



## wwPDB EM Validation Summary Report ⓘ

Jul 28, 2025 – 03:59 PM EDT

PDB ID : 9PD8 / pdb\_00009pd8  
EMDB ID : EMD-71529  
Title : 22bin20S complex (NSF-alphaSNAP-2:2 syntaxin-1a:SNAP-25), hydrolyzing, class 21  
Authors : White, K.I.; Brunger, A.T.  
Deposited on : 2025-06-30  
Resolution : 4.23 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

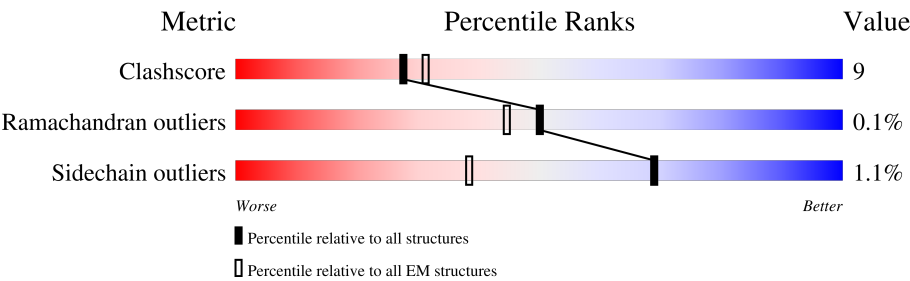
EMDB validation analysis : 0.0.1.dev126  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.23 Å.

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





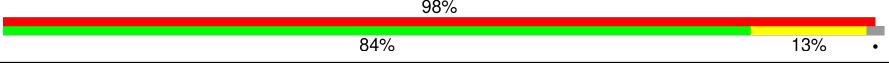
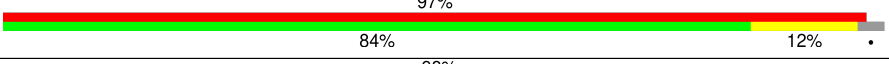
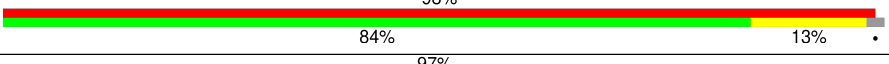


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	747	<div><div>33%</div><div>75%</div><div>21%</div><div>• •</div></div>
1	B	747	<div><div>32%</div><div>75%</div><div>21%</div><div>• •</div></div>
1	C	747	<div><div>31%</div><div>74%</div><div>23%</div><div>•</div></div>
1	D	747	<div><div>8%</div><div>56%</div><div>16%</div><div>28%</div></div>
1	E	747	<div><div>15%</div><div>59%</div><div>12%</div><div>28%</div></div>
1	F	747	<div><div>47%</div><div>79%</div><div>16%</div><div>5%</div></div>
2	I	518	<div><div>13%</div><div>8%</div><div>6%</div><div>86%</div></div>
2	J	518	<div><div>12%</div><div>8%</div><div>•</div><div>88%</div></div>

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Mol	Chain	Length	Quality of chain
3	G	267	
3	H	267	
4	K	296	
4	L	296	
4	M	296	
4	N	296	
5	O	13	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 85172 atoms, of which 42768 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	723	Total	C	H	N	O	S	5	0
			11425	3571	5779	981	1063	31		
1	B	723	Total	C	H	N	O	S	1	0
			11385	3560	5757	977	1060	31		
1	C	724	Total	C	H	N	O	S	7	0
			11486	3587	5809	991	1068	31		
1	D	536	Total	C	H	N	O	S	7	0
			8522	2652	4327	735	785	23		
1	E	535	Total	C	H	N	O	S	1	0
			8463	2636	4297	726	781	23		
1	F	706	Total	C	H	N	O	S	0	0
			11143	3490	5635	955	1033	30		

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	ASN	-	expression tag	UNP P18708
B	-2	GLY	-	expression tag	UNP P18708
B	-1	ALA	-	expression tag	UNP P18708
B	0	ASN	-	expression tag	UNP P18708
C	-2	GLY	-	expression tag	UNP P18708
C	-1	ALA	-	expression tag	UNP P18708
C	0	ASN	-	expression tag	UNP P18708
D	-2	GLY	-	expression tag	UNP P18708
D	-1	ALA	-	expression tag	UNP P18708
D	0	ASN	-	expression tag	UNP P18708
E	-2	GLY	-	expression tag	UNP P18708
E	-1	ALA	-	expression tag	UNP P18708
E	0	ASN	-	expression tag	UNP P18708
F	-2	GLY	-	expression tag	UNP P18708
F	-1	ALA	-	expression tag	UNP P18708
F	0	ASN	-	expression tag	UNP P18708

- Molecule 2 is a protein called Synaptosomal-associated protein 25, Synaptosomal-associated protein 25, Synaptosomal-associated protein 25, Alpha-soluble NSF attachment protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	J	61	Total	C	H	N	O	S	0	0
			971	292	484	84	107	4		
2	I	70	Total	C	H	N	O	S	0	0
			1099	333	546	97	119	4		

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

- Molecule 3 is a protein called Syntaxin-1A.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	G	63	Total	C	H	N	O	S	0	0
			1023	320	506	89	103	5		
3	H	68	Total	C	H	N	O	S	0	0
			1100	345	544	94	112	5		

- Molecule 4 is a protein called Alpha-soluble NSF attachment protein isoform X2.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	K	289	Total	C	H	N	O	S	0	0
			4503	1435	2231	378	441	18		
4	L	287	Total	C	H	N	O	S	0	0
			4467	1424	2212	375	438	18		
4	M	289	Total	C	H	N	O	S	0	0
			4503	1435	2231	378	441	18		
4	N	287	Total	C	H	N	O	S	0	0
			4467	1424	2212	375	438	18		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	0	GLY	-	expression tag	UNP A0A8C2LIB4
K	44	ILE	MET	conflict	UNP A0A8C2LIB4
K	244	MET	VAL	conflict	UNP A0A8C2LIB4
L	0	GLY	-	expression tag	UNP A0A8C2LIB4
L	44	ILE	MET	conflict	UNP A0A8C2LIB4
L	244	MET	VAL	conflict	UNP A0A8C2LIB4
M	0	GLY	-	expression tag	UNP A0A8C2LIB4
M	44	ILE	MET	conflict	UNP A0A8C2LIB4
M	244	MET	VAL	conflict	UNP A0A8C2LIB4

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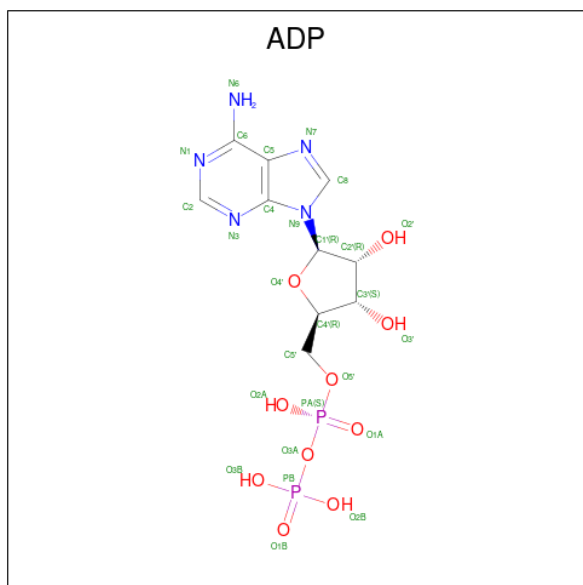
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Chain	Residue	Modelled	Actual	Comment	Reference
N	0	GLY	-	expression tag	UNP A0A8C2LIB4
N	44	ILE	MET	conflict	UNP A0A8C2LIB4
N	244	MET	VAL	conflict	UNP A0A8C2LIB4

- Molecule 5 is a protein called unknown sequence.

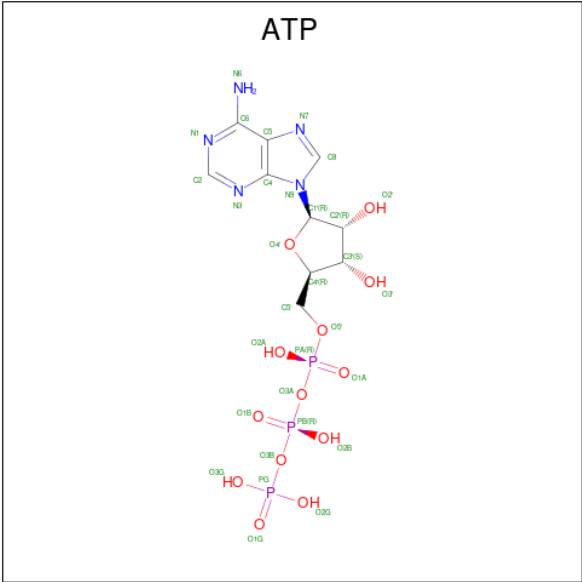
Mol	Chain	Residues	Atoms					AltConf	Trace
5	O	13	Total	C	H	N	O	0	0
			119	39	54	13	13		

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).



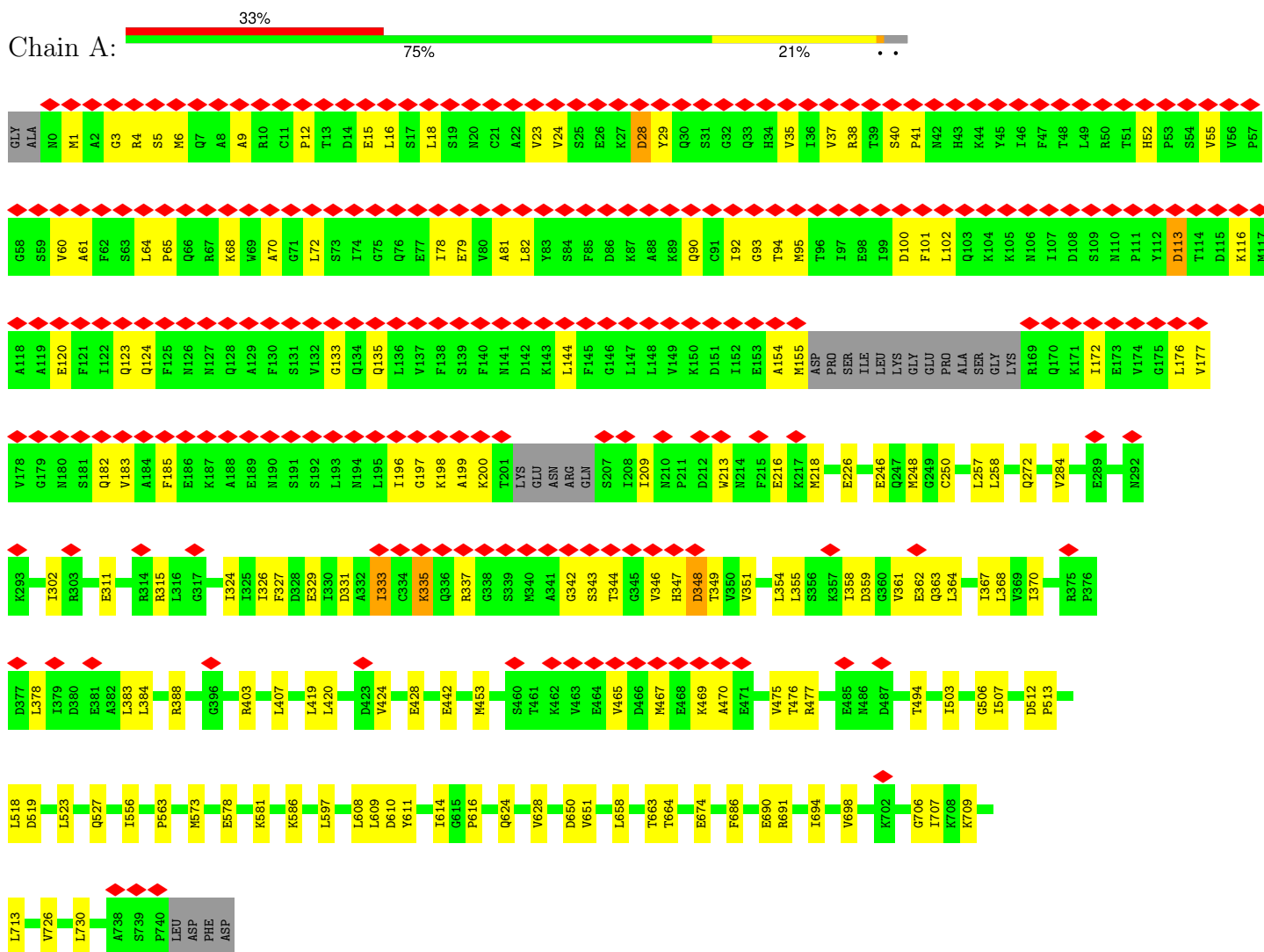
Mol	Chain	Residues	Atoms						AltConf
7	A	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
7	B	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
7	C	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
7	D	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
7	E	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
7	E	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3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



