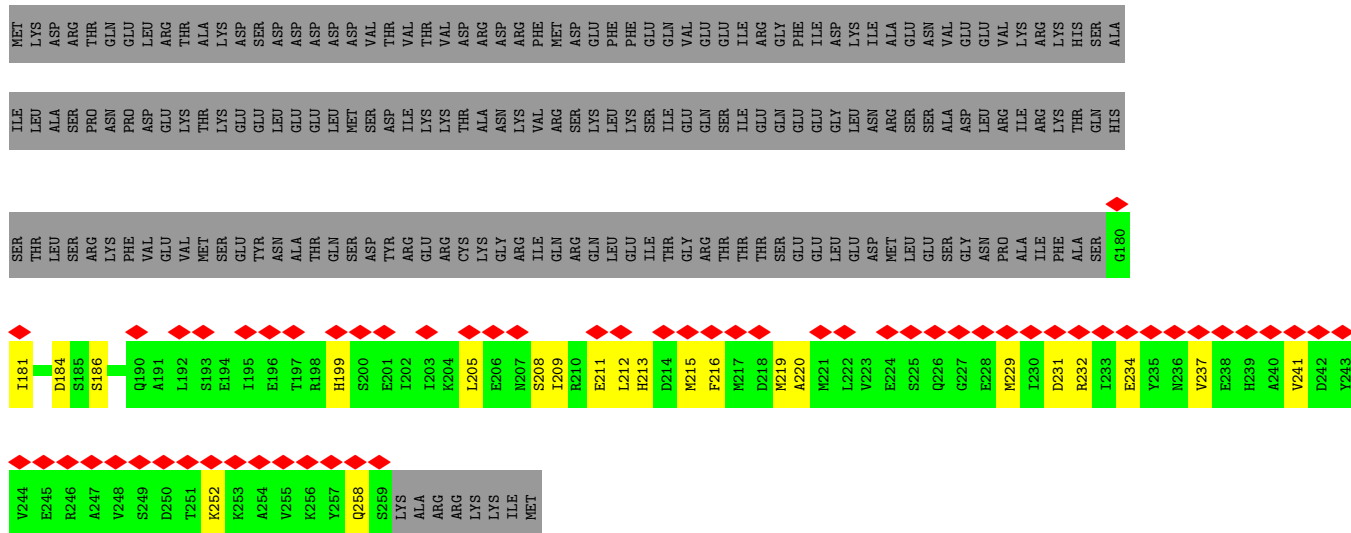


• Molecule 2: Syntaxin-1A

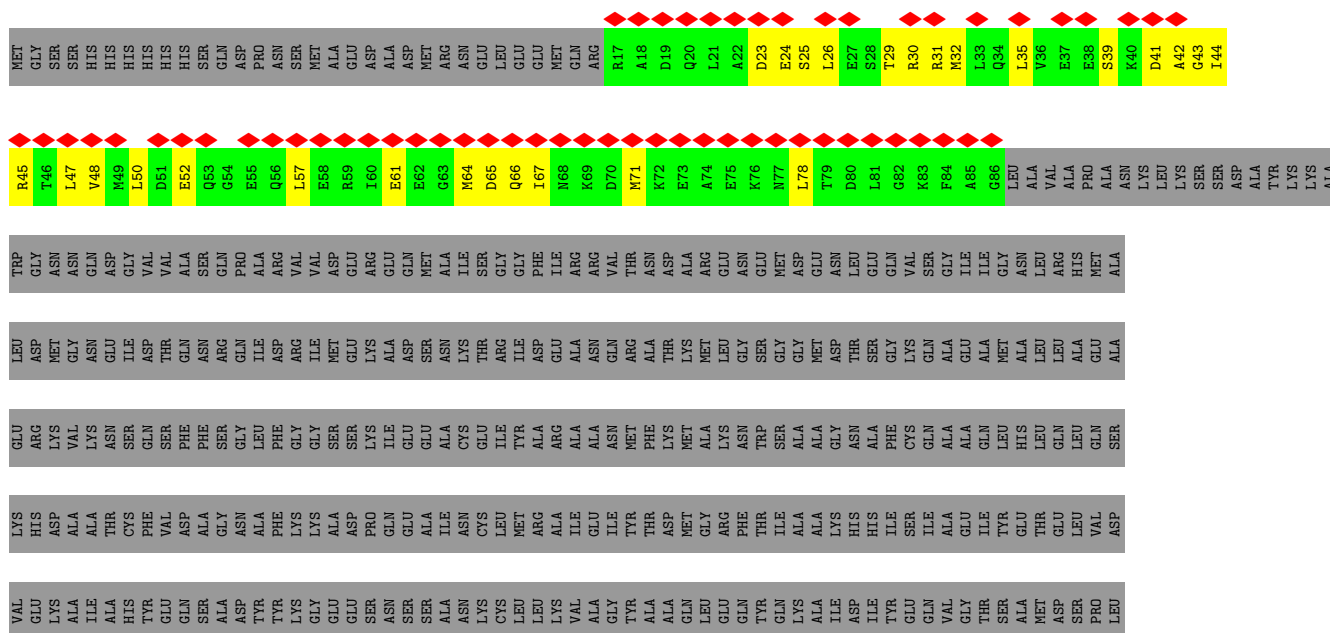




• Molecule 2: Syntaxin-1A



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



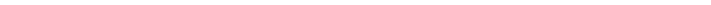
SER	THR	THR	GLU	SER	VAL	LYS	GLY	TYR	PHE	ASP	SER	ILE	SER	ARG	LEU	GLN	TRP	THR	THR	MET	LEU	ASN	LEU	ARG	ILE	LYS	ALA	LYS	LEU	GLN	ILE	GLY	ASP	GLY	GLU	ASP	PRO	PHE	LEU	DEU	ASP	CYS	HIS	LEU	ALA	LYS	ASP	LYS	VAL	ASP
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- Molecule 3: Synaptosomal-associated protein 25, Synaptosomal-associated protein 25, Alpha-soluble NSF attachment protein chimera

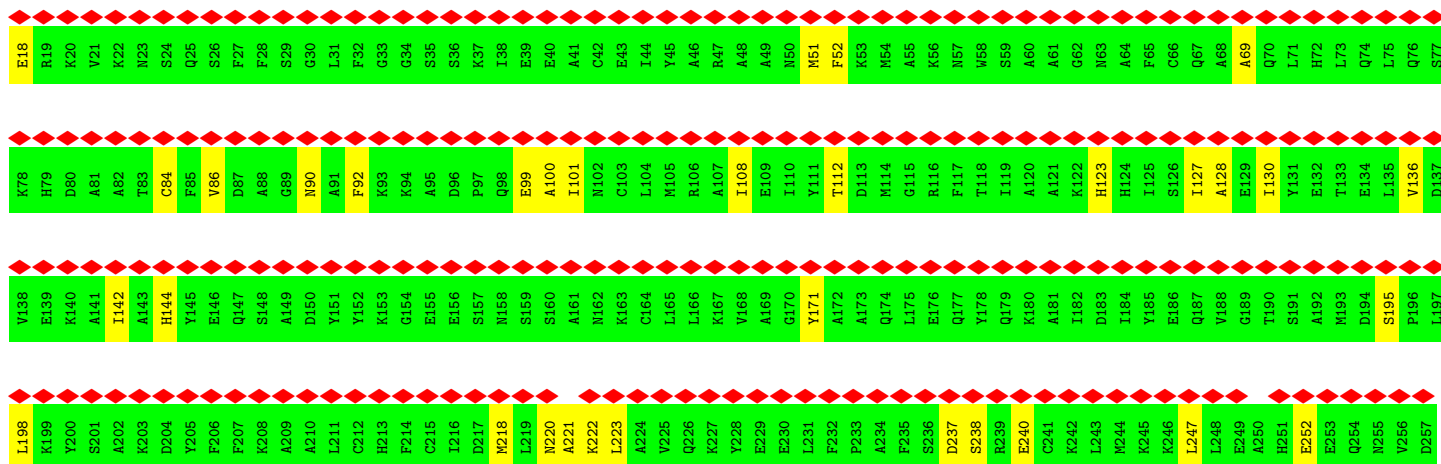
Chain J:  13% 9% 87%

LEU	VAL	LYS	GLU	LEU	ASP	TRP	R45
GLY	GLY	HIS	ARG	ASP	GLY	GLY	R46
THR	LYS	ASP	THR	MET	GLY	ASP	T46
GLU	ALA	ALA	VAL	GLY	ASN	ASN	L47
SER	ALA	ALA	ILE	ASN	GLN	GLN	V48
VAL	LYS	THR	ASN	GLU	ASP	GLY	M49
LYS	HIS	CYS	THR	ILE	GLY	VAL	L50
ASP	THR	PHE	GLN	ASP	THR	VAL	D51
GLU	GLY	VAL	ASN	THR	ALA	ALA	E52
THR	GLN	ASP	PHE	GLN	ASN	SER	Q53
PHE	SER	LYS	ALA	GLY	ARG	GLN	G54
ILE	ALA	GLY	SER	ALA	PRO	ALA	E55
SER	ASP	ASN	GLY	ILE	ALA	ALA	E56
ARG	TYR	ALA	PHE	LEU	ARG	VAL	Q56
LEU	TYR	PHE	LEU	ASP	ARG	VAL	L57
CYS	GLY	LYS	GLY	ILE	VAL	VAL	E58
ASP	GLY	ALA	GLY	MET	GLU	GLU	R59
THR	GLU	ASP	SER	GLU	GLY	ARG	I60
MET	SER	PRO	LYS	LYS	ARG	GLU	E61
THR	ASN	GLN	ILE	ALA	GLU	GLN	E62
MET	ASN	GLU	GLU	ASP	GLN	GLN	E63
LEU	SER	ALA	GLU	SER	MET	MET	G63
ALA	ALA	ILE	ALA	ASN	ALA	ALA	M64
LEU	LYS	ASN	CYS	LYS	ILE	SER	D65
ILE	LYS	CYS	GLY	THR	ARG	GLY	Q66
LYS	CYS	LEU	ILE	ARG	GLY	GLY	I67
VAL	LEU	MET	TYR	ILE	GLY	ILE	N68
GLY	LEU	ARG	ALA	ASP	GLU	ILE	R69
ASP	ALA	ILE	ALA	ALA	ARG	ARG	K69
GLU	GLY	ILE	ASN	GLN	VAL	VAL	D70
LEU	TYR	TYR	MET	ARG	THR	THR	M71
GLU	ALA	THR	PHE	ALA	ASN	ALA	K72
GLU	ALA	ASP	LYS	THR	ASP	ASP	E73
ASP	GLN	MET	GLY	LYS	ALA	ALA	A74
ARG	LEU	GLY	ALA	MET	ARG	GLU	E75
LEU	GLY	LYS	LEU	GLY	GLY	ASN	K76
ASP	GLN	PHE	ASN	THR	ASP	GLN	T77
SER	THR	ARG	THR	SER	GLU	GLU	L78
THR	THR	THR	THR	GLY	ASN	ASP	T79
ARG	GLN	THR	THR	THR	GLY	LEU	D80
GLY	GLN	ILE	THR	GLY	GLY	GLU	L81
GLU	LYS	ALA	ALA	GLY	MET	VAL	G82
CYS	ALA	LYS	ALA	ASP	ASN	GLN	K83
LYS	ILE	LYS	ILE	THR	THR	SER	PHE
LEU	ASP	HIS	ASN	SER	GLY	GLY	ALA
MET	ILE	HIS	ALA	THR	THR	ILE	ALA
LYS	TYR	ILE	THR	PHE	GLY	ILE	GLY
LYS	GLU	SER	LYS	GLY	GLN	GLY	LEU
LEU	GLN	ILE	ALA	GLN	GLN	VAL	ALA
LEU	VAL	ALA	GLY	ALA	ALA	ALA	ALA
ALA	THR	ILE	GLY	ALA	ALA	ALA	ALA
HIS	SER	TYR	GLN	LEU	ALA	ILE	ALA
GLY	THR	GLU	ALA	MET	HIS	GLY	ALA
GLU	ASP	THR	THR	GLY	GLU	GLY	ALA
ASN	SER	GLN	GLN	GLN	LEU	LEU	ALA
VAL	PRO	VAL	VAL	LEU	ALA	HIS	PRO
ASP	LEU	ASP	LEU	GLY	GLY	GLY	ASN
							ASN
							LYS
							LEU
							LYS
							K40
							D41
							SER
							SER
							ASP
							G43
							A42
							ALA
							TYR
							LYS
							LYS
							A18
							D19
							Q20
							L21
							A22
							D23
							E24
							S25
							L26</