### 3 Residue-property plots

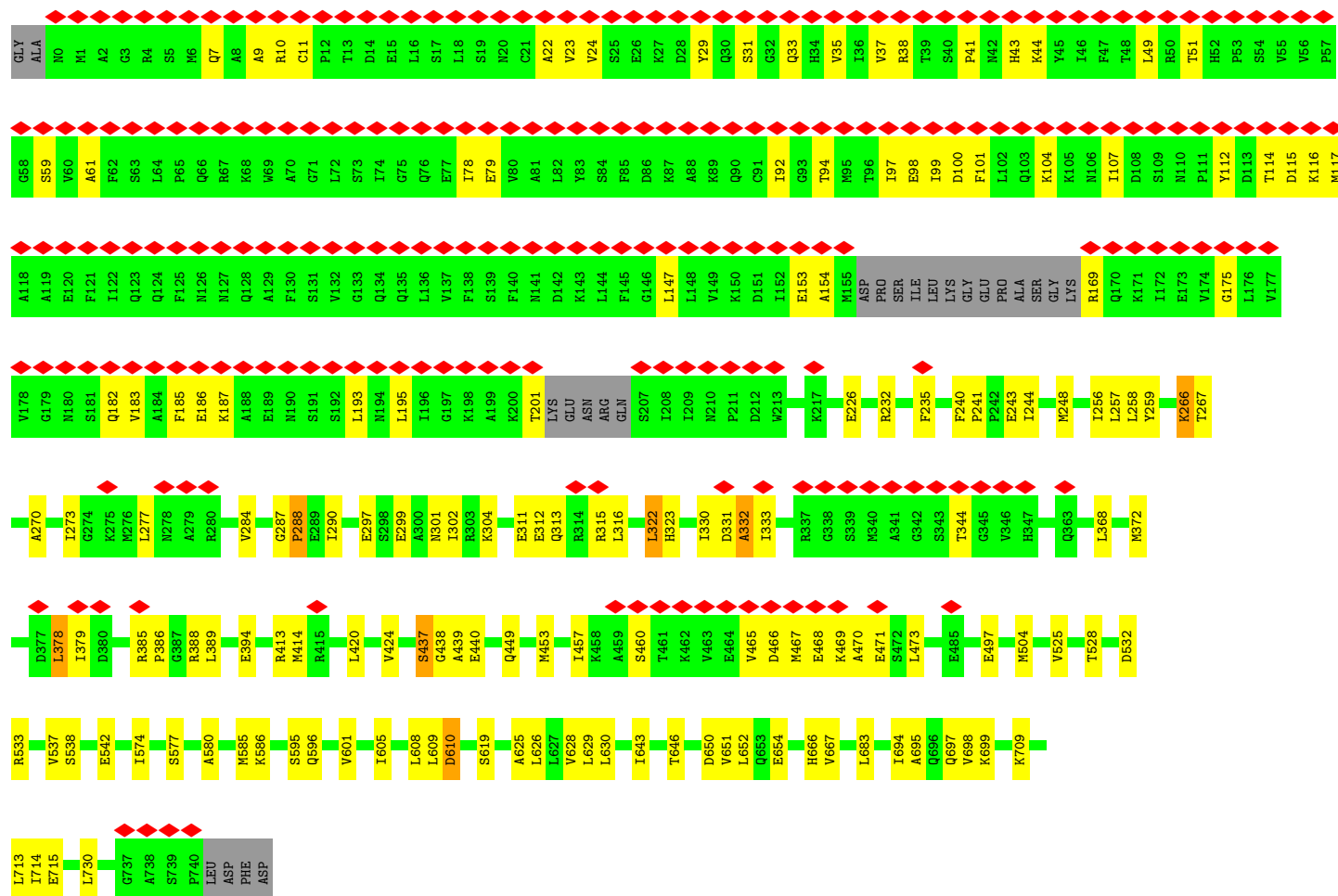
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

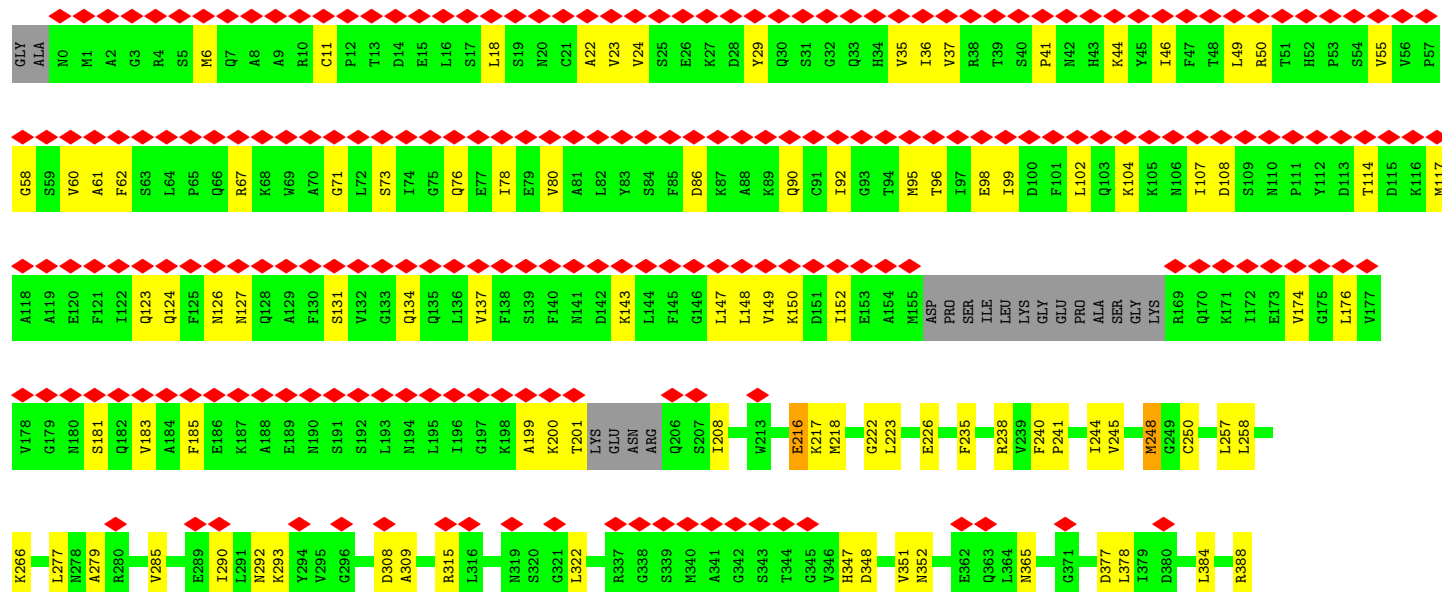
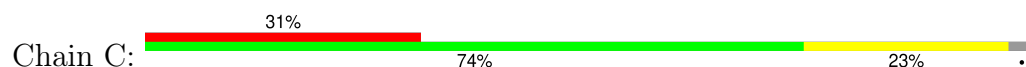


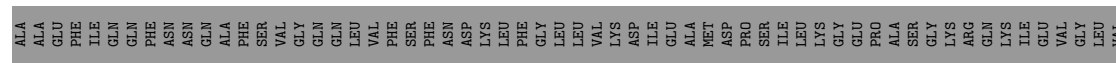
#### • Molecule 1: Vesicle-fusing ATPase

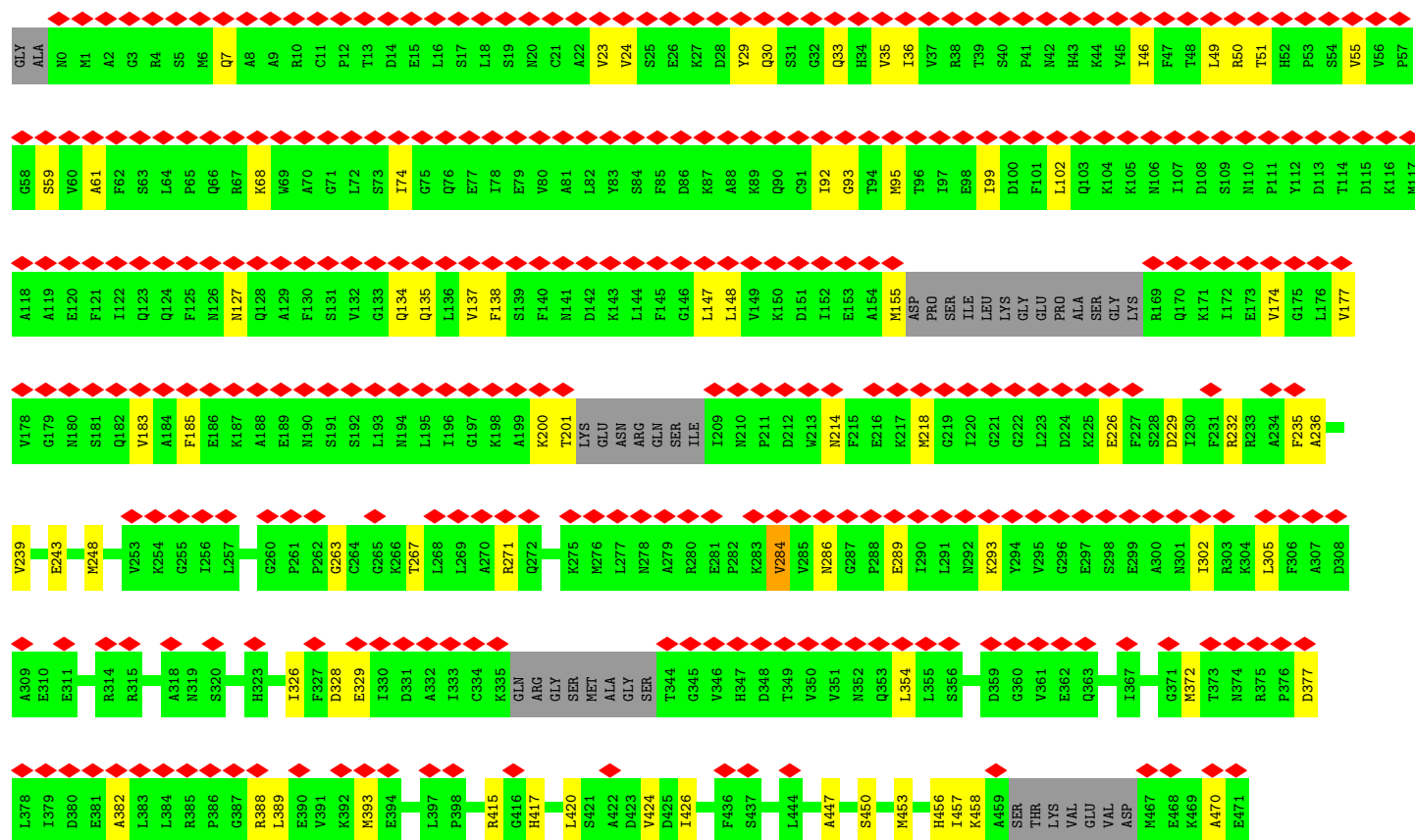




● Molecule 1: Vesicle-fusing ATPase









[illegible]

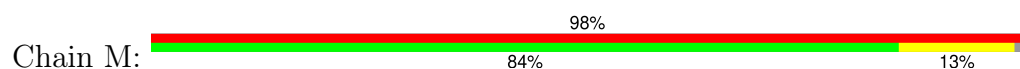
- Molecule 3: Syntaxin-1A

[illegible]

V241	D242	Y243	V244	E245	R246	A247	V248	S249	D250	T251	K252	R253	A254	V255	K256	Y257	Q258	S259	LYS	ALA	ARG	ARG	LYS	LYS	ILE	MET
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- Molecule 3: Syntaxin-1A

[illegible]




E240	C241	K242	L243	M244	K245	K246	L247	L248	E249	A250	H251	E252	E253	Q254	N255	V256	D257	S258	Y259	T260	E261	S262	V263	C264	E265	Y266	D267	S268	I269	S270	R271	L272	D273	Q274	W275	L276	T277	T278	M279	L280	L281	R282	I283	K284	K285	T286	L287	Q288	GLY	ASP	GLU	GLU	ASP	LEU	ARG				
K180	A181	D182	D183	I184	Y185	E186	Q187	V188	G189	T190	S191	A192	M193	D194	S195	P196	L197	L198	K199	Y200	S201	A202	K203	D204	Y205	F206	F207	K208	A209	A210	L211	C212	H213	F214	C215	I216	D217	M218	L219	N220	A221	K222	L223	A224	V225	Q226	K227	Y228	E229	E230	L231	F232	P233	A234	F235	S236	D237	S238	R239
A120	A121	K122	H123	H124	I125	S126	I127	E128	E129	T130	Y131	E132	T133	E134	L135	V136	D137	V138	E139	K140	A141	I142	A143	H144	Y145	E146	Q147	S148	A149	D150	Y151	Y152	K153	G154	E155	E156	S157	N158	S159	S160	A161	N162	K163	C164	L165	L166	K167	V168	A169	G170	Y171	A172	A173	Q174	L175	E176	Q177	Y178	Q179
A60	A61	G62	N63	A64	F65	C66	Q67	A68	A69	Q70	L71	H72	L73	Q74	L75	Q76	S77	K78	H79	D80	A81	A82	T83	C84	F85	W86	D87	A88	G89	N90	A91	F92	K93	K94	A95	D96	P97	Q98	E99	A100	I101	N102	C103	L104	M105	R106	A107	I108	E109	I110	Y111	T112	D113	M114	G115	R116	F117	T118	I119
G0	M1	D2	T3	S4	G5	K6	Q7	A8	E9	A10	M11	A12	L13	L14	A15	E16	A17	E18	R19	V21	K22	N23	S24	Q25	S26	F27	F28	S29	G30	L31	F32	G33	G34	S35	S36	K37	I38	E39	E40	A41	C42	E43	I44	Y45	A46	R47	A48	A49	N50	M51	F52	K53	M54	A55	K56	N57	W58	S59	

• Molecule 4: Alpha-soluble NSF attachment protein isoform X2

Chain N:

<

• Molecule 5: unknown sequence

Chain O: 

X1	X2	X7	X12	X13
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## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	32677	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	1.256	Depositor
Minimum map value	-0.544	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.048	Depositor
Recommended contour level	0.3	Depositor
Map size ( $\text{\AA}$ )	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 ( $\text{\AA}$ )	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, 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	0.34	1/5761 (0.0%)	0.54	0/7762
1	B	0.34	0/5720	0.55	0/7708
1	C	0.33	1/5793 (0.0%)	0.54	0/7804
1	D	0.39	0/4301	0.63	0/5796
1	E	0.34	1/4233 (0.0%)	0.55	0/5704
1	F	0.22	0/5593	0.41	0/7535
2	I	0.17	0/553	0.36	0/735
2	J	0.19	0/486	0.44	0/645
3	G	0.16	0/523	0.41	0/700
3	H	0.27	0/562	0.48	0/753
4	K	0.23	0/2312	0.41	0/3107
4	L	0.10	0/2295	0.25	0/3084
4	M	0.12	0/2312	0.28	0/3107
4	N	0.15	0/2295	0.36	0/3084
All	All	0.30	3/42739 (0.0%)	0.49	0/57524

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	733	LEU	C-N	7.97	1.44	1.33
1	A	362	GLU	C-N	5.69	1.44	1.34
1	C	681	GLU	C-N	5.28	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	5646	5779	5750	127	0
1	B	5628	5757	5756	126	0
1	C	5677	5809	5780	135	0
1	D	4195	4327	4275	97	0
1	E	4166	4297	4293	69	0
1	F	5508	5635	5639	85	0
2	I	553	546	546	42	0
2	J	487	484	483	26	0
3	G	517	506	505	23	0
3	H	556	544	544	29	0
4	K	2272	2231	2231	30	0
4	L	2255	2212	2212	23	0
4	M	2272	2231	2231	33	0
4	N	2255	2212	2212	44	0
5	O	65	54	15	0	0
6	A	27	12	12	0	0
6	B	27	12	12	1	0
6	C	27	12	12	0	0
6	D	27	12	12	3	0
6	F	27	12	12	1	0
7	A	31	12	12	4	0
7	B	31	12	12	0	0
7	C	31	12	12	1	0
7	D	31	12	12	1	0
7	E	62	24	24	3	0
7	F	31	12	12	0	0
All	All	42404	42768	42616	805	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 805 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)
1:E:652:LEU:HD12	1:E:657:MET:HE2	1.44	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:259:TYR:CZ	1:D:392:LYS:HE2	2.00	0.96
1:D:259:TYR:CE2	1:D:392:LYS:HG2	2.04	0.93
1:A:329:GLU:HG2	1:A:331:ASP:OD1	1.74	0.86
1:A:690:GLU:HG3	1:A:726:VAL:CG1	2.06	0.84

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	722/747 (97%)	679 (94%)	41 (6%)	2 (0%)	37	72
1	B	718/747 (96%)	669 (93%)	46 (6%)	3 (0%)	30	67
1	C	725/747 (97%)	692 (95%)	33 (5%)	0	100	100
1	D	541/747 (72%)	498 (92%)	43 (8%)	0	100	100
1	E	534/747 (72%)	499 (93%)	35 (7%)	0	100	100
1	F	696/747 (93%)	672 (97%)	24 (3%)	0	100	100
2	I	68/518 (13%)	67 (98%)	1 (2%)	0	100	100
2	J	59/518 (11%)	59 (100%)	0	0	100	100
3	G	61/267 (23%)	61 (100%)	0	0	100	100
3	H	66/267 (25%)	66 (100%)	0	0	100	100
4	K	287/296 (97%)	279 (97%)	8 (3%)	0	100	100
4	L	285/296 (96%)	276 (97%)	9 (3%)	0	100	100
4	M	287/296 (97%)	279 (97%)	8 (3%)	0	100	100
4	N	285/296 (96%)	280 (98%)	5 (2%)	0	100	100
All	All	5334/7236 (74%)	5076 (95%)	253 (5%)	5 (0%)	50	83

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	332	ALA
1	A	198	LYS
1	B	610	ASP
1	A	333	ILE
1	B	290	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	624/638 (98%)	616 (99%)	8 (1%)	65	77
1	B	619/638 (97%)	611 (99%)	8 (1%)	65	77
1	C	627/638 (98%)	619 (99%)	8 (1%)	65	77
1	D	465/638 (73%)	451 (97%)	14 (3%)	36	57
1	E	457/638 (72%)	451 (99%)	6 (1%)	65	77
1	F	605/638 (95%)	603 (100%)	2 (0%)	91	92
2	I	60/430 (14%)	60 (100%)	0	100	100
2	J	55/430 (13%)	55 (100%)	0	100	100
3	G	58/245 (24%)	58 (100%)	0	100	100
3	H	62/245 (25%)	62 (100%)	0	100	100
4	K	237/243 (98%)	236 (100%)	1 (0%)	89	91
4	L	235/243 (97%)	235 (100%)	0	100	100
4	M	237/243 (98%)	236 (100%)	1 (0%)	89	91
4	N	235/243 (97%)	235 (100%)	0	100	100
All	All	4576/6150 (74%)	4528 (99%)	48 (1%)	69	82

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	606	GLU
1	D	725	ARG
1	D	609	LEU

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Mol	Chain	Res	Type
1	D	720	MET
1	D	736	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	347	HIS
1	F	675	GLN
1	E	417	HIS
1	F	34	HIS
4	K	187	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

12 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	$\# Z  > 2$
6	ADP	D	802	-	24,29,29	0.91	1 (4%)	29,45,45	1.25	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	ATP	C	801	-	28,33,33	0.88	2 (7%)	34,52,52	0.83	1 (2%)
7	ATP	B	801	-	28,33,33	0.82	1 (3%)	34,52,52	0.84	1 (2%)
7	ATP	D	801	-	28,33,33	0.64	0	34,52,52	0.90	1 (2%)
6	ADP	F	802	-	24,29,29	0.91	0	29,45,45	1.25	2 (6%)
6	ADP	B	802	-	24,29,29	0.75	0	29,45,45	0.76	1 (3%)
7	ATP	E	802	-	28,33,33	0.66	0	34,52,52	0.97	1 (2%)
7	ATP	F	801	-	28,33,33	0.65	0	34,52,52	0.87	1 (2%)
7	ATP	E	801	-	28,33,33	0.66	0	34,52,52	0.93	1 (2%)
6	ADP	C	802	-	24,29,29	0.73	0	29,45,45	0.74	1 (3%)
7	ATP	A	802	-	28,33,33	0.67	0	34,52,52	0.91	1 (2%)
6	ADP	A	801	-	24,29,29	0.89	0	29,45,45	1.24	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
6	ADP	D	802	-	-	1/12/32/32	0/3/3/3
7	ATP	C	801	-	-	5/18/38/38	0/3/3/3
7	ATP	B	801	-	-	1/18/38/38	0/3/3/3
7	ATP	D	801	-	-	6/18/38/38	0/3/3/3
6	ADP	F	802	-	-	3/12/32/32	0/3/3/3
6	ADP	B	802	-	-	3/12/32/32	0/3/3/3
7	ATP	E	802	-	-	5/18/38/38	0/3/3/3
7	ATP	F	801	-	-	4/18/38/38	0/3/3/3
7	ATP	E	801	-	-	4/18/38/38	0/3/3/3
6	ADP	C	802	-	-	0/12/32/32	0/3/3/3
7	ATP	A	802	-	-	5/18/38/38	0/3/3/3
6	ADP	A	801	-	-	2/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	801	ATP	C1'-N9	-2.34	1.44	1.49
7	C	801	ATP	C1'-N9	-2.25	1.44	1.49
7	C	801	ATP	PB-O2B	-2.06	1.45	1.55
6	D	802	ADP	O4'-C1'	2.06	1.43	1.40

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	802	ADP	N3-C2-N1	-4.22	122.94	128.67
6	D	802	ADP	N3-C2-N1	-4.17	123.01	128.67
6	A	801	ADP	N3-C2-N1	-4.13	123.06	128.67
6	A	801	ADP	C4-C5-N7	-2.57	106.63	109.34
6	F	802	ADP	C4-C5-N7	-2.52	106.68	109.34

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	802	ADP	C5'-O5'-PA-O1A
7	A	802	ATP	C5'-O5'-PA-O1A
7	A	802	ATP	C5'-O5'-PA-O3A
7	C	801	ATP	C5'-O5'-PA-O1A
7	C	801	ATP	C5'-O5'-PA-O2A

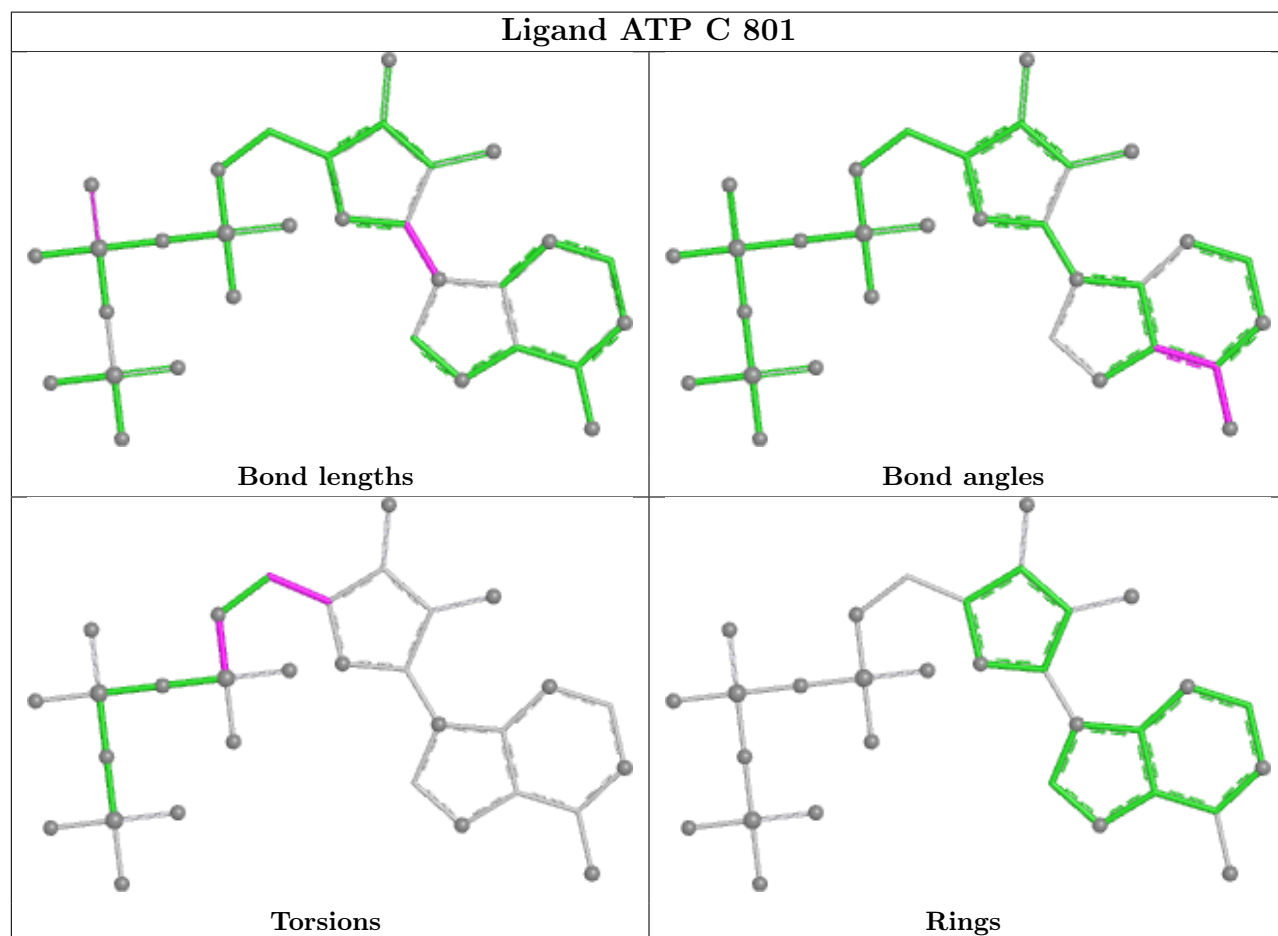
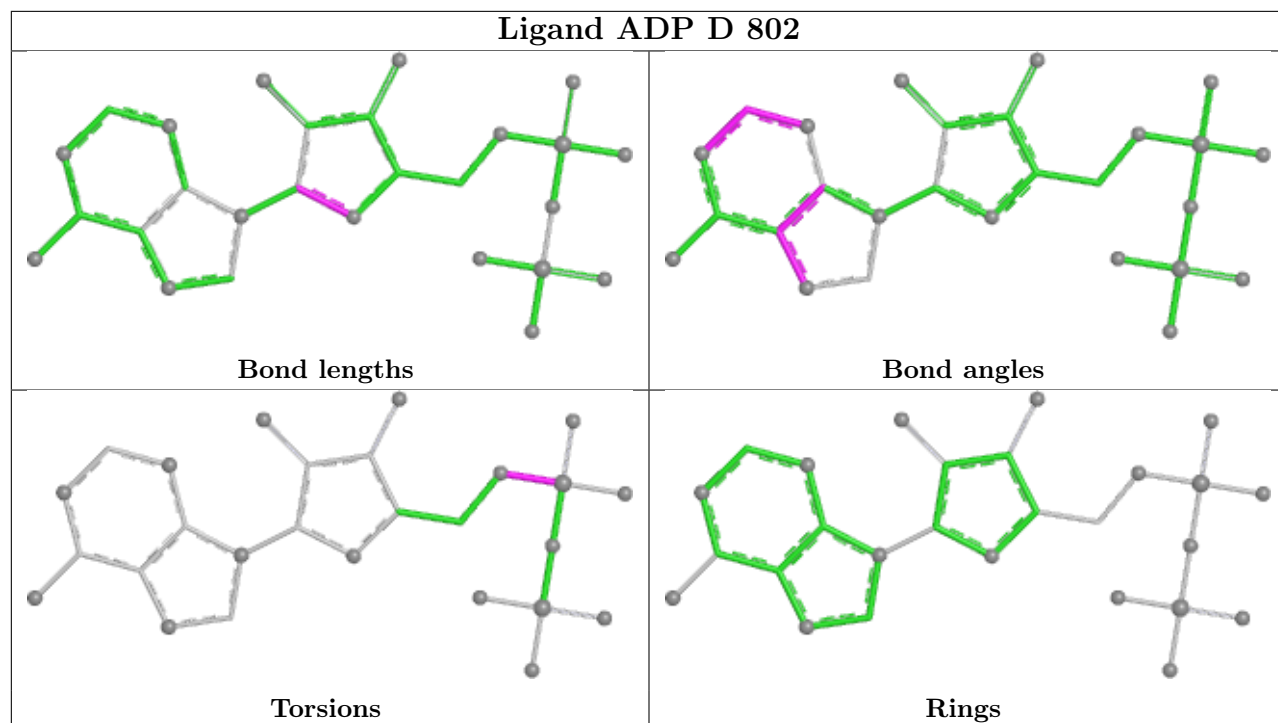
There are no ring outliers.