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

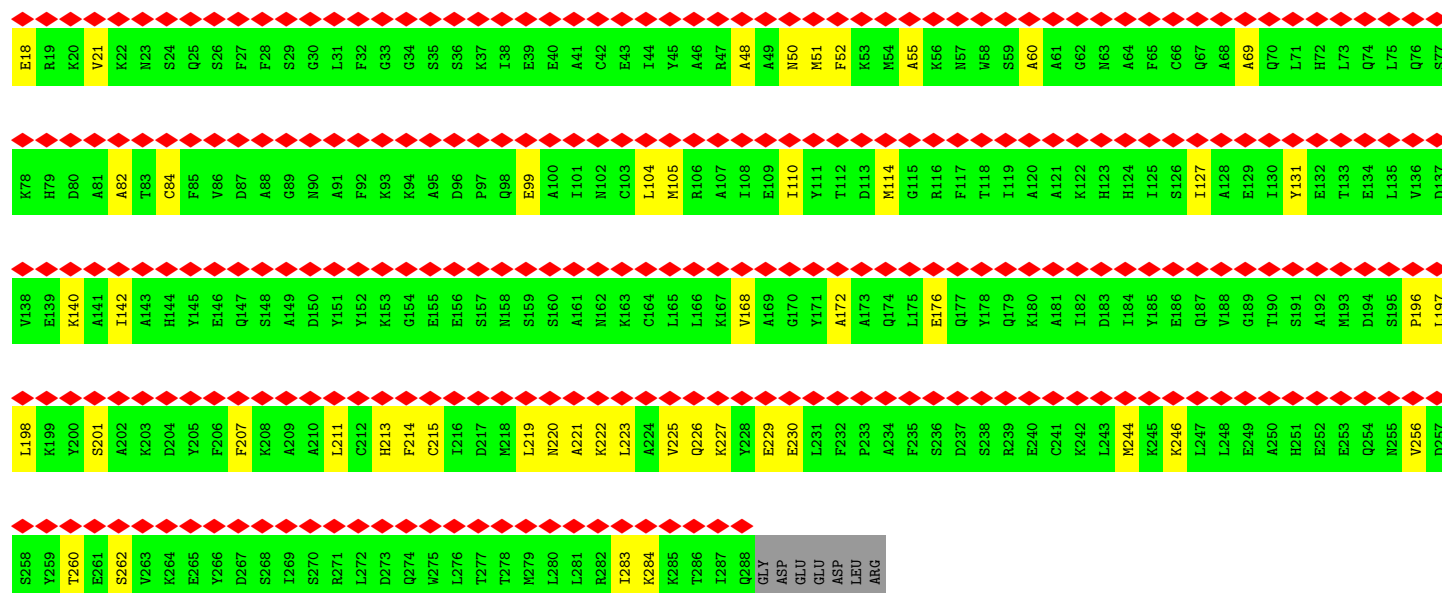
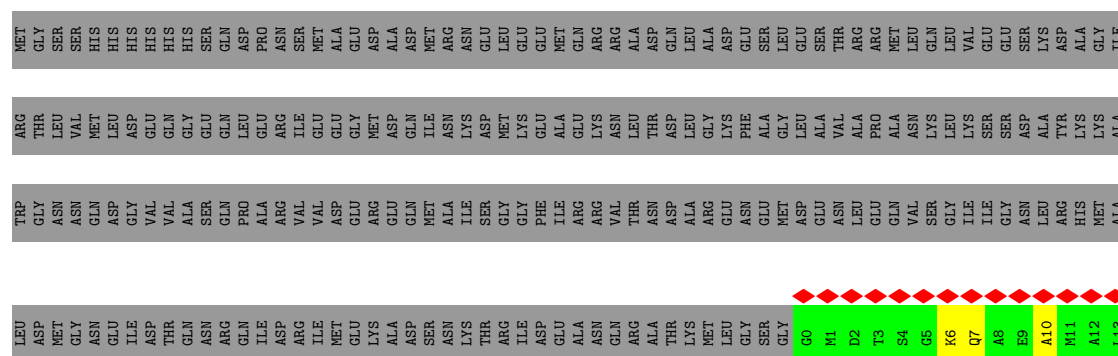
Chain K:  56% 43% 12% 44%

[illegible]

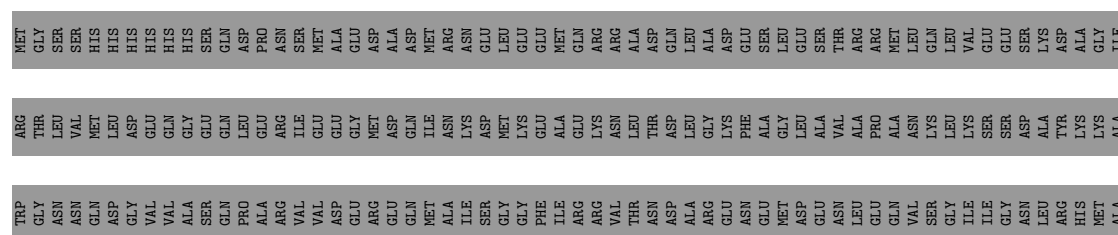
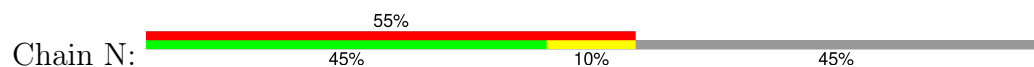




- Molecule 3: Synaptosomal-associated protein 25, Synaptosomal-associated protein 25, Alpha-soluble NSF attachment protein chimera



- 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	A82	K22	ASN
S263	K203	A143	T83	N23	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	F28	ILE
S270	A210	D150	G89	S29	ASP
K271	L211	Y151	A91	S29	ARG
L272	C212	Y152	F92	G30	ILE
D273	H213	K153	K93	L31	MET
Q274	F214	G154	K94	F32	GLY
W275	C215	E155	A95	G33	LYS
L276	I216	E156	D96	G34	ALA
T277	D217	S157	P97	G34	ASP
T278	M218	N158	Q98	S35	SER
M279	L219	S159	E99	S35	ASN
L280	N220	S160	A100	S36	LYS
L281	A221	A161	I101	K37	ASN
R282	K222	N162	N102	E40	GLN
L283	L223	K163	C103	A41	ARG
K284	A224	C164	L104	E43	ALA
K285	V225	L165	M105	I44	ALA
T286	Q226	L166	Y45	Y45	THR
ILE	K227	K167	R106	A46	LYS
GLN	Y228	V168	A107	R47	LYS
GLY	E229	A169	I108	Y47	MET
ASP	E230	G170	E109	A48	LEU
GLU	L231	Y171	Y111	A49	GLY
ASP	F232	A172	T112	N50	SER
LEU	P233	A173	D113	M51	GLY
ARG	A234	Q174	M114	F52	GLY
	F235	L175	G115	K53	G0
	S236	E176	R116	M54	M1
	D237	Q177	F117	A55	T3
	S238	Y178	T118	K56	S4
	R239	Q179	I119	N57	C5
	E240	K180	A120	W58	R6
	C241	A181	A121	S59	Q7
	K242	I182	K122	A60	A8
	L243	D183	H123	A61	E9
	M244	I184	H124	G62	M1
	K245	Y185	I125	N63	A12
	K246	E186	S126	A64	L13
	L247	Q187	I127	F65	L14
	L248	V188	A128	C66	A15
	E249	G189	E129	Q67	E16
	A250	T190	I130	A68	A17
	H251	S191	Y131	A69	
	E252	A192	E132	Q70	
	E253	M193	T133	L71	
	Q254	D194	E134	W73	
	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 (Å)	322.224, 322.224, 322.224	wwPDB
Map dimensions	294, 294, 294	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: PO4, ATP, ADP

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...

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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	F	802	-	24,29,29	0.89	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	E	802	-	28,33,33	0.75	0	34,52,52	0.96	2 (5%)
4	ADP	D	802	-	24,29,29	0.84	0	29,45,45	1.26	2 (6%)
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%)
5	ATP	A	802	-	28,33,33	0.72	0	34,52,52	0.88	1 (2%)
5	ATP	C	801	-	28,33,33	0.81	0	34,52,52	0.89	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
4	ADP	A	801	-	24,29,29	0.88	0	29,45,45	1.25	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%)

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

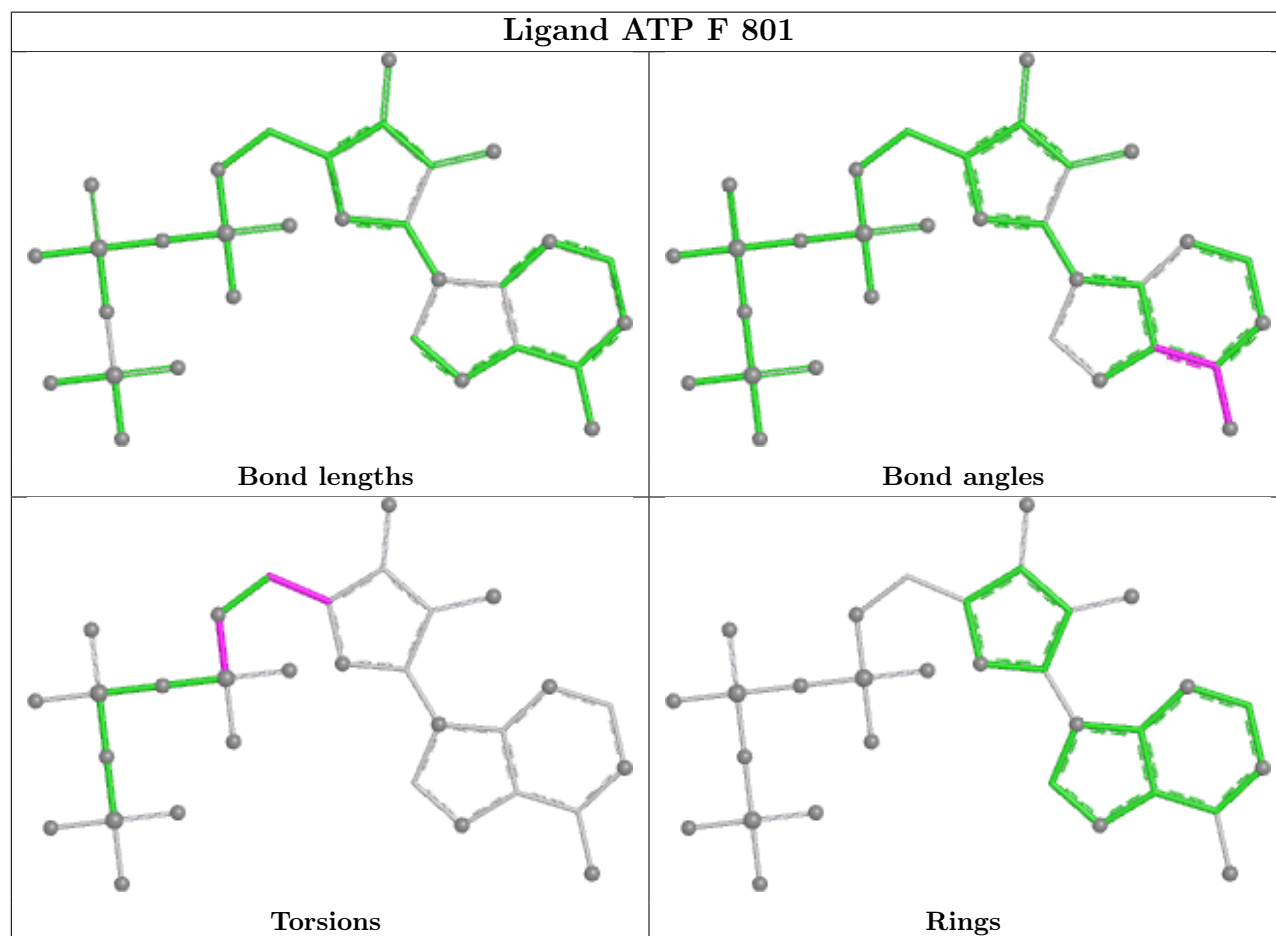
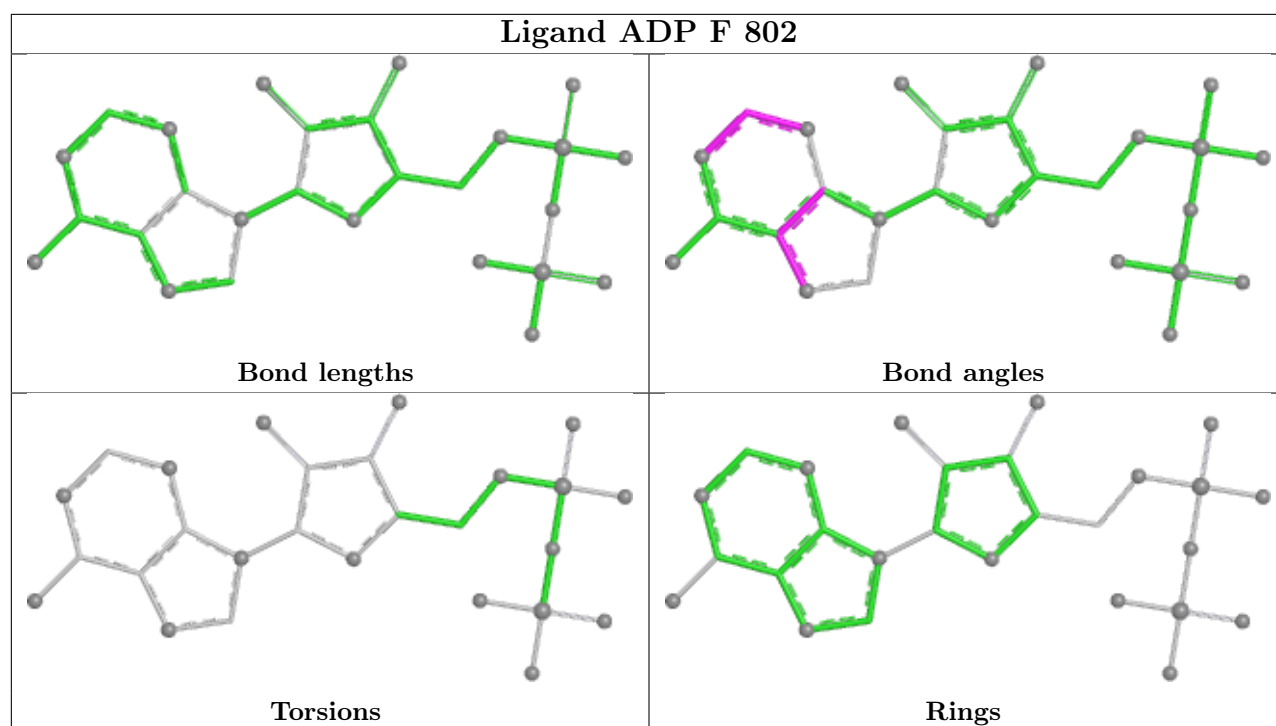
Mol	Chain	Res	Type	Atoms
4	B	802	ADP	C5'-O5'-PA-O1A
4	C	802	ADP	C5'-O5'-PA-O3A
4	D	802	ADP	C5'-O5'-PA-O1A
4	D	802	ADP	C5'-O5'-PA-O3A
5	A	802	ATP	PB-O3B-PG-O2G

There are no ring outliers.