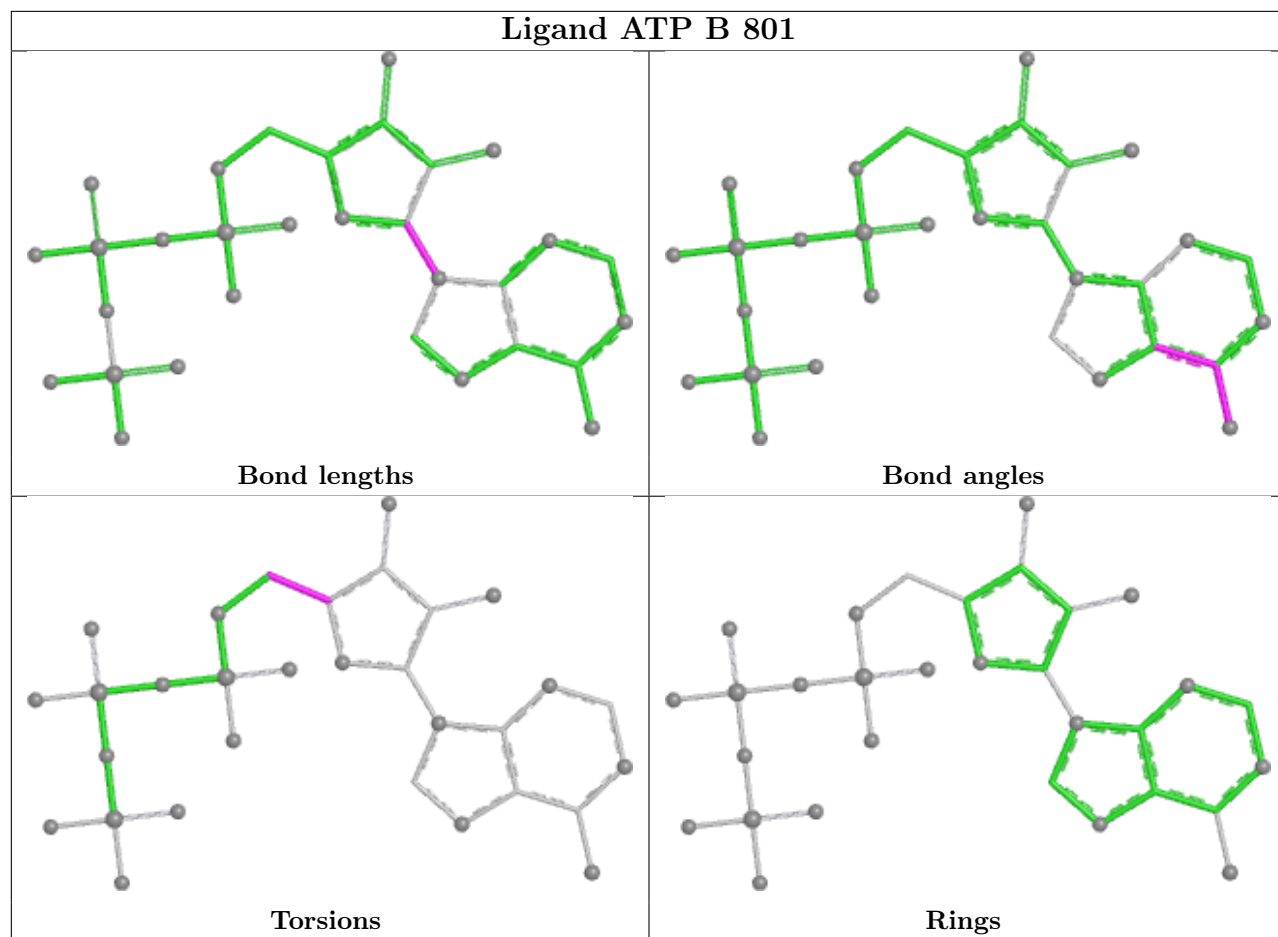
7 monomers are involved in 14 short contacts:

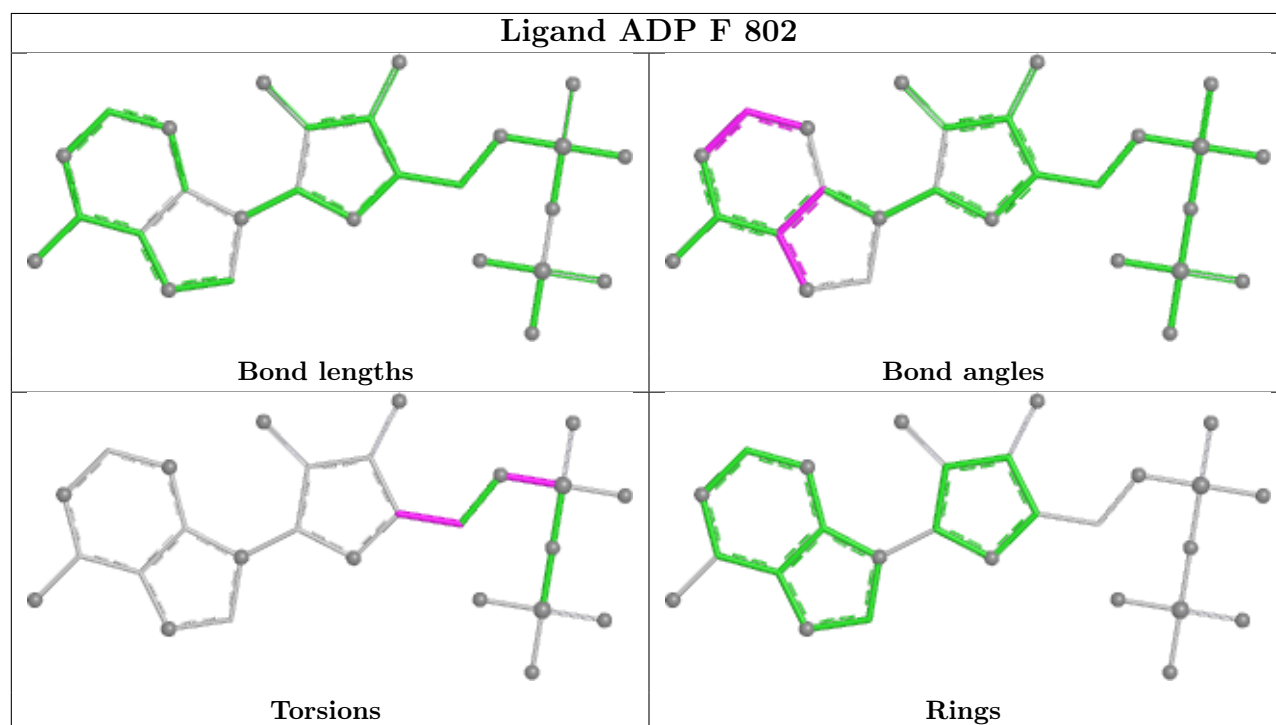
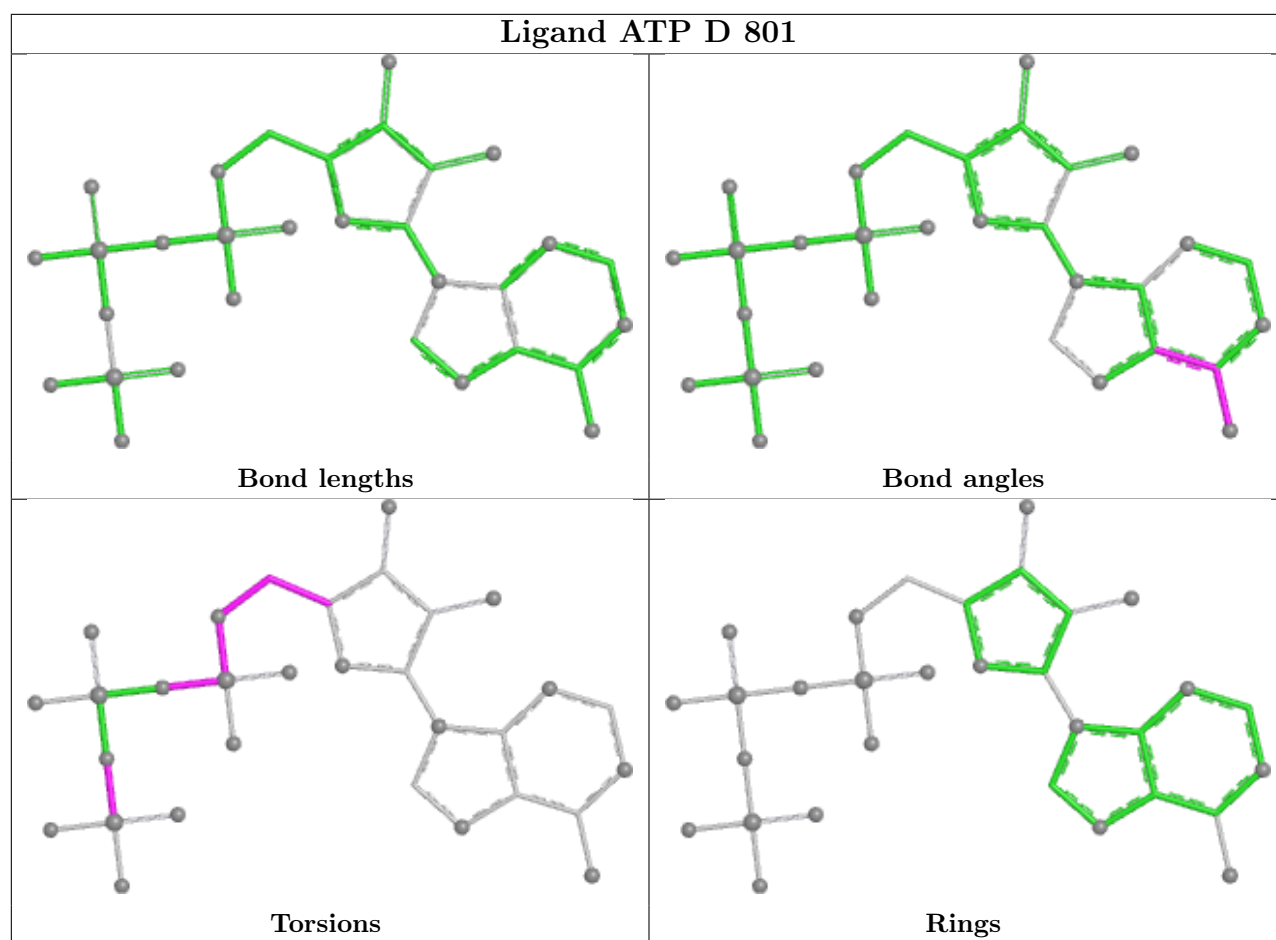
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	802	ADP	3	0
7	C	801	ATP	1	0
7	D	801	ATP	1	0
6	F	802	ADP	1	0
6	B	802	ADP	1	0
7	E	802	ATP	3	0
7	A	802	ATP	4	0

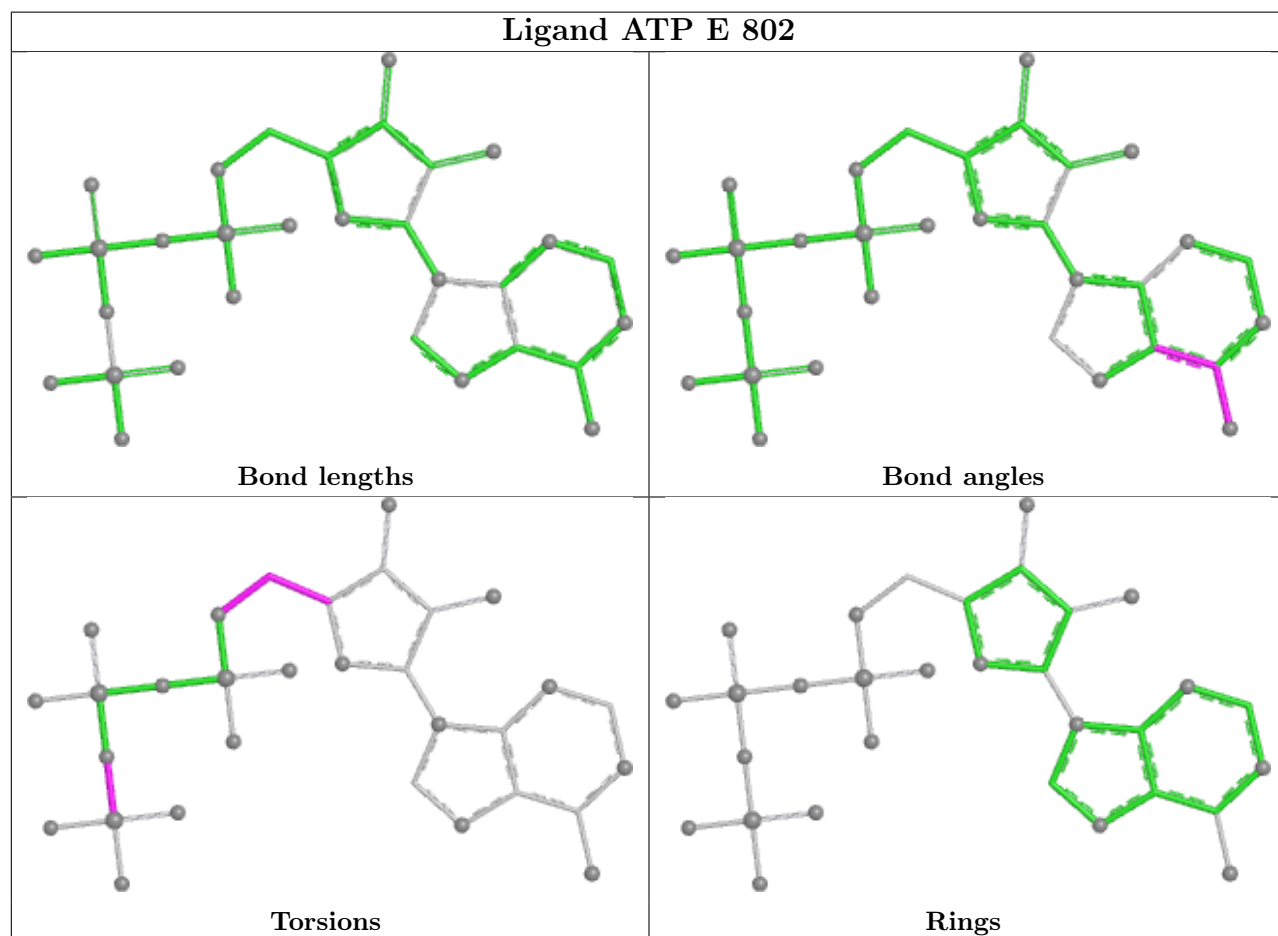
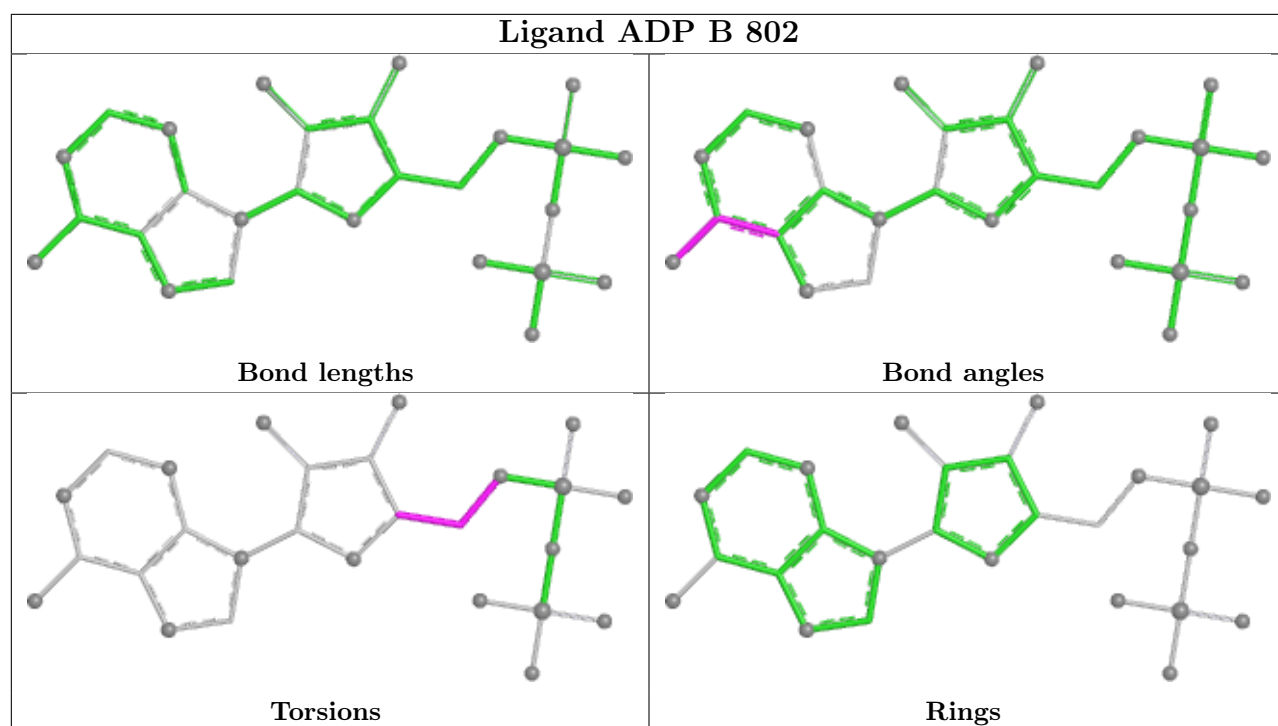
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

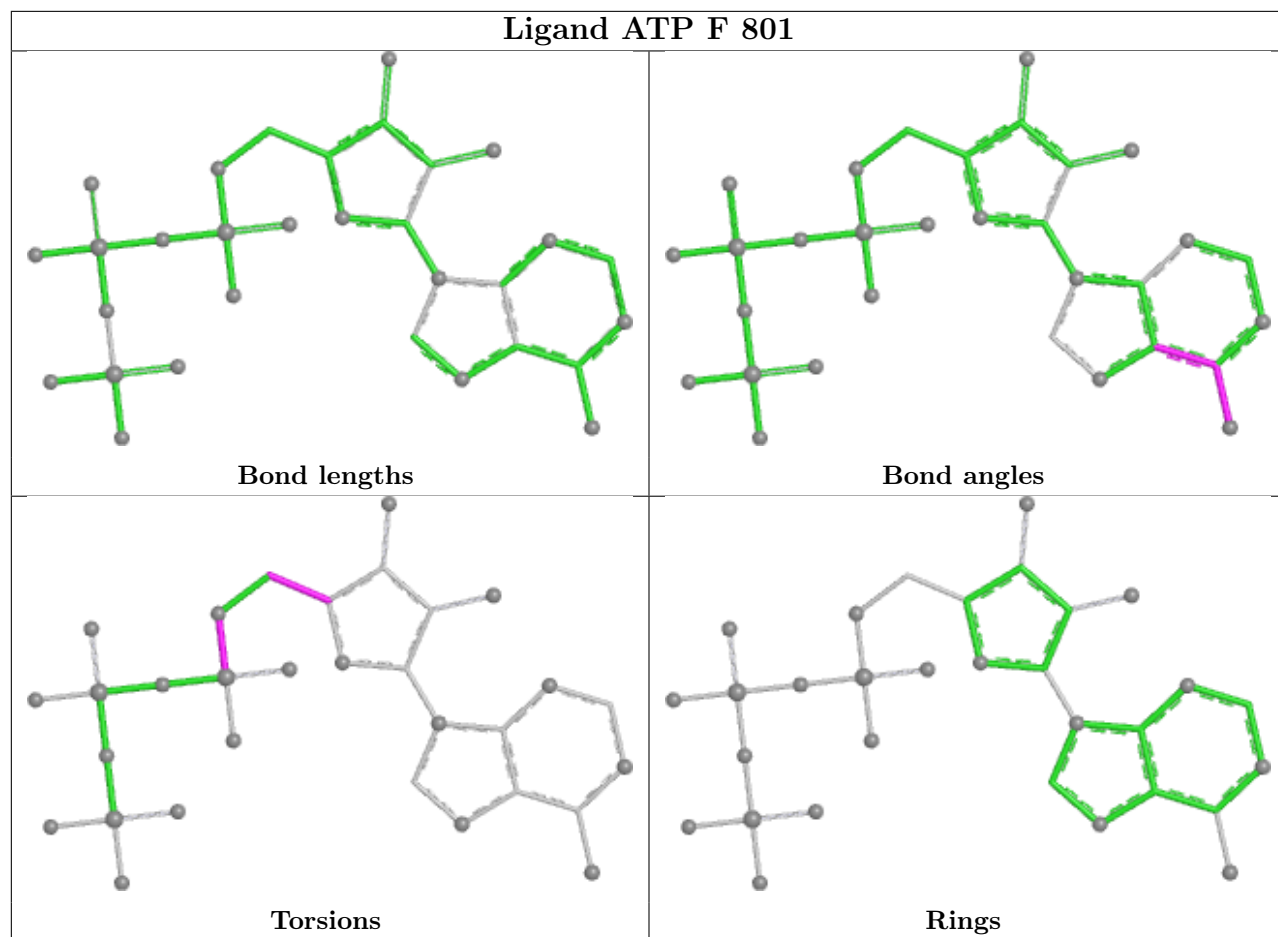




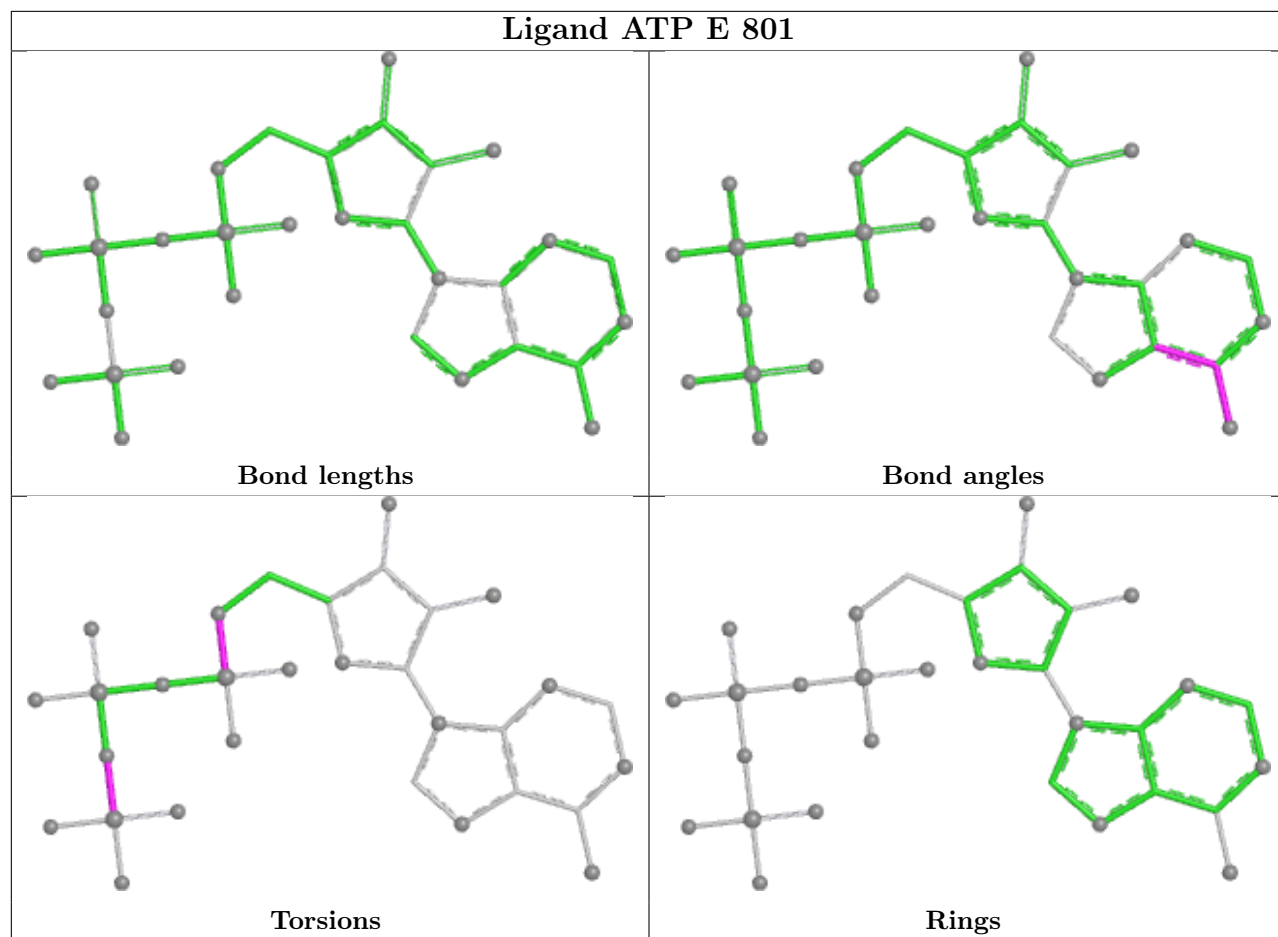




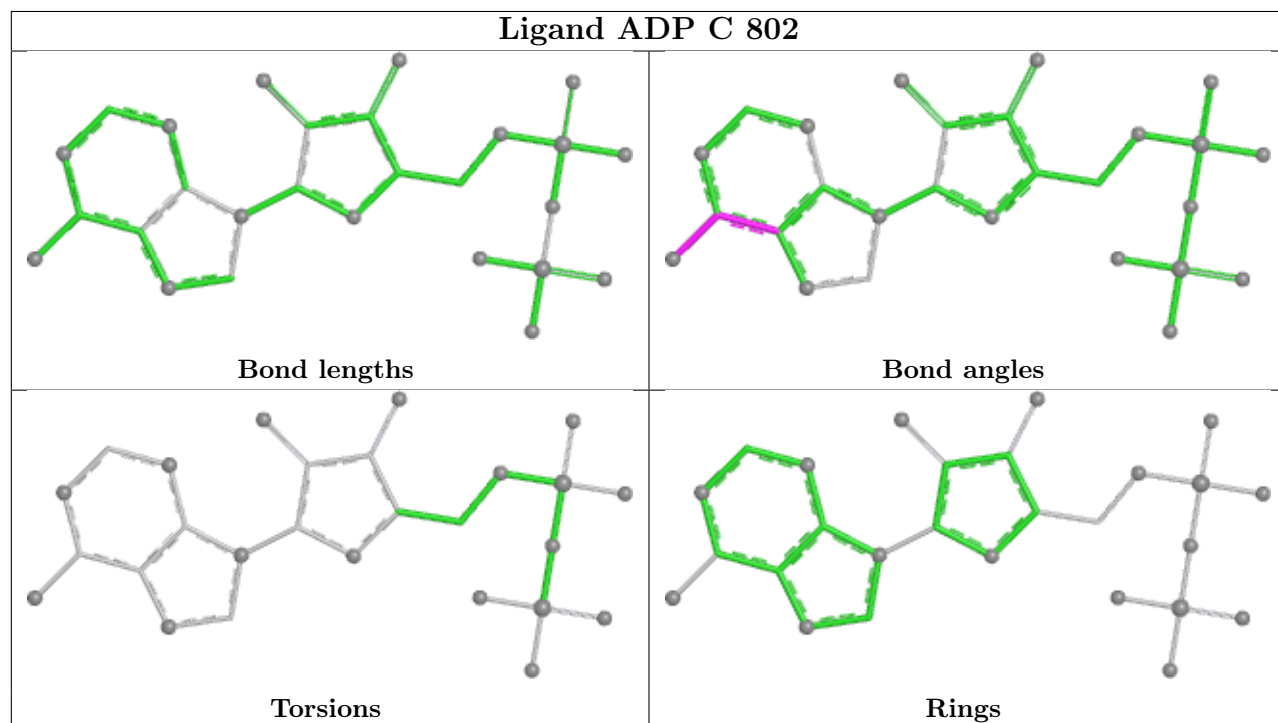


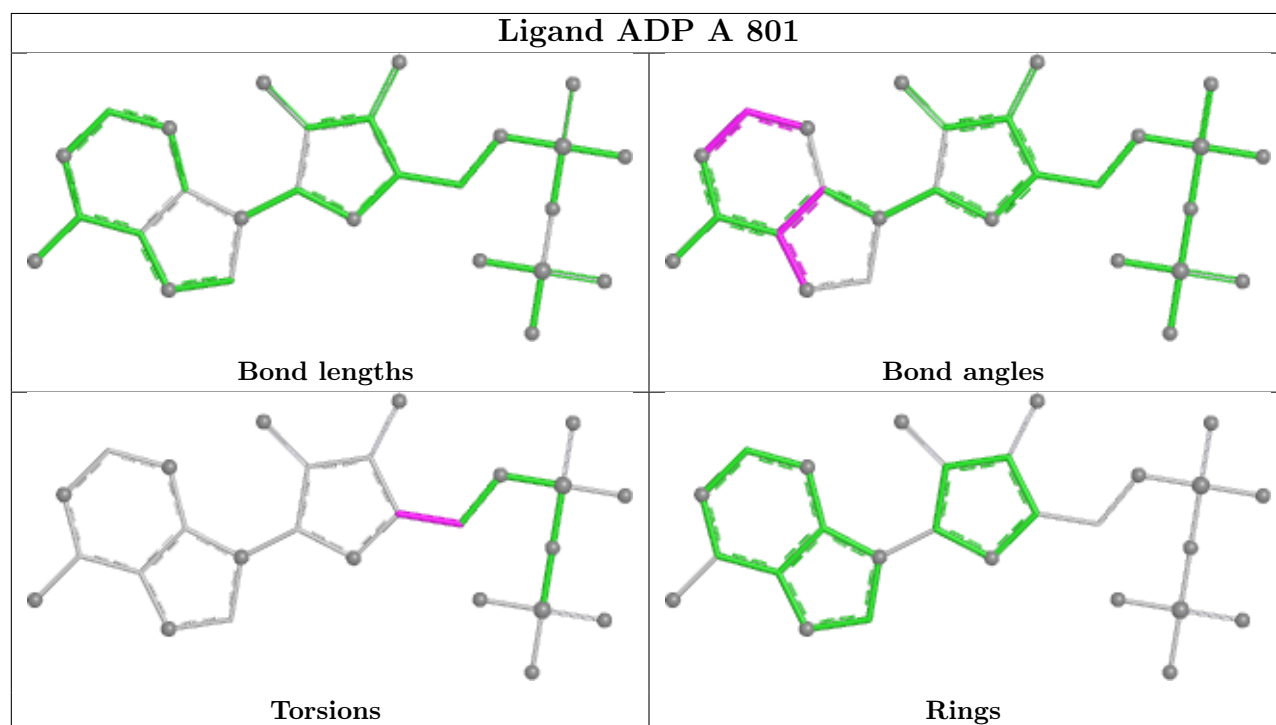
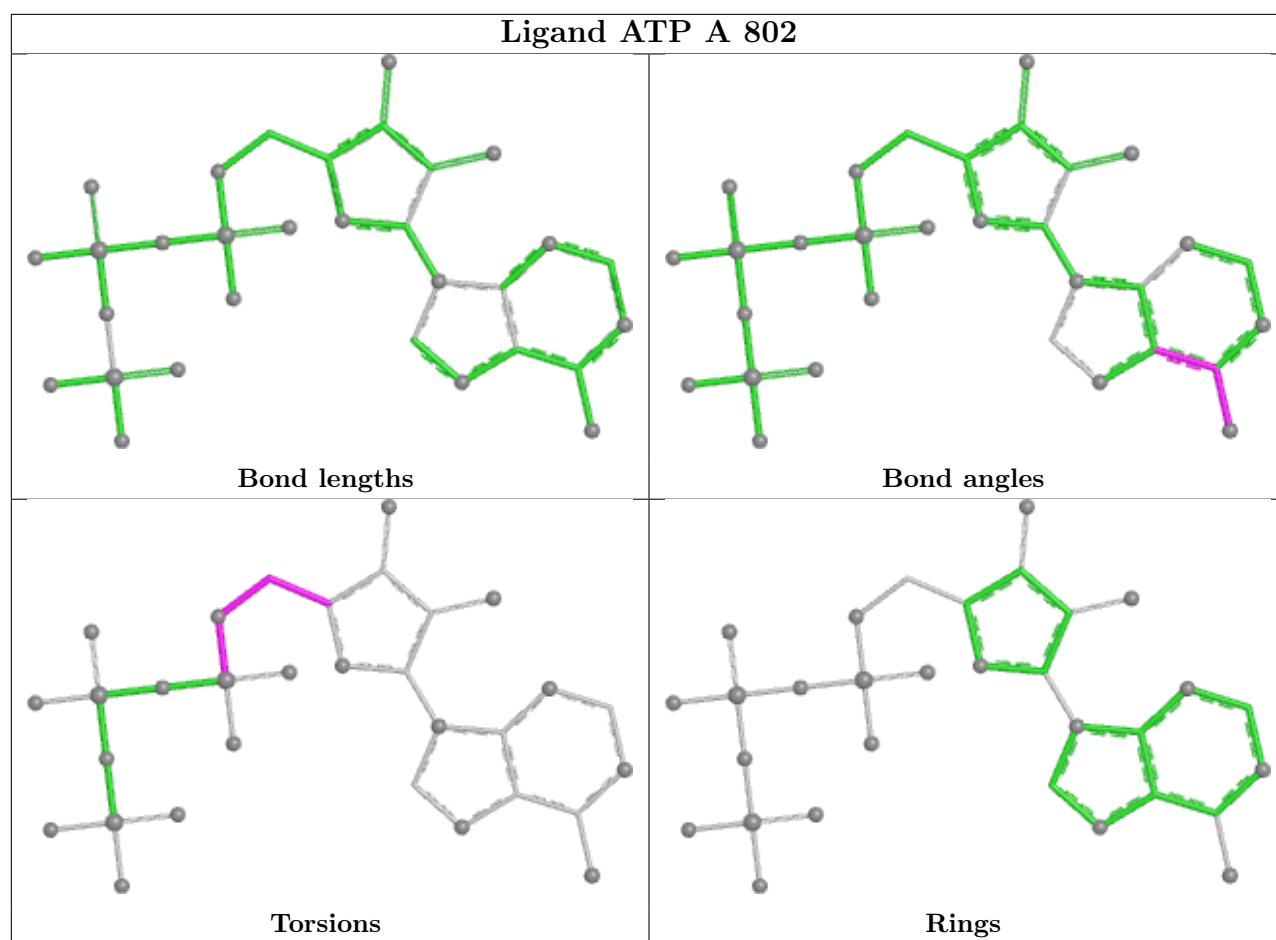


## Ligand ATP E 801



## Ligand ADP C 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.



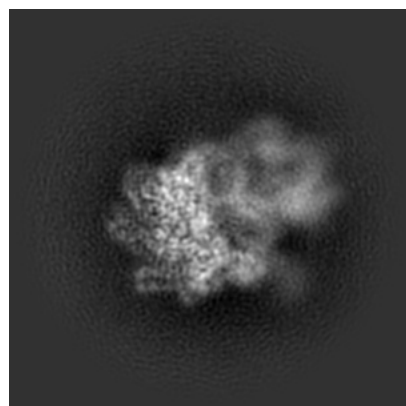
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71529. These allow visual inspection of the internal detail of the map and identification of artifacts.

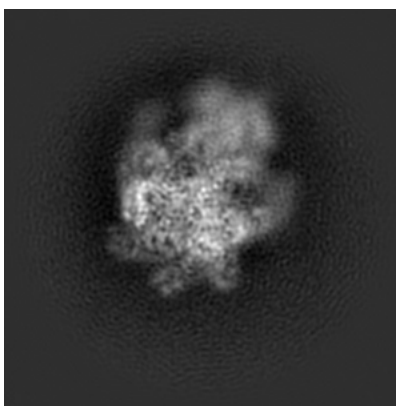
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

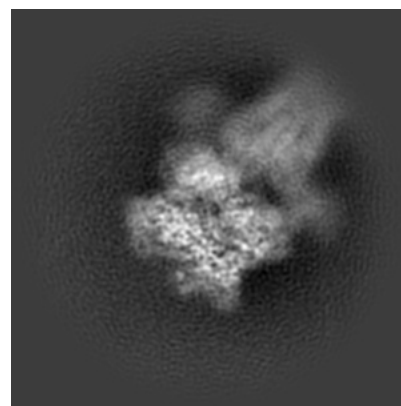
#### 6.1.1 Primary map



X

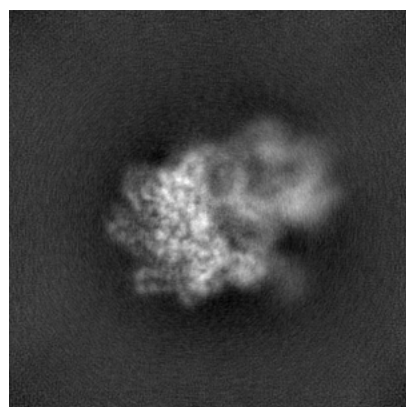


Y

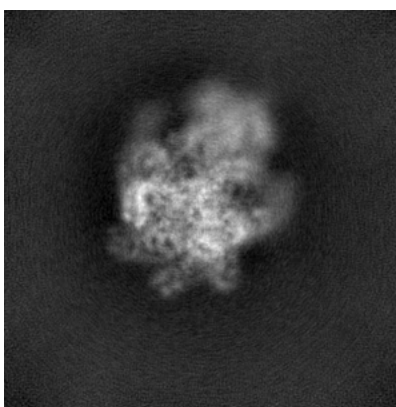


Z

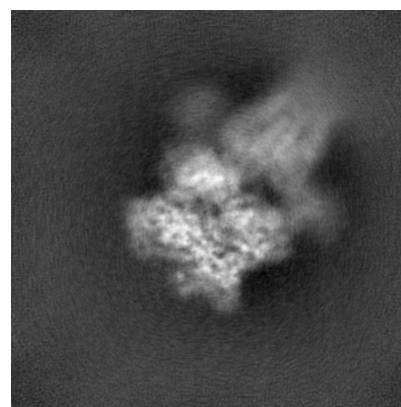
#### 6.1.2 Raw map



X



Y

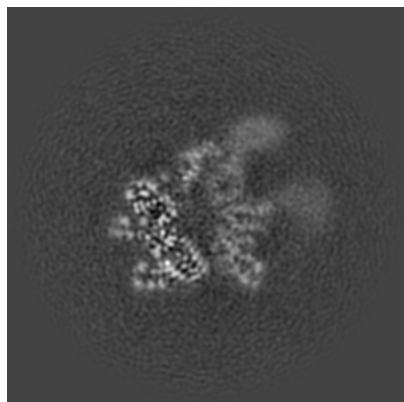


Z

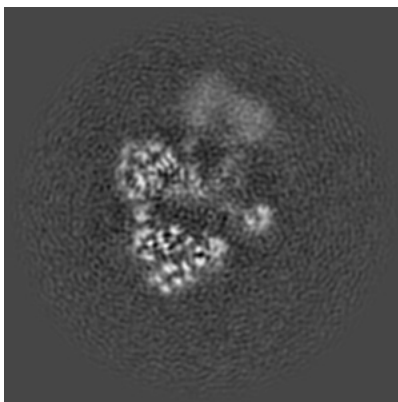
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