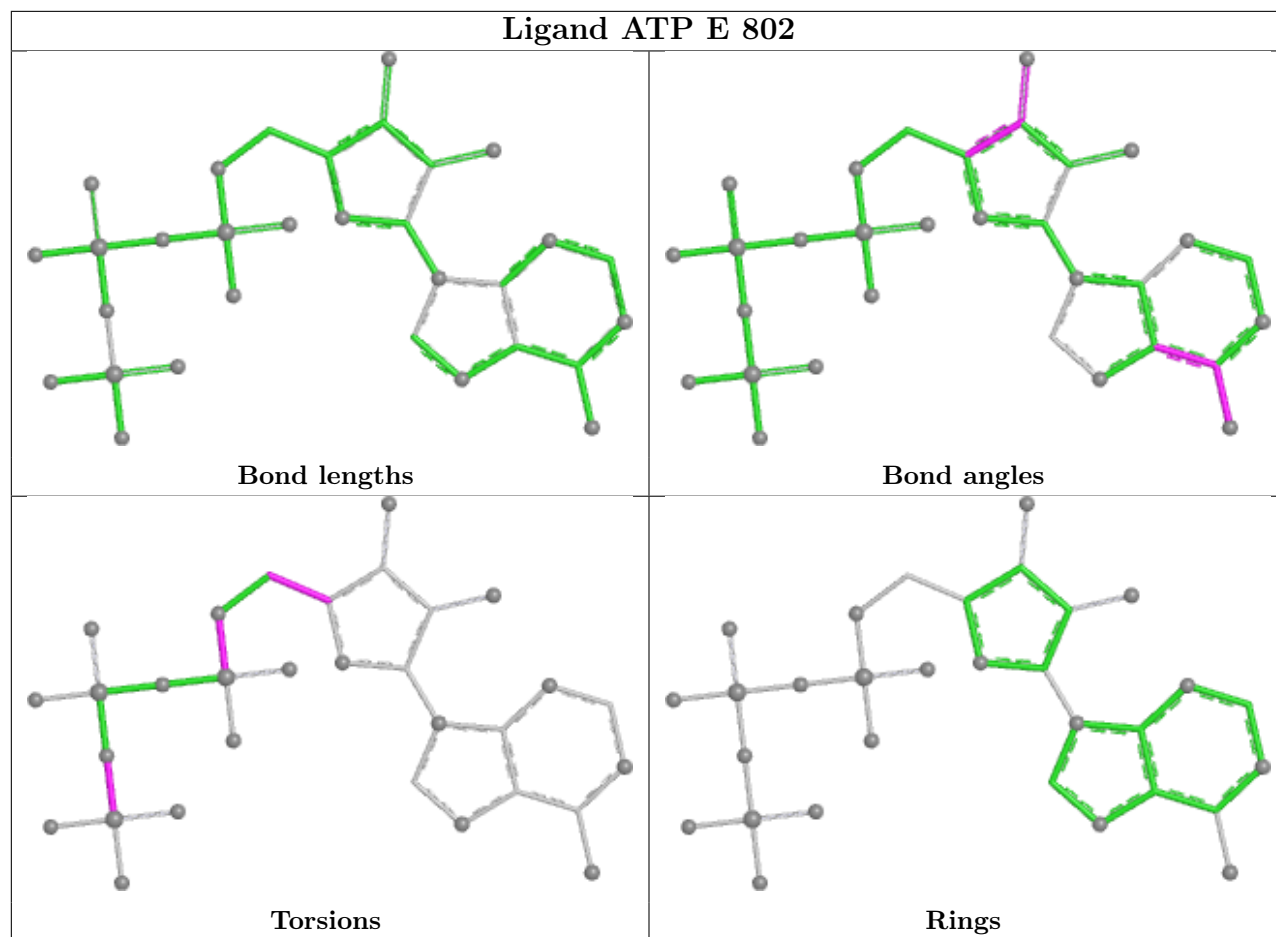
7 monomers are involved in 8 short contacts:

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

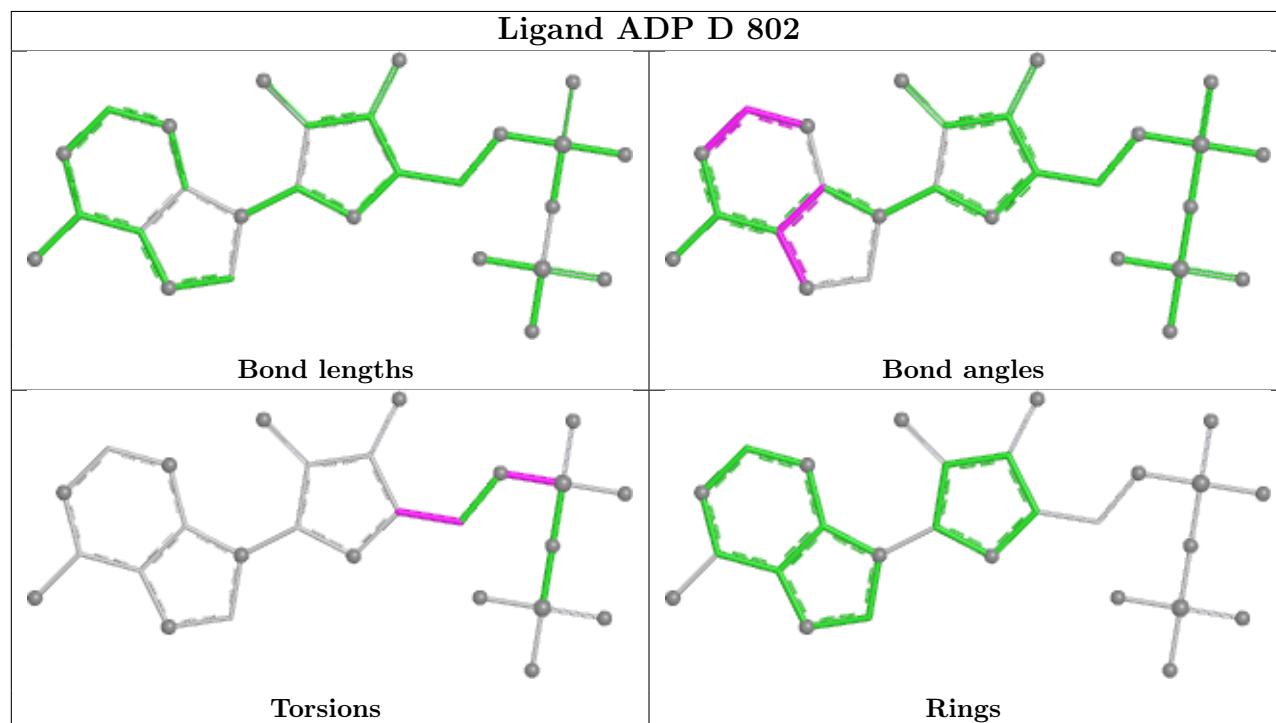
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

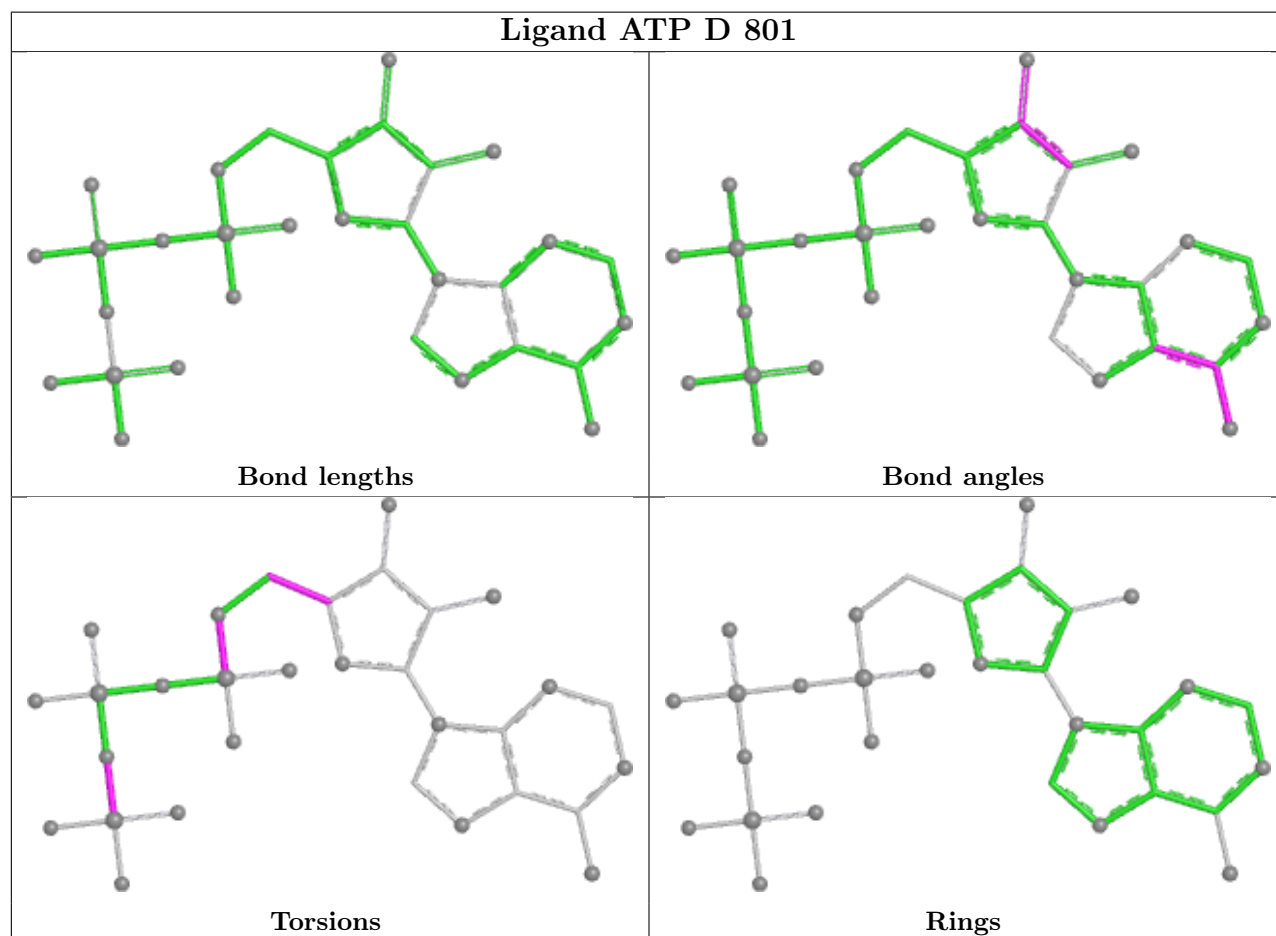
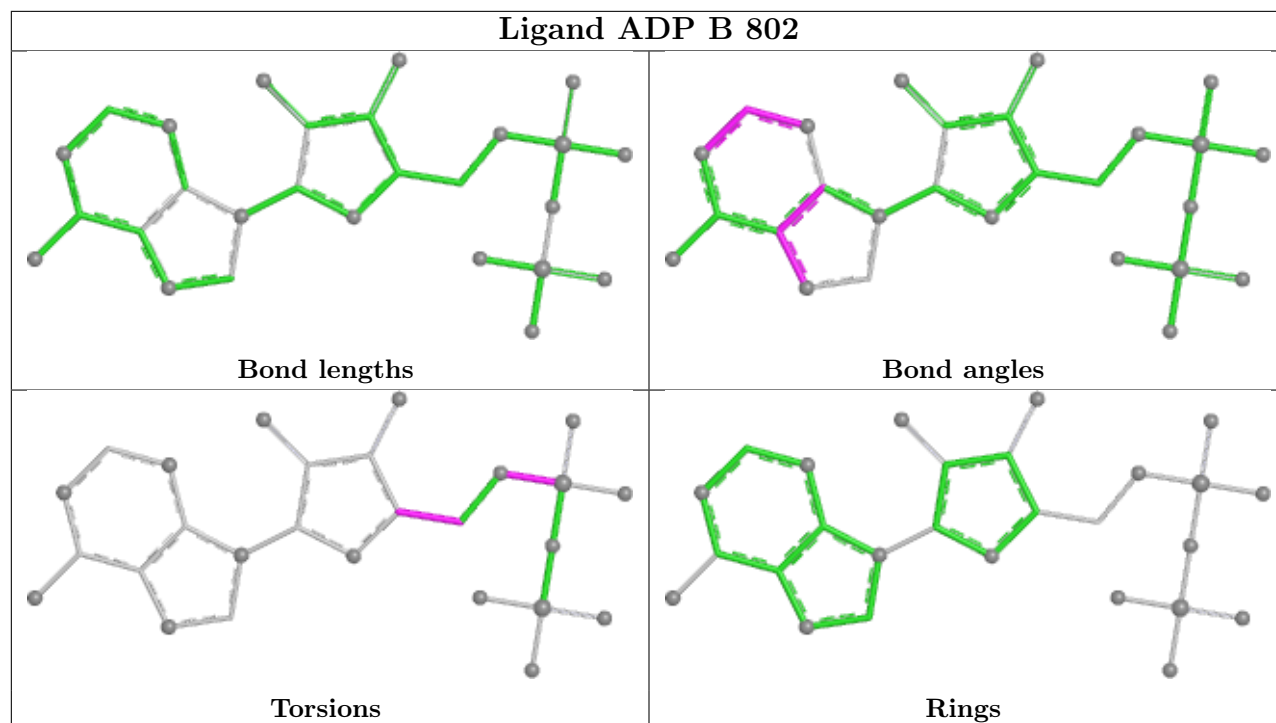