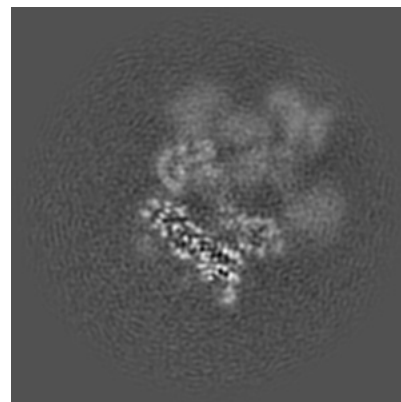
### 6.2.1 Primary map



X Index: 147

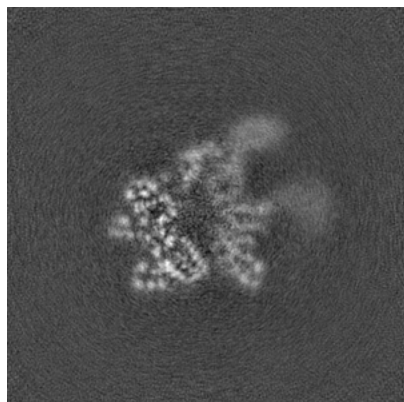


Y Index: 147

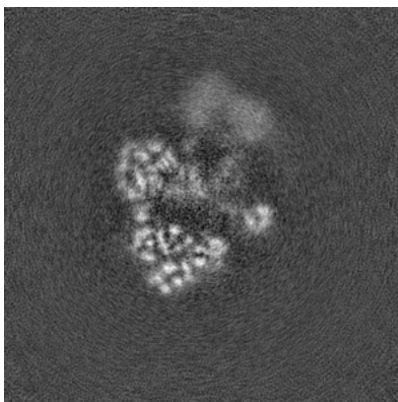


Z Index: 147

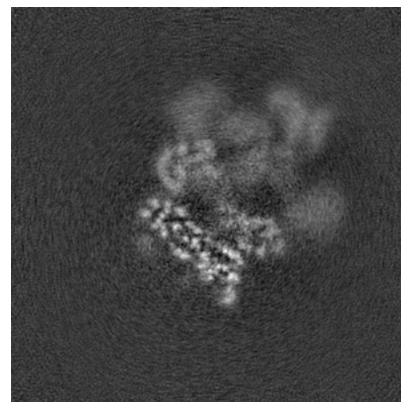
### 6.2.2 Raw map



X Index: 147



Y Index: 147

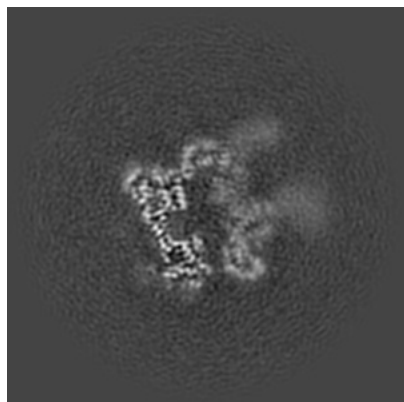


Z Index: 147

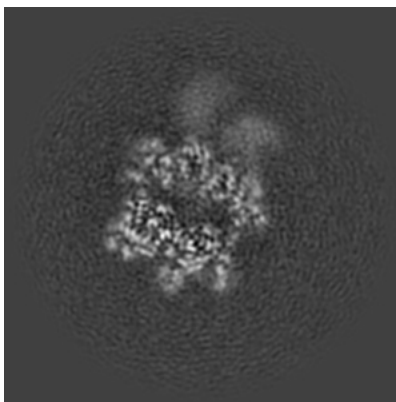
The images above show central slices of the map in three orthogonal directions.

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

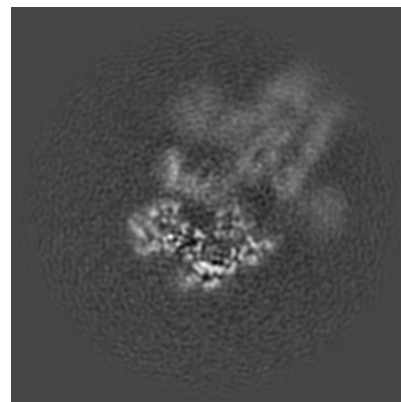
### 6.3.1 Primary map



X Index: 137

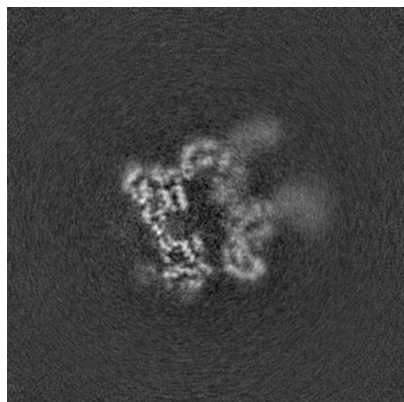


Y Index: 135

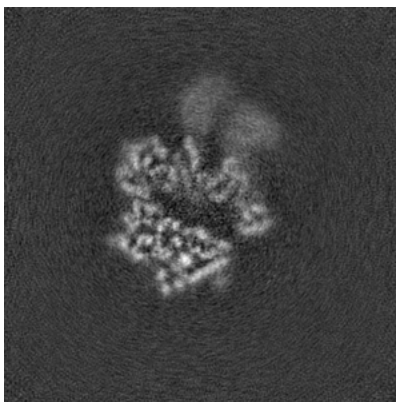


Z Index: 156

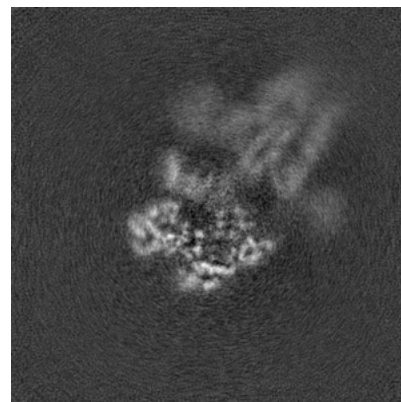
### 6.3.2 Raw map



X Index: 137



Y Index: 141

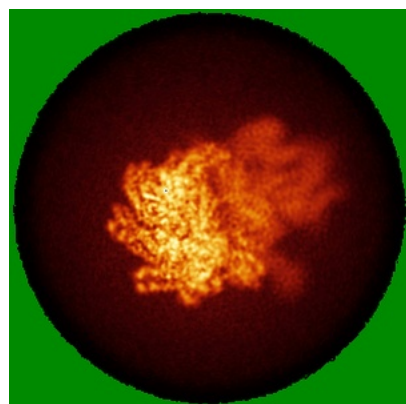


Z Index: 157

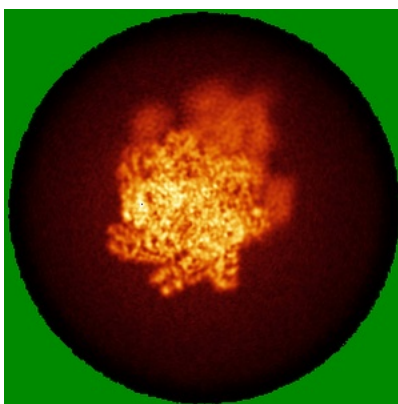
The images above show the largest variance slices of the map in three orthogonal directions.