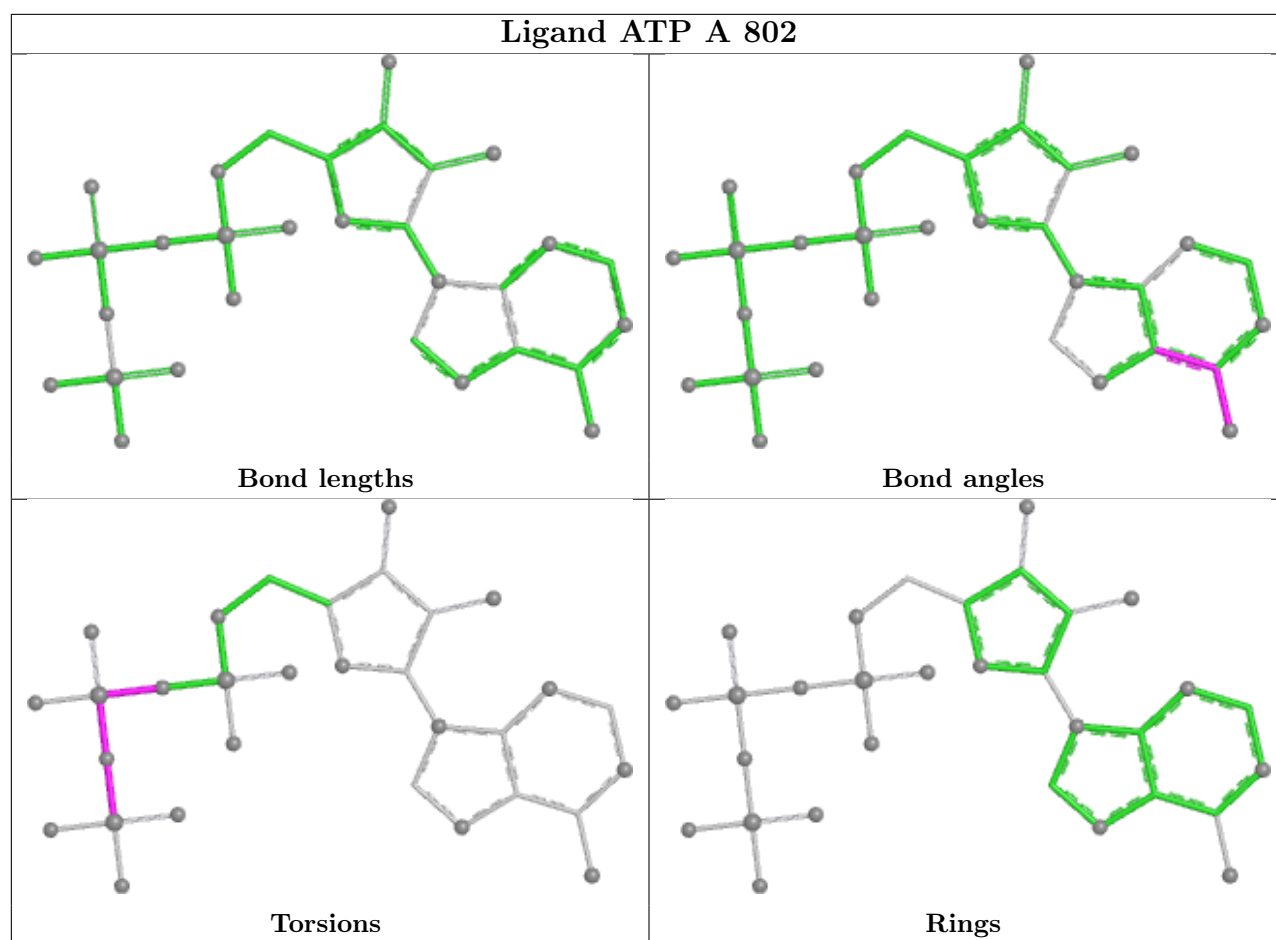
Ligand ATP E 802

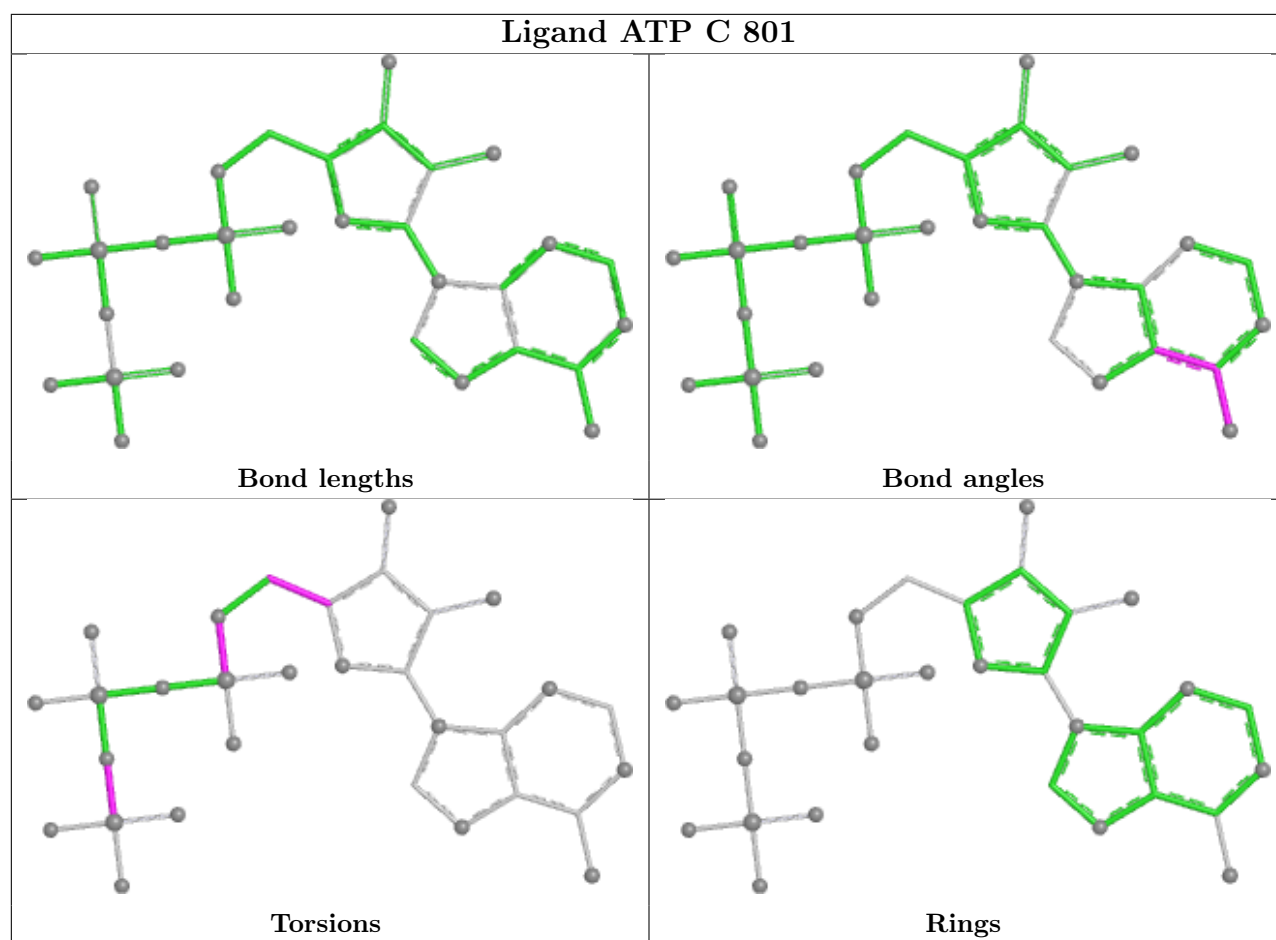


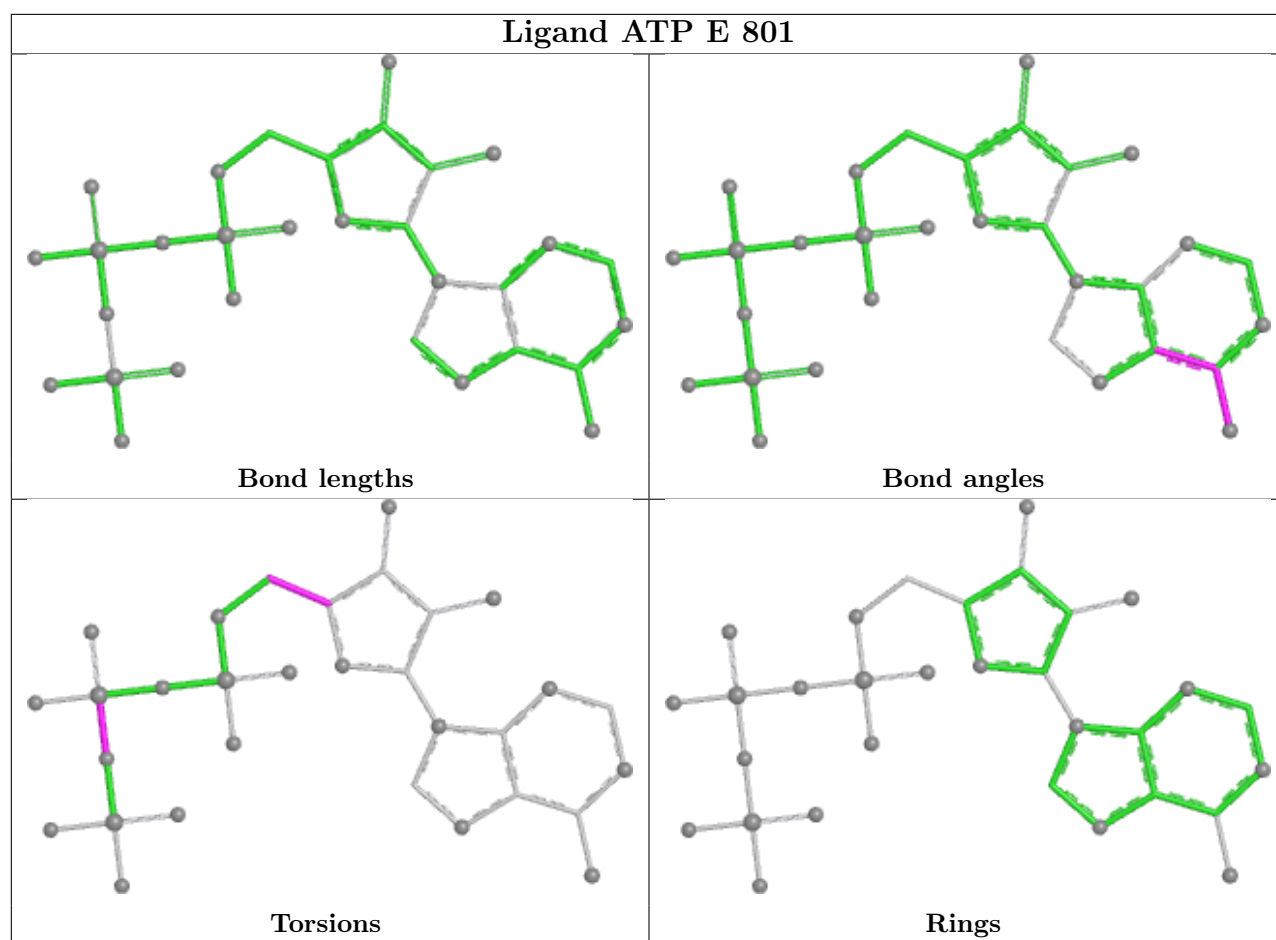
Ligand ADP D 802



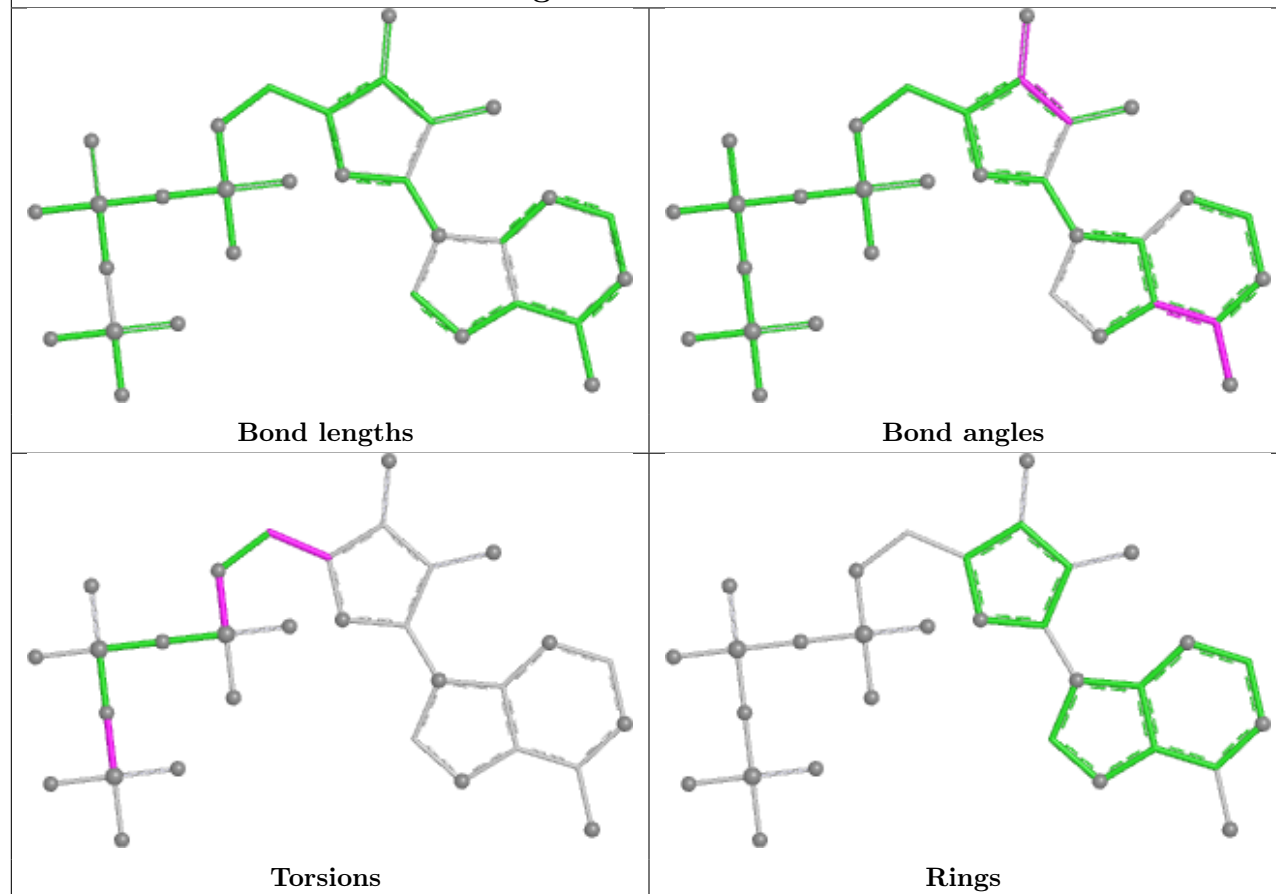




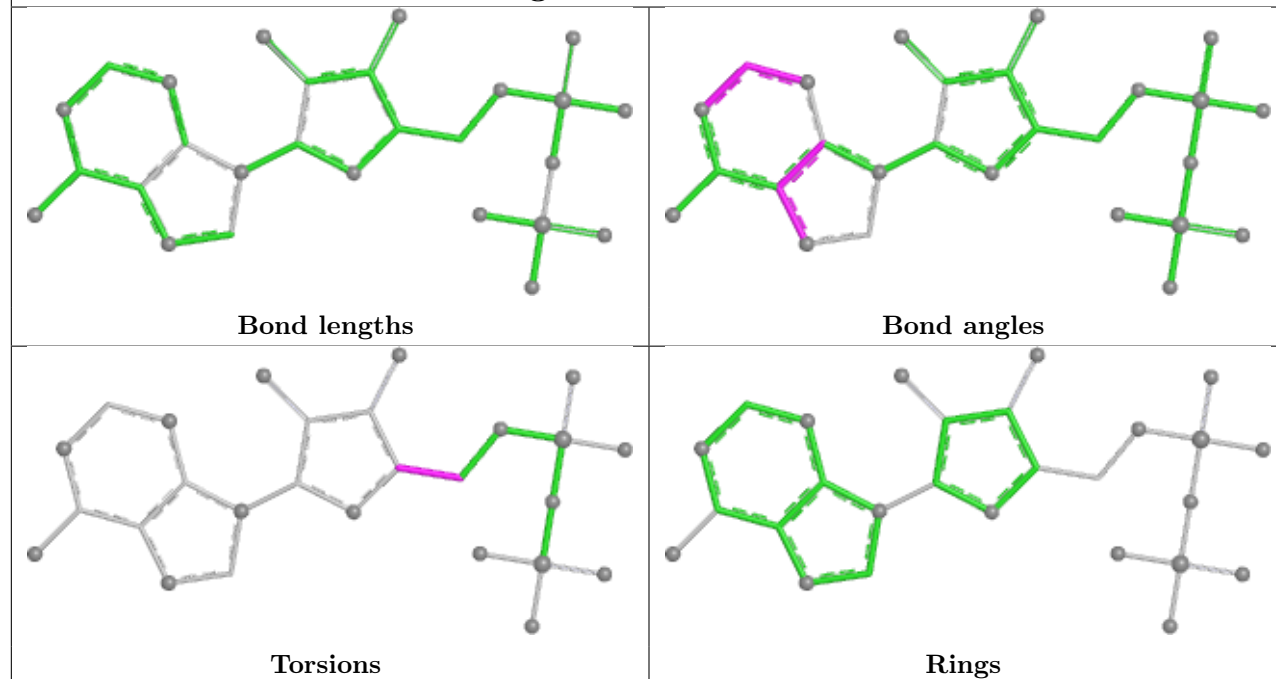


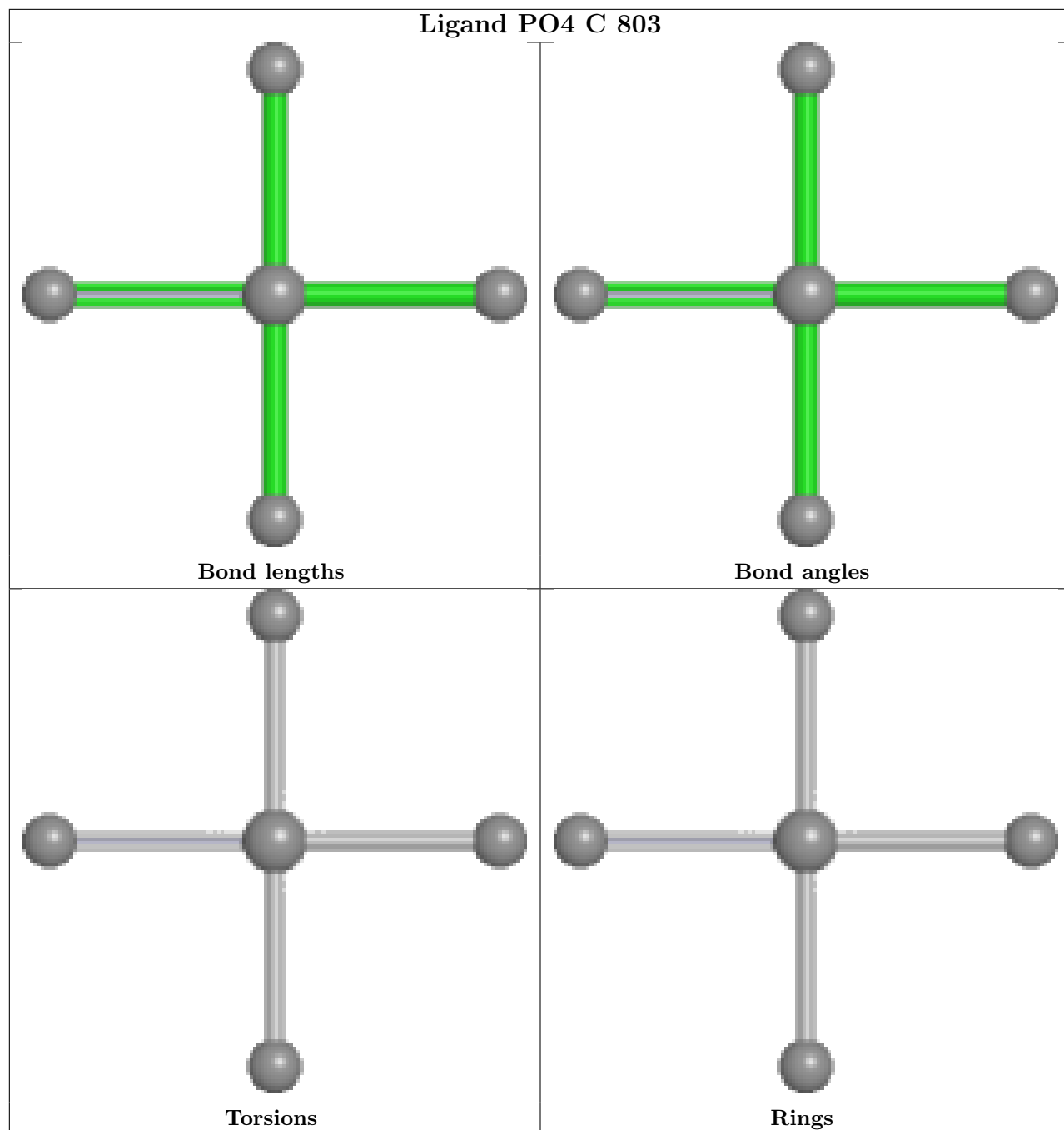


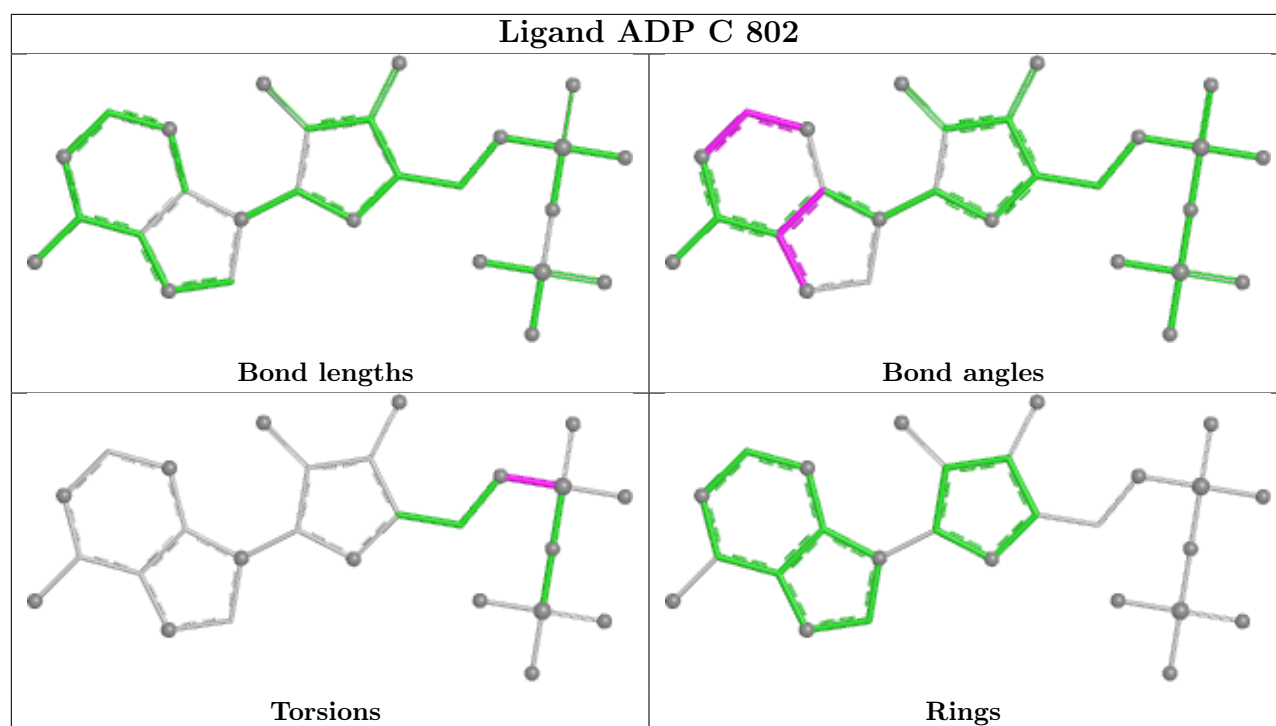
Ligand ATP B 801



Ligand ADP A 801







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.