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

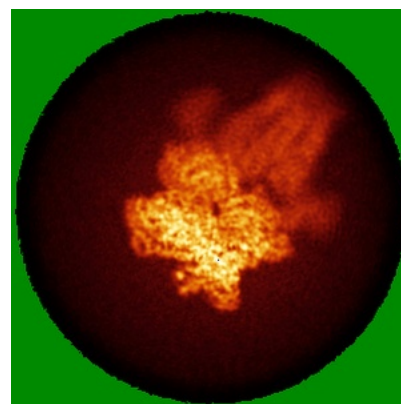
### 6.4.1 Primary map



X

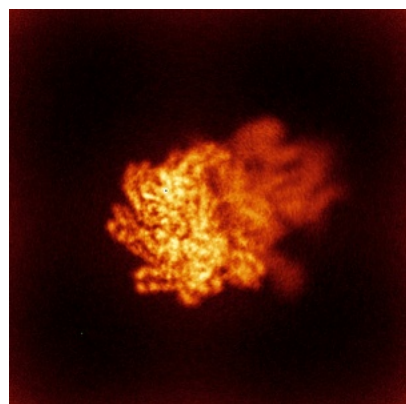


Y

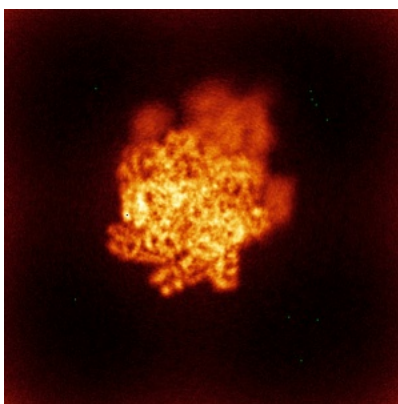


Z

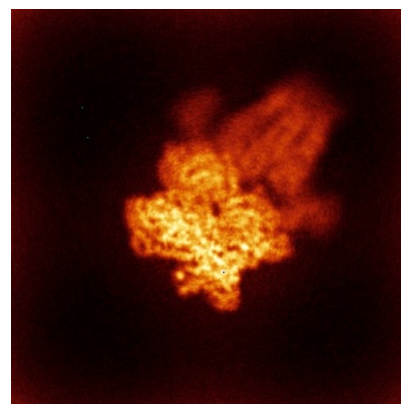
### 6.4.2 Raw map



X



Y



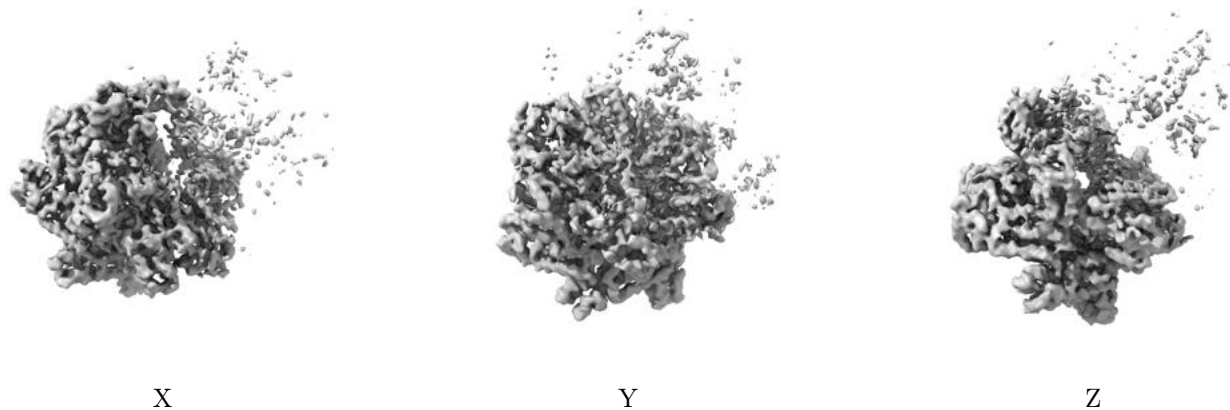
Z

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.

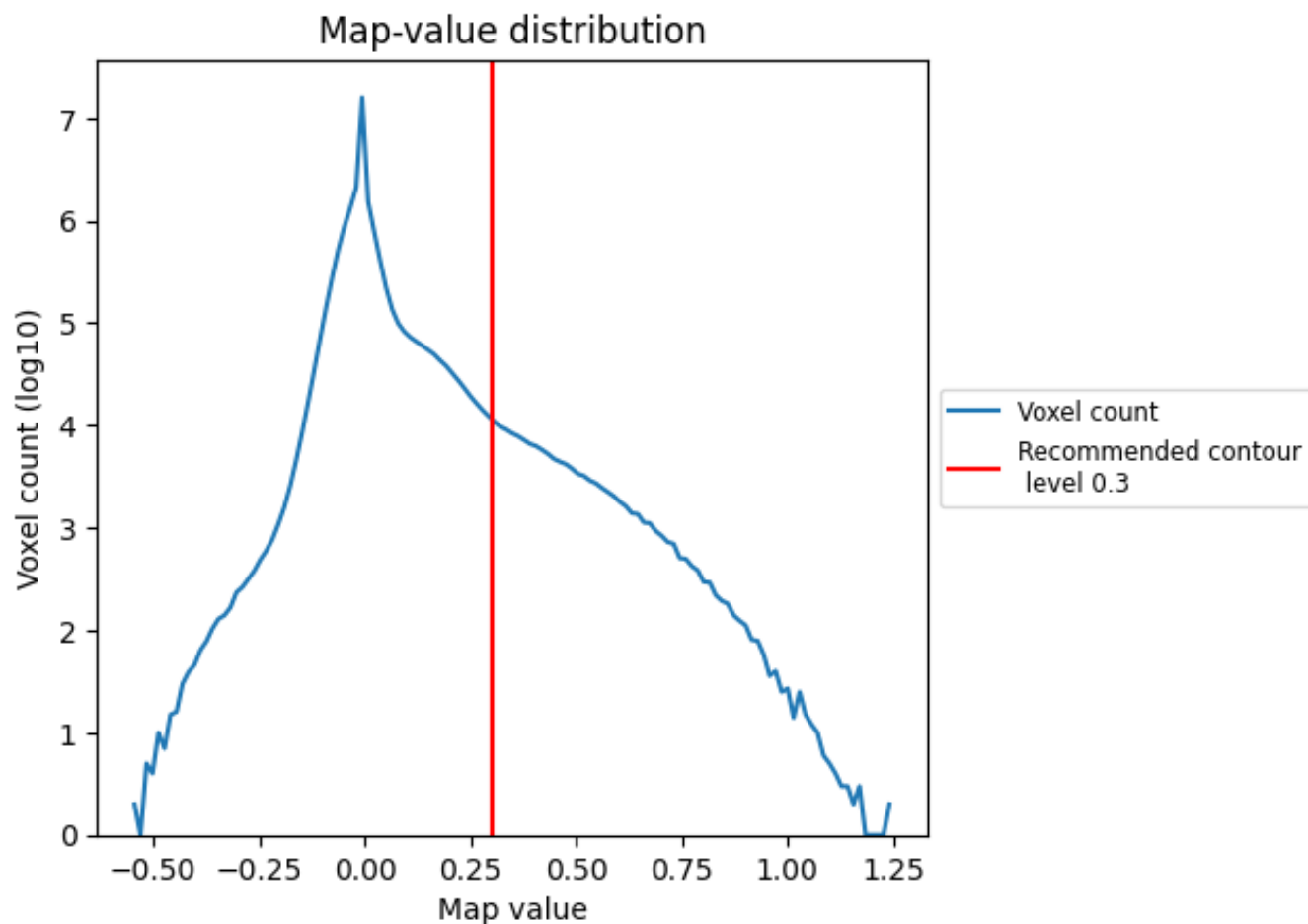
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

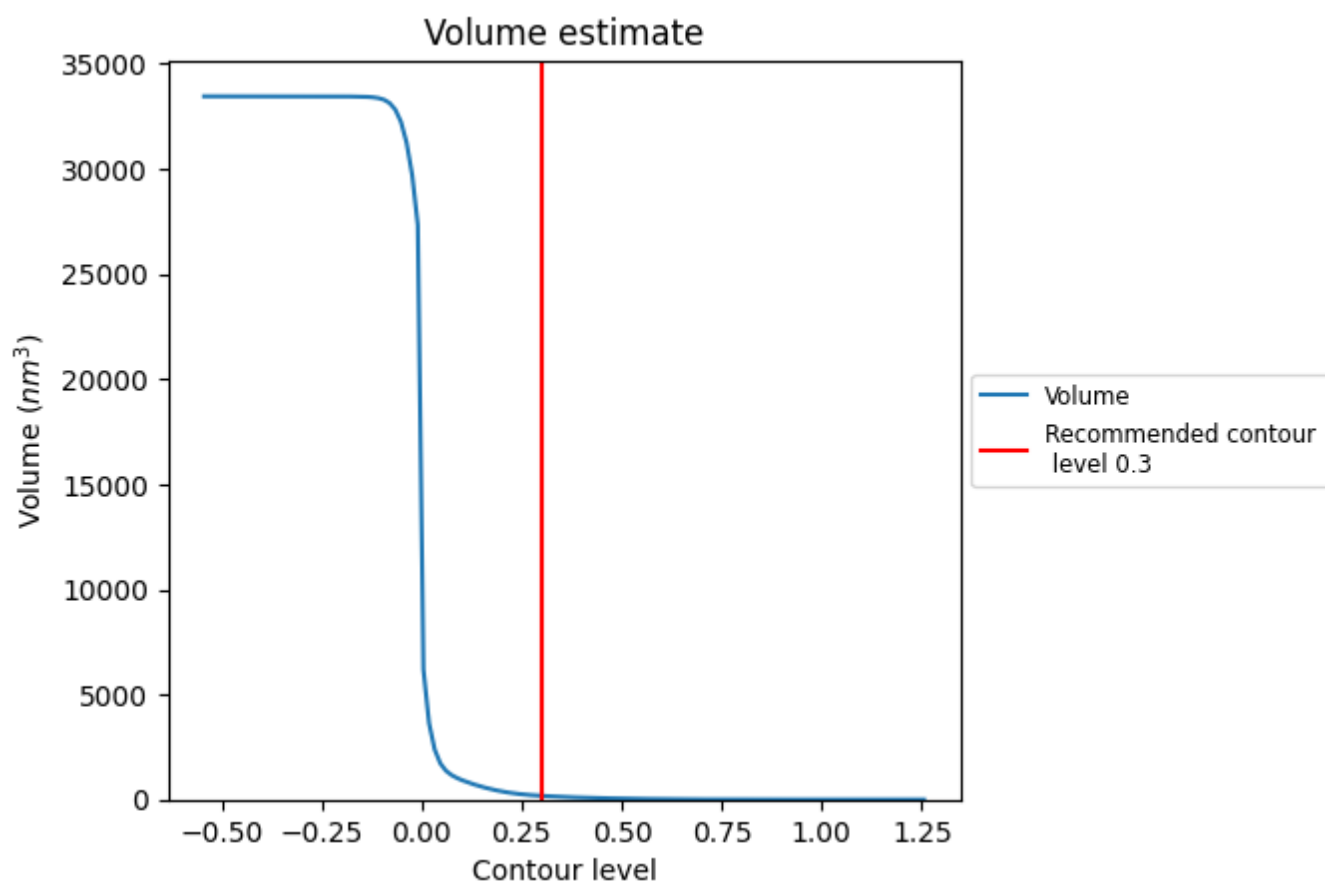
This section contains the results of statistical analysis of the map.

### 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.

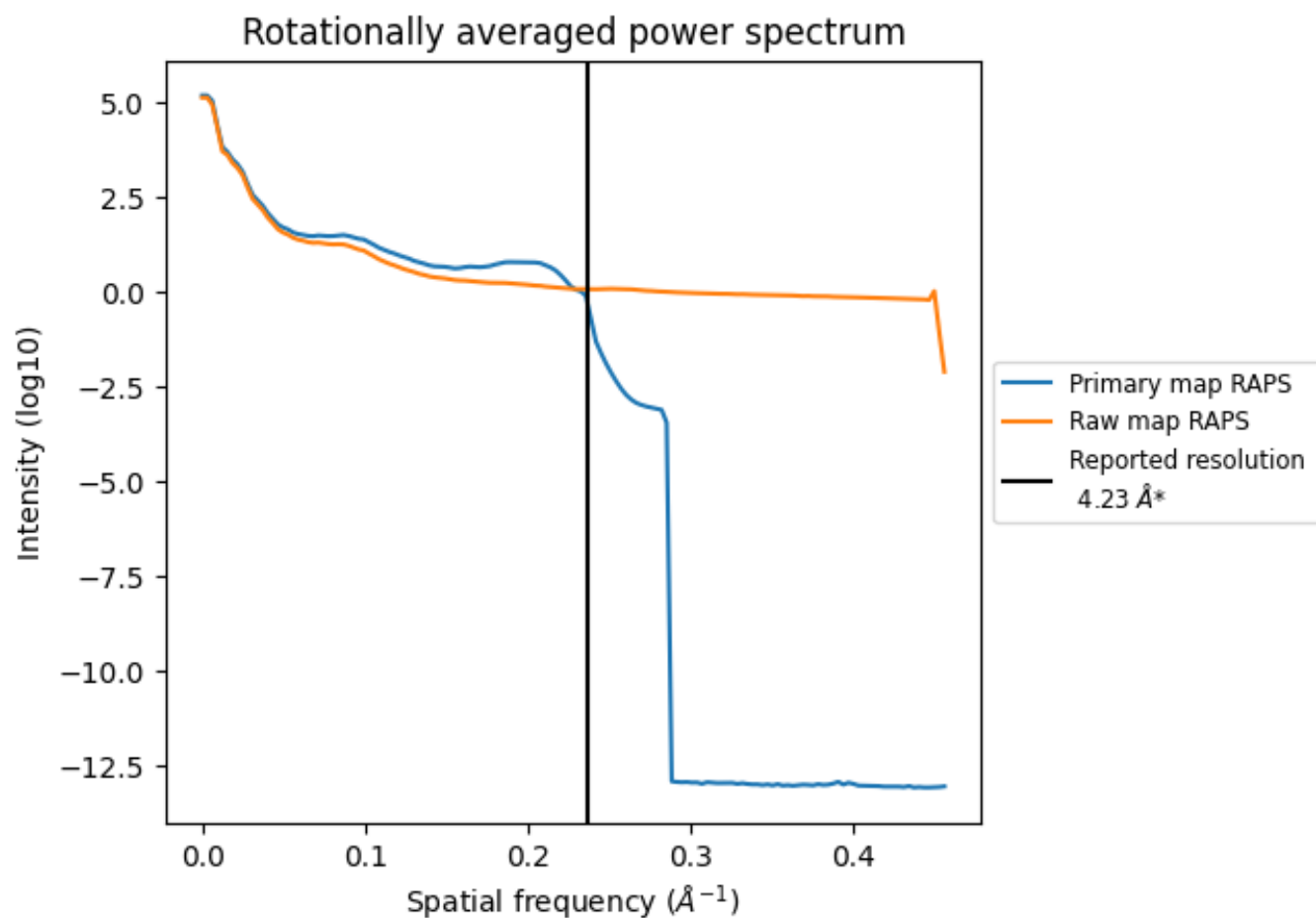
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 177 nm<sup>3</sup>; this corresponds to an approximate mass of 160 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 ⓘ