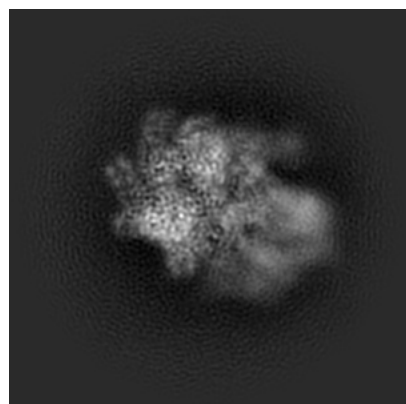
6 Map visualisation [i](#)

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.

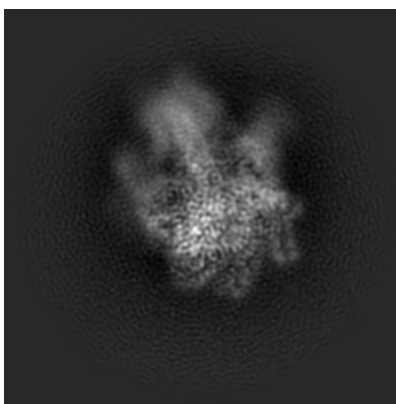
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

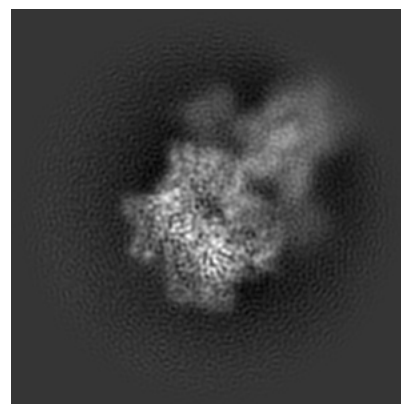
6.1.1 Primary map



X

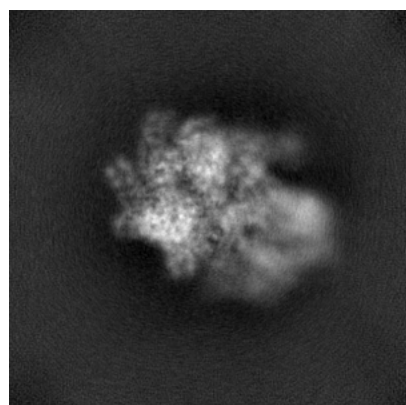


Y

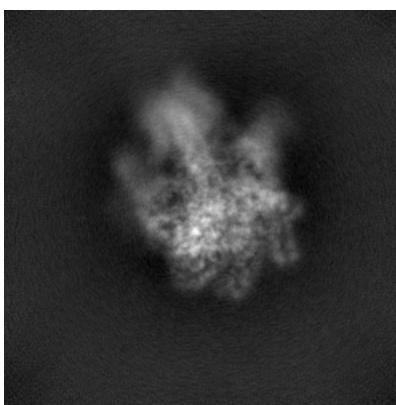


Z

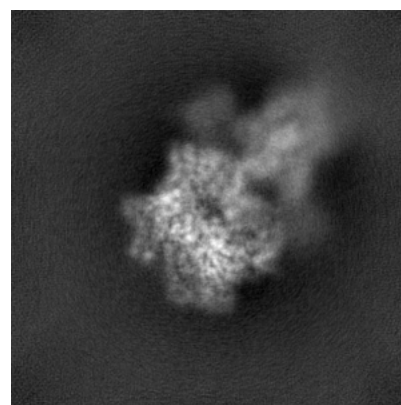
6.1.2 Raw map



X



Y

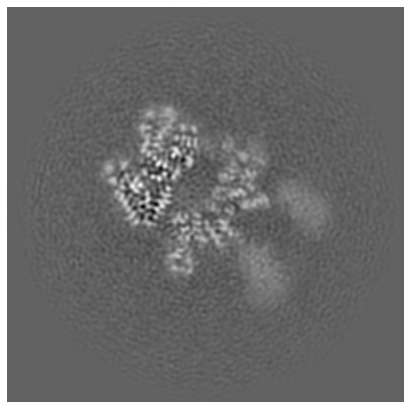


Z

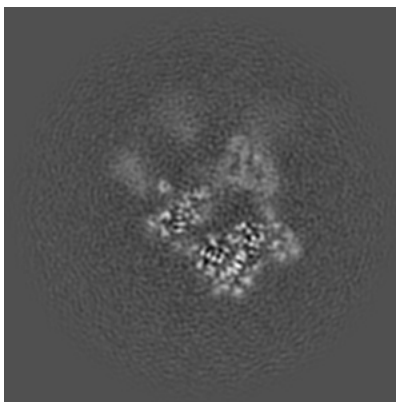
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

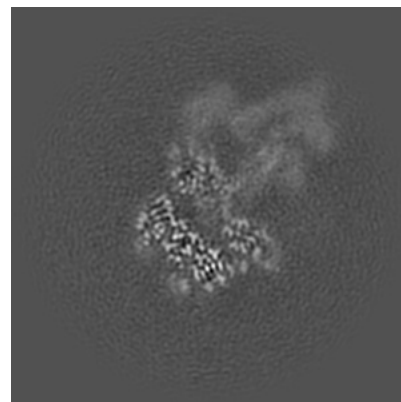
6.2.1 Primary map



X Index: 147

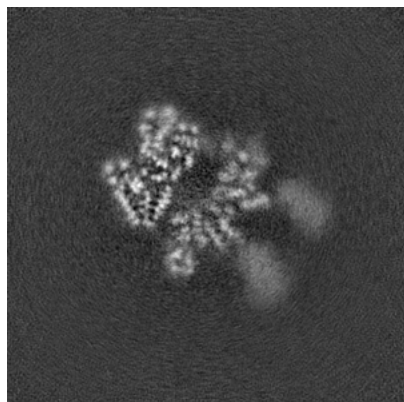


Y Index: 147

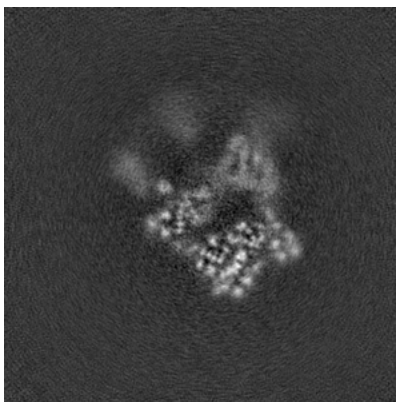


Z Index: 147

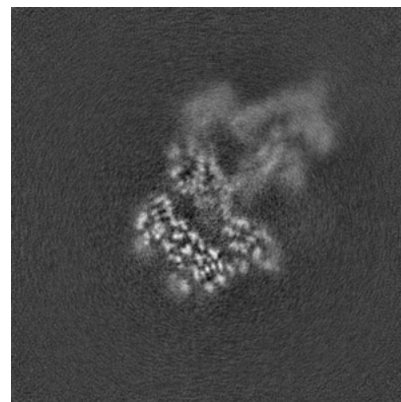
6.2.2 Raw map



X Index: 147



Y Index: 147

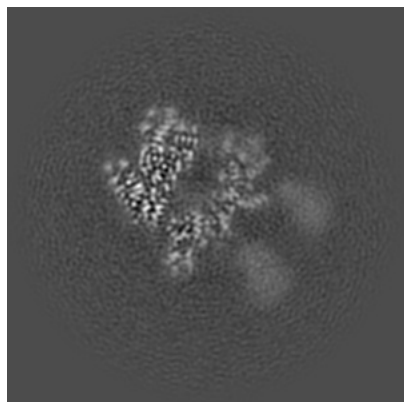


Z Index: 147

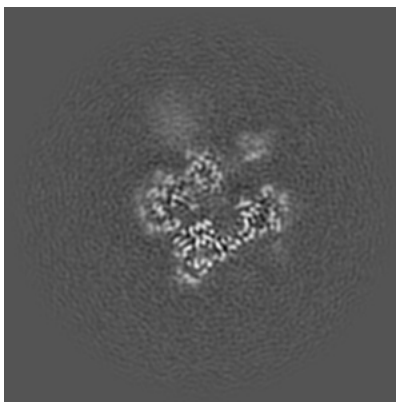
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

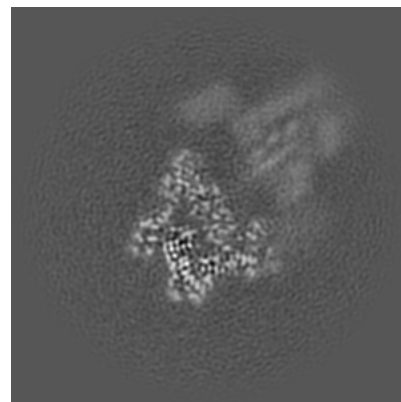
6.3.1 Primary map



X Index: 149

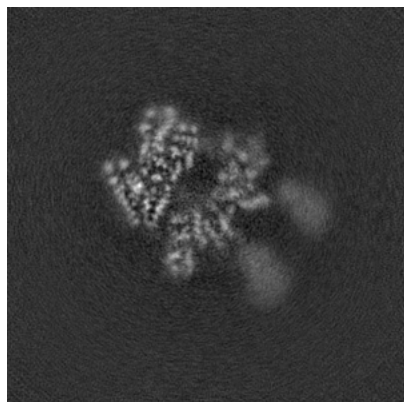


Y Index: 126

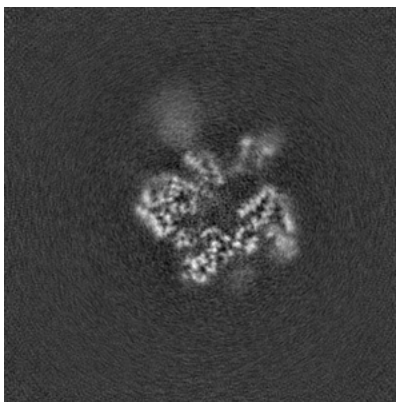


Z Index: 138

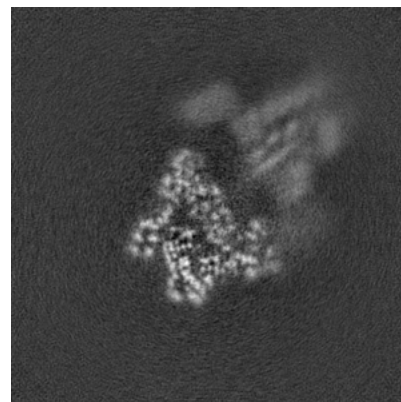
6.3.2 Raw map



X Index: 148



Y Index: 132

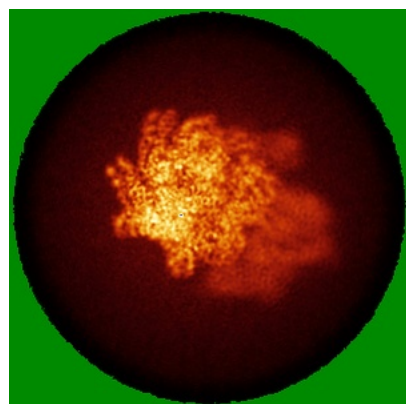


Z Index: 138

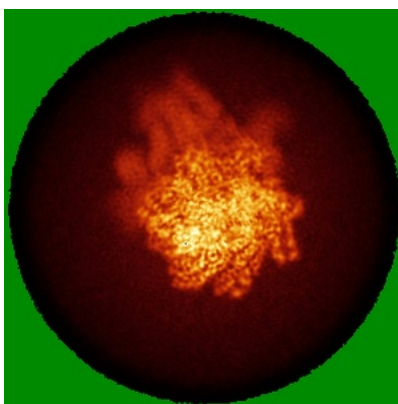
The images above show the largest variance slices of the map in three orthogonal directions.

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

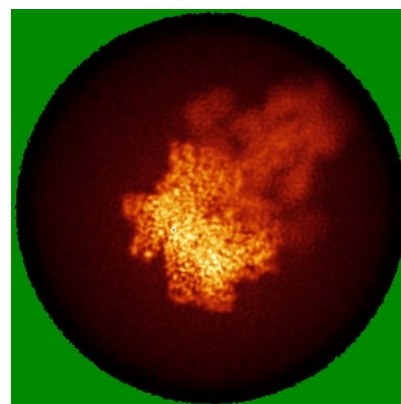
6.4.1 Primary map



X

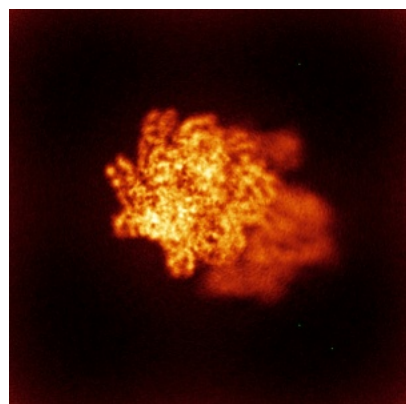


Y

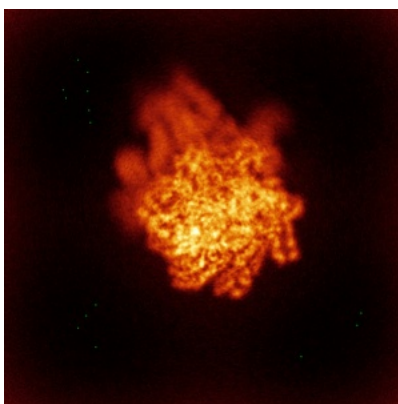


Z

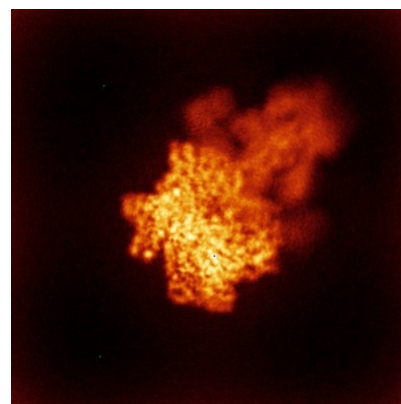
6.4.2 Raw map



X



Y

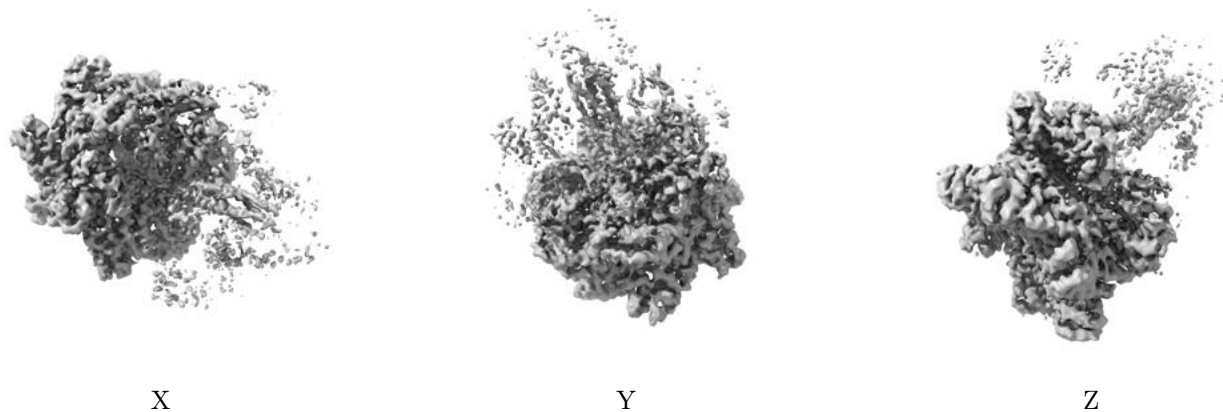


Z

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.

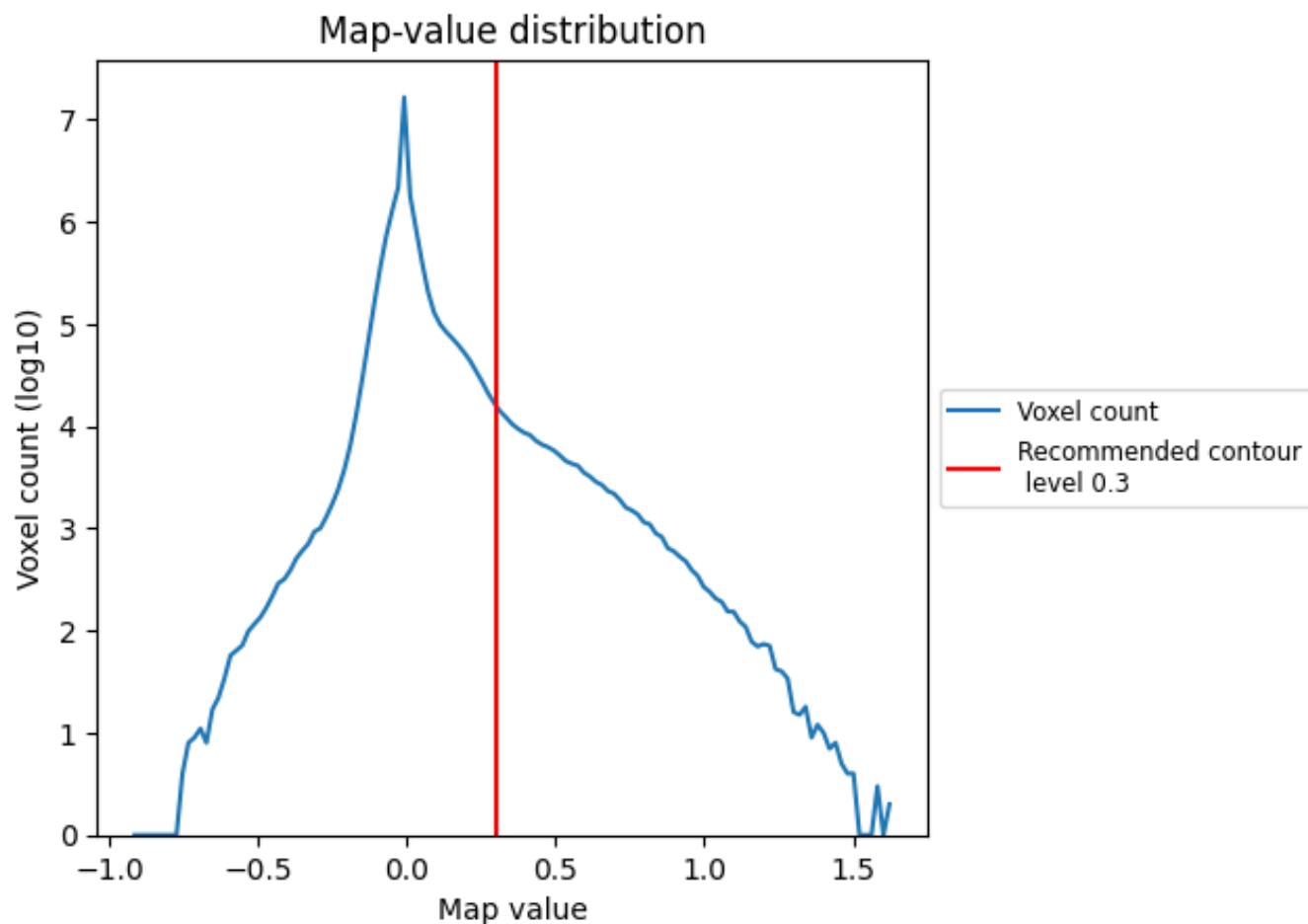
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

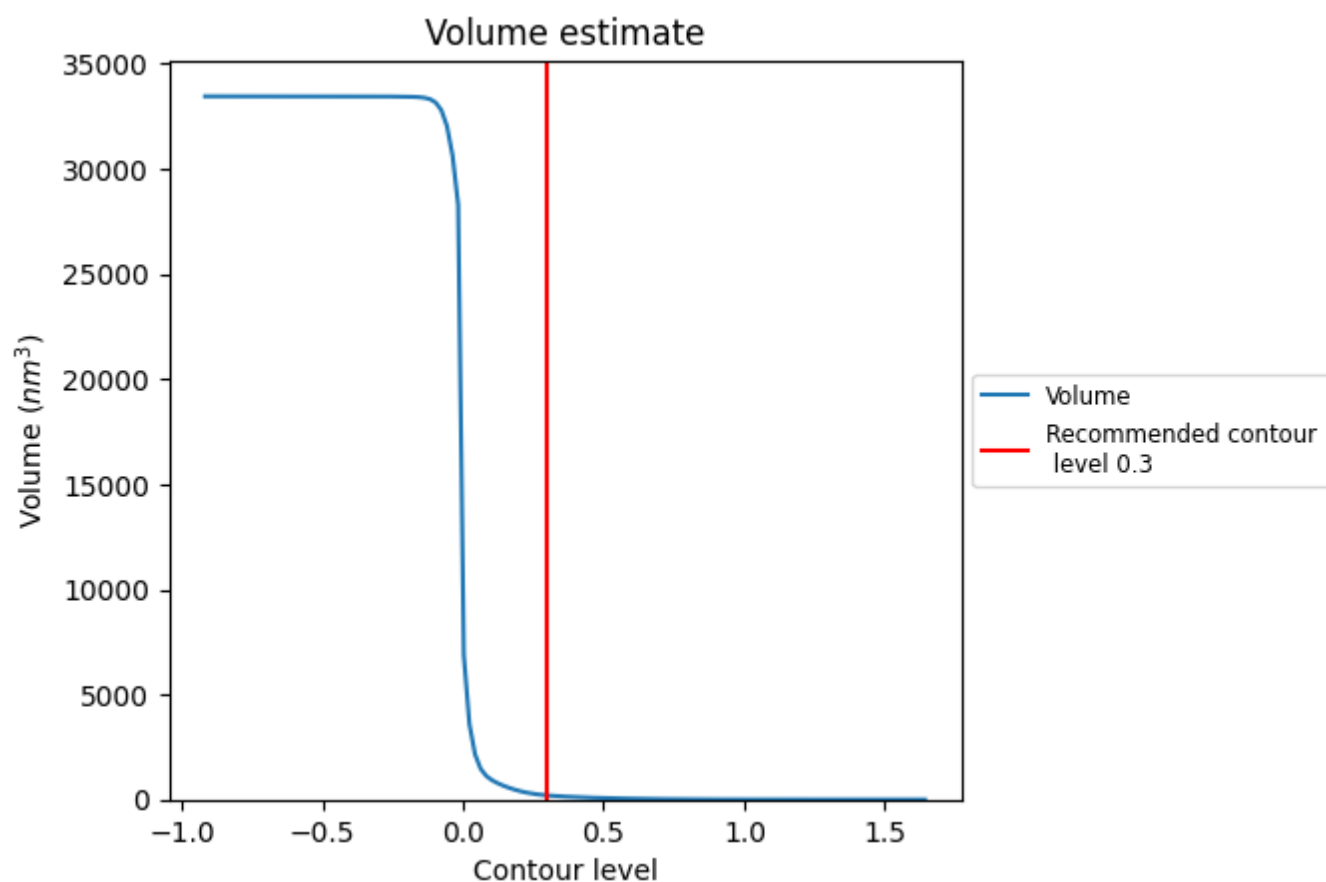
This section contains the results of statistical analysis of the map.

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.

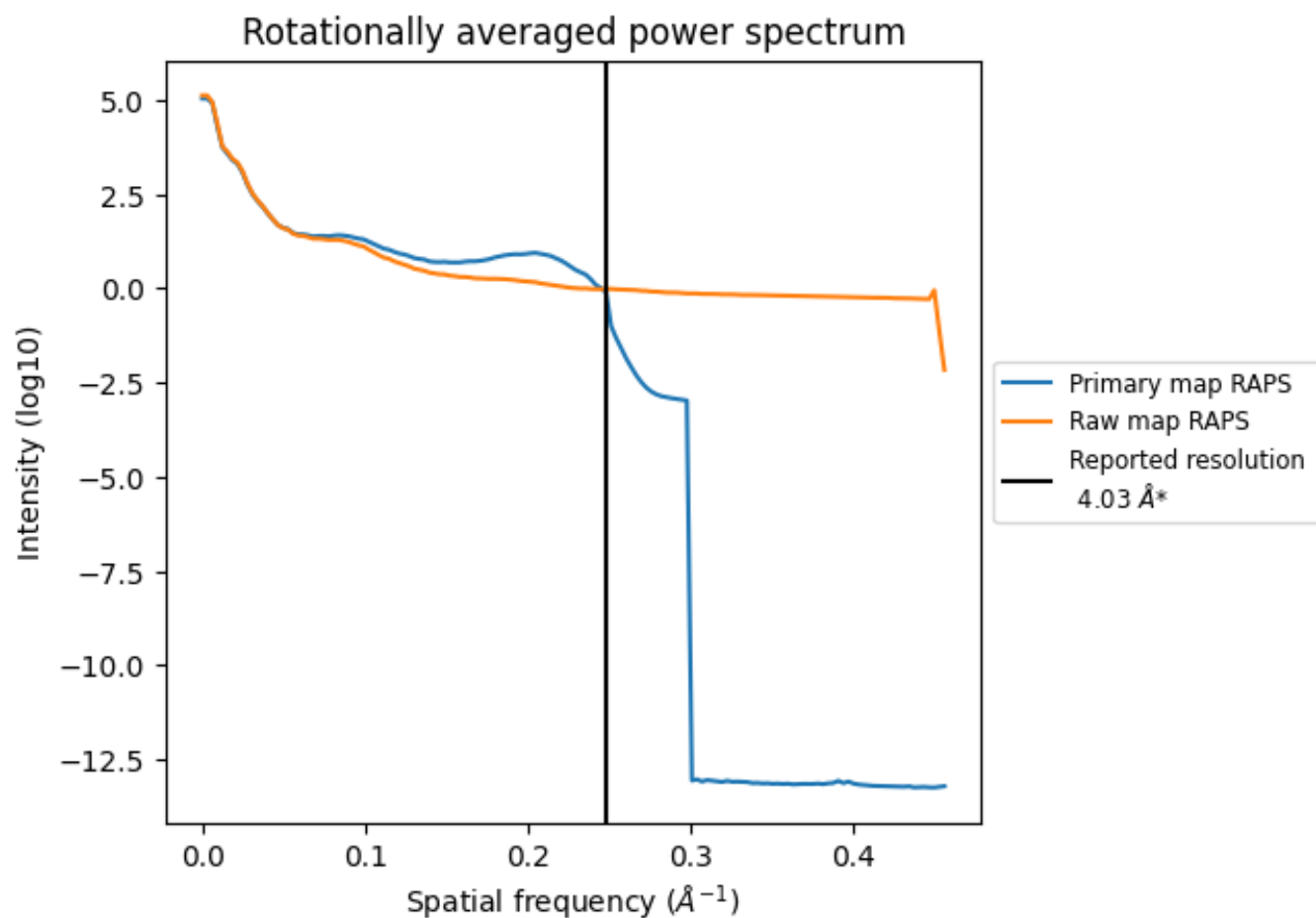
7.2 Volume estimate [i](#)