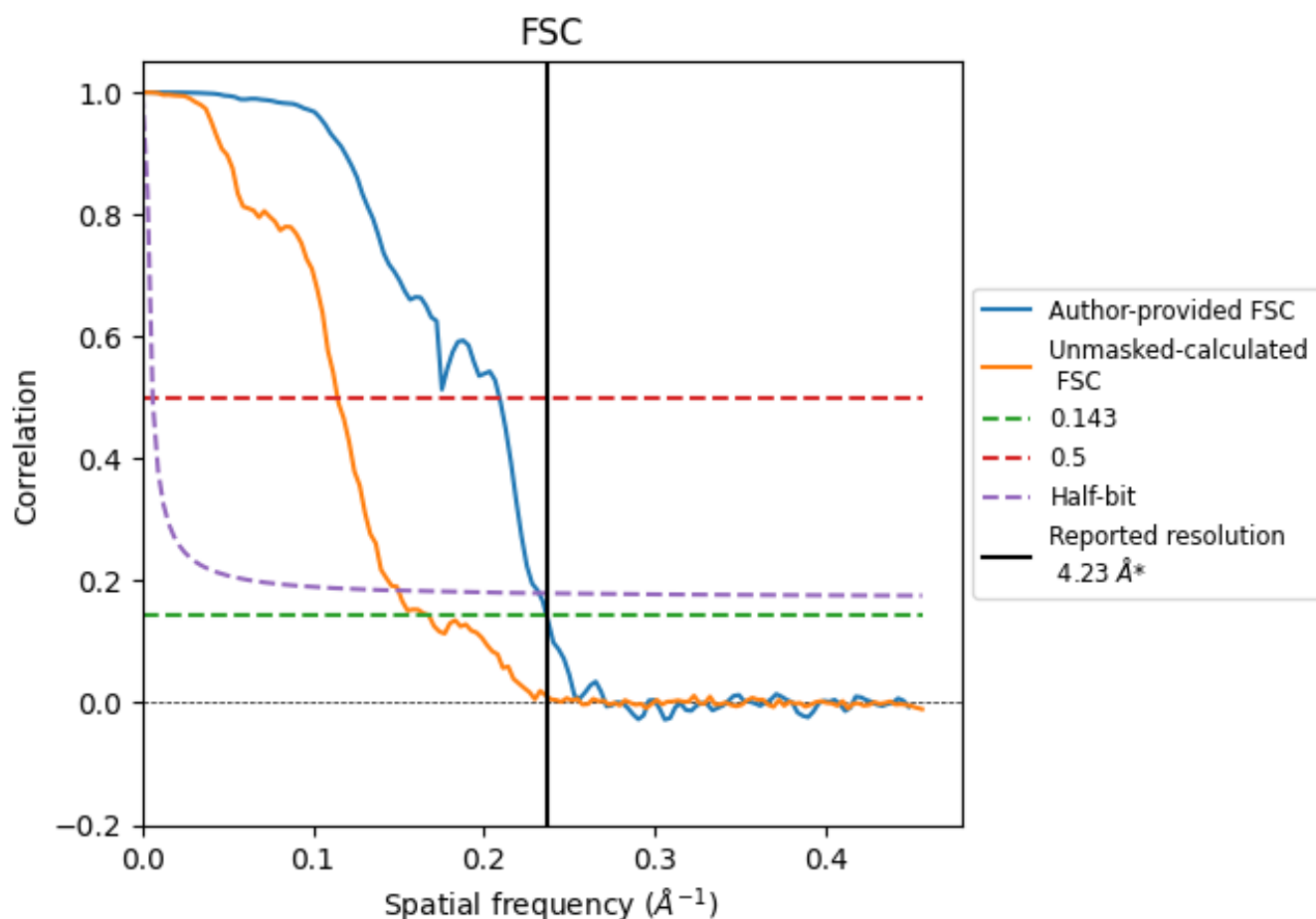
\*Reported resolution corresponds to spatial frequency of 0.236 Å<sup>-1</sup>



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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.236  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

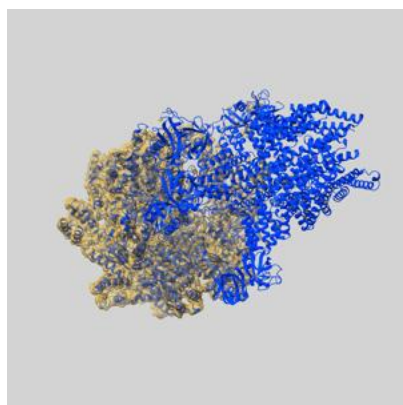
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.23	-	-
Author-provided FSC curve	4.23	4.79	4.31
Unmasked-calculated*	5.96	8.75	6.68

\*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 5.96 differs from the reported value 4.23 by more than 10 %

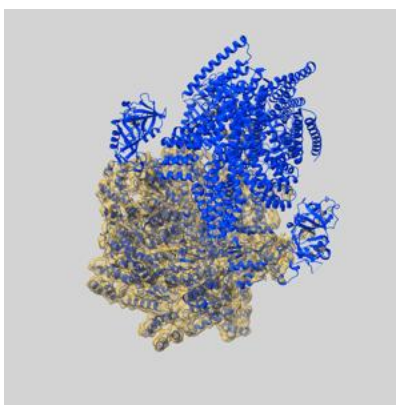
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-71529 and PDB model 9PD8. Per-residue inclusion information can be found in section [3](#) on page [9](#).

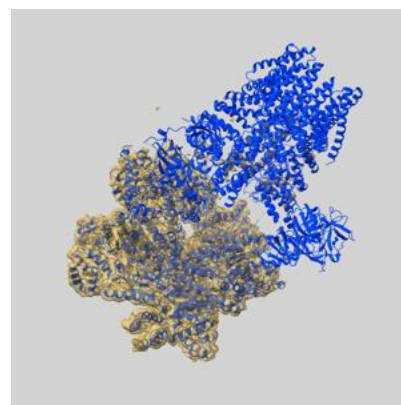
### 9.1 Map-model overlay [i](#)



X



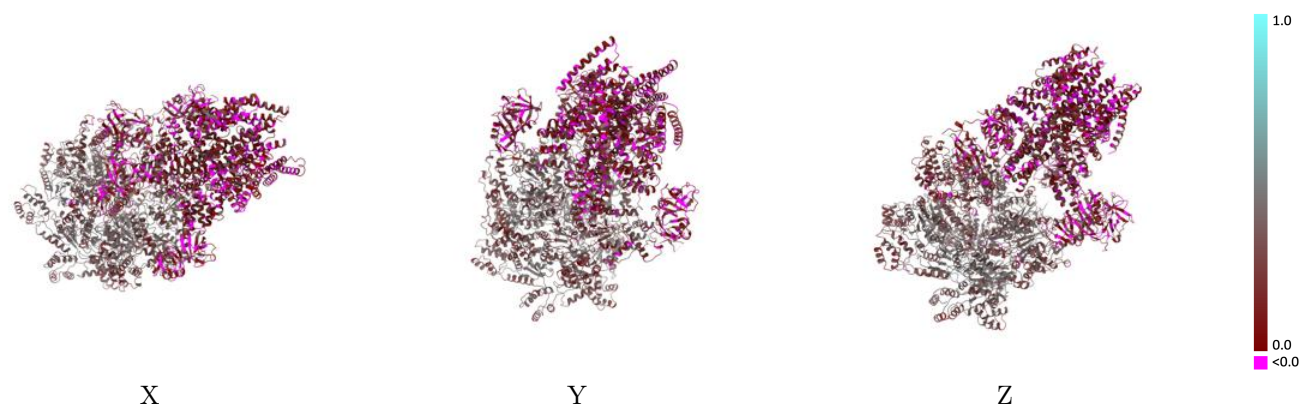
Y



Z

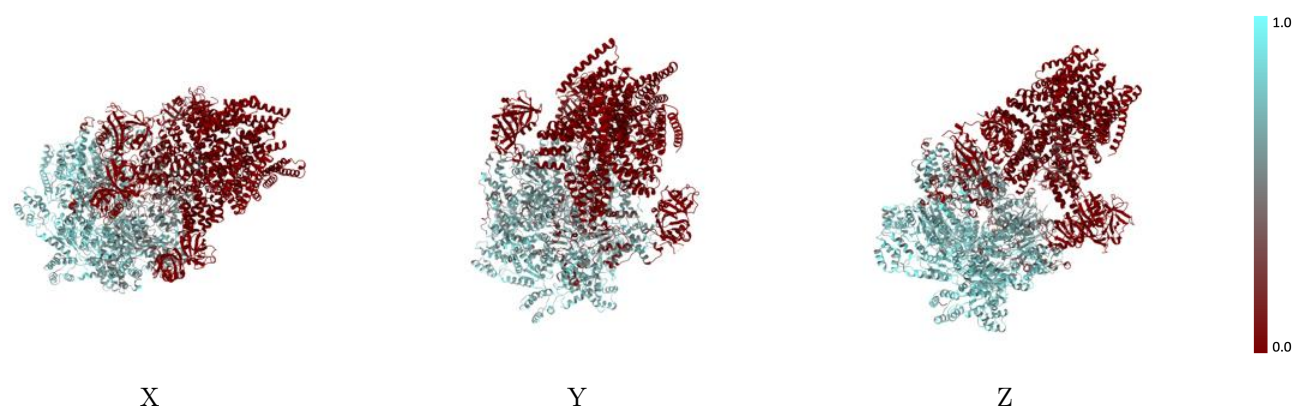
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



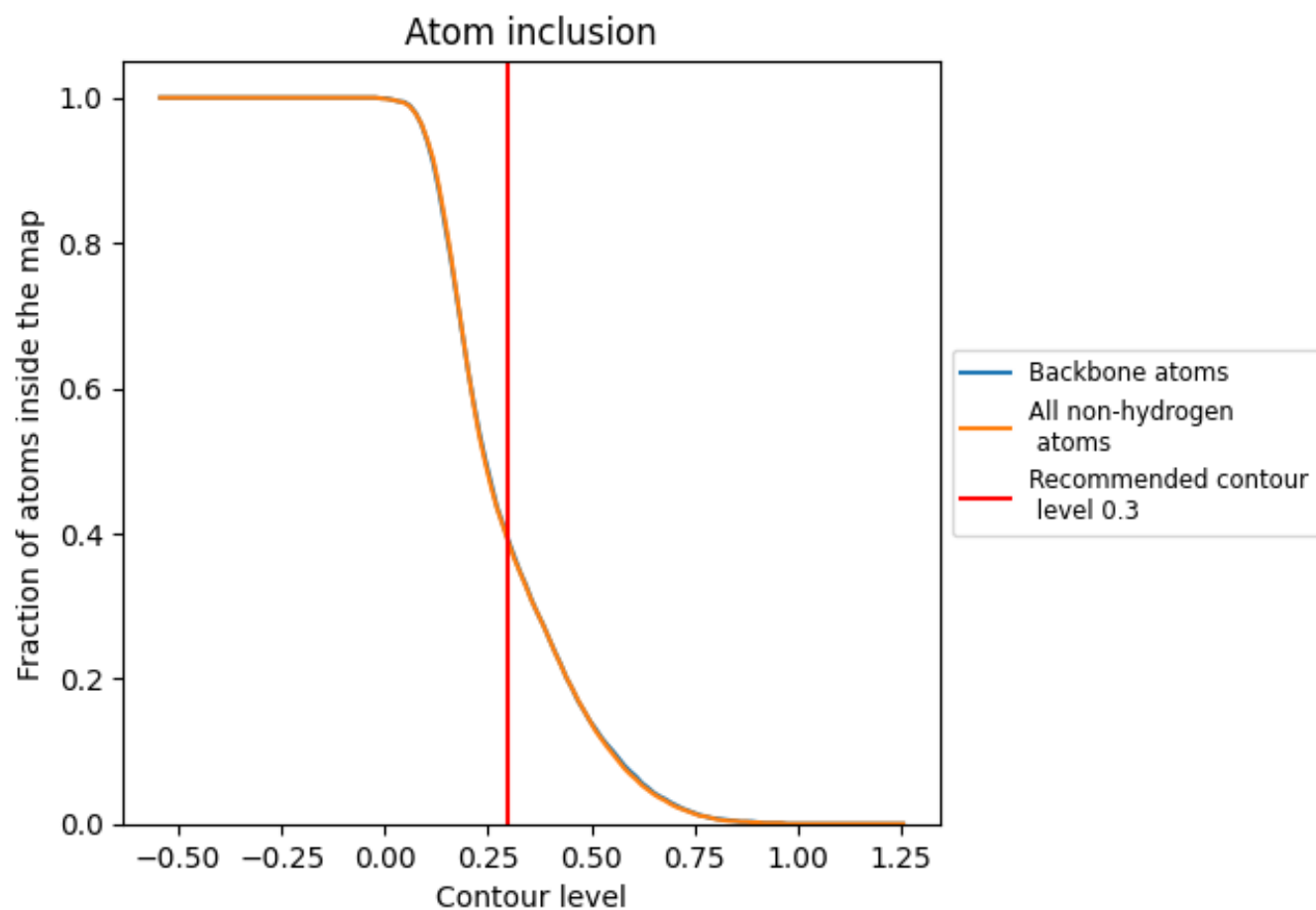
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 39% of all backbone atoms