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 ⓘ

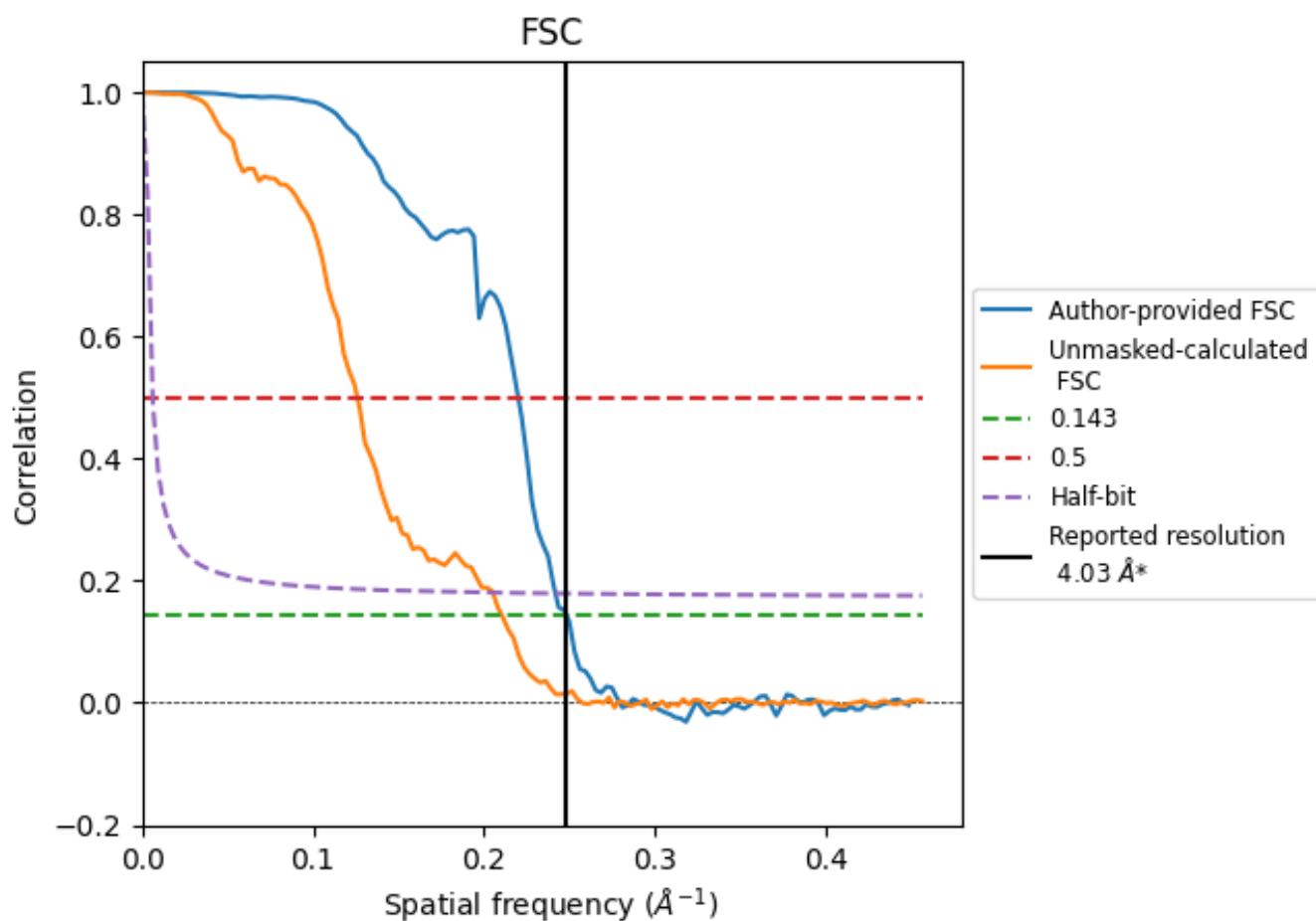


*Reported resolution corresponds to spatial frequency of 0.248 Å⁻¹

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](#)

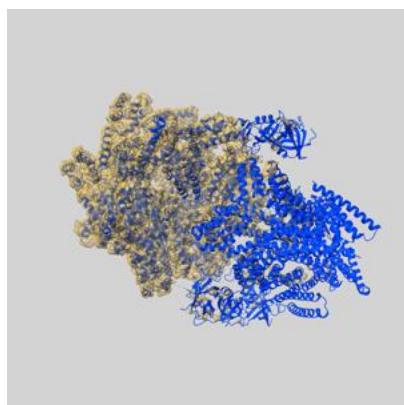
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.03	-	-
Author-provided FSC curve	4.03	4.55	4.14
Unmasked-calculated*	4.75	7.94	4.88

*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 %

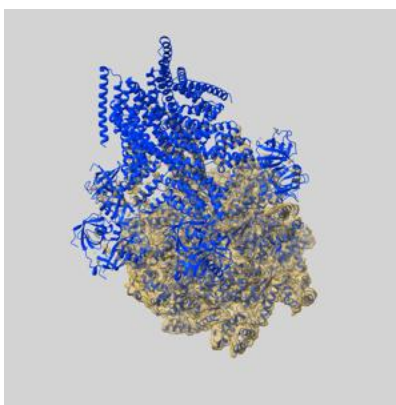
9 Map-model fit [i](#)

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](#).

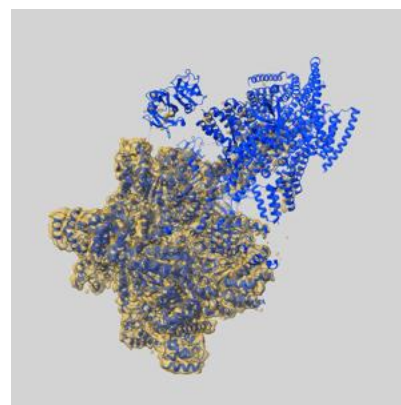
9.1 Map-model overlay [i](#)



X



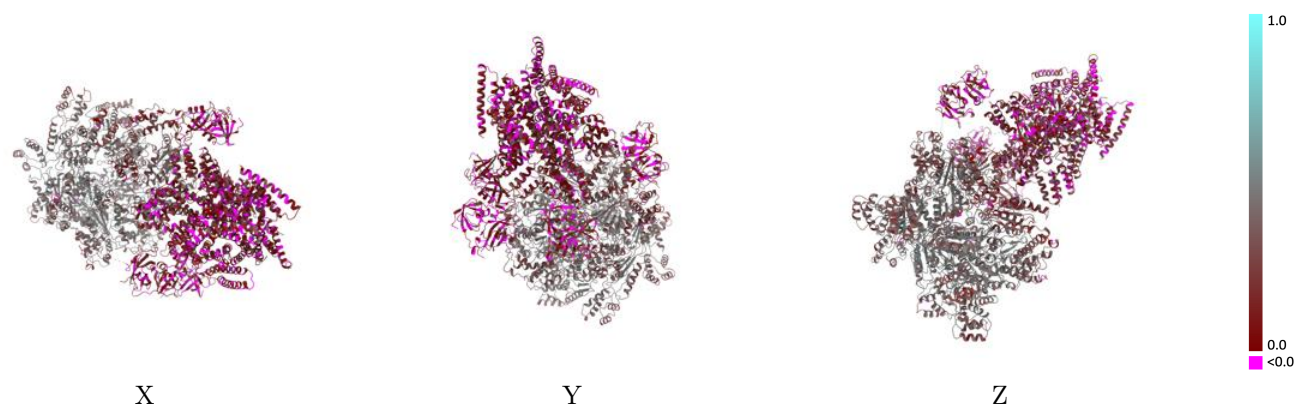
Y



Z

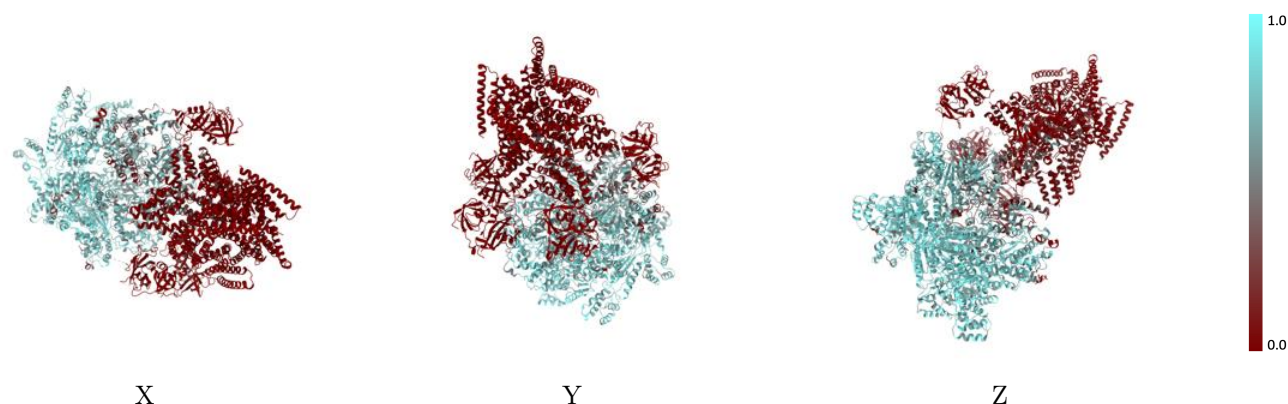
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



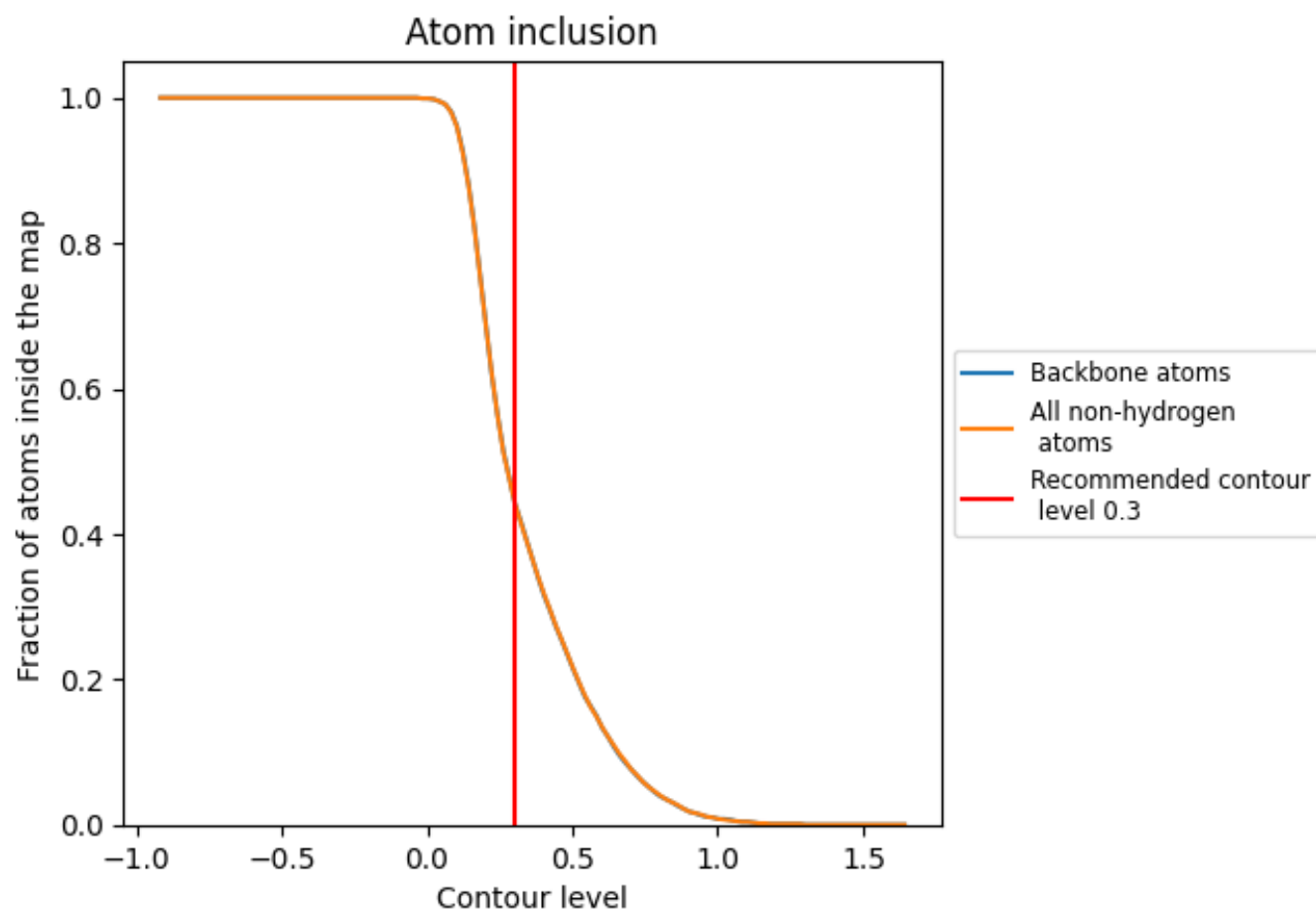
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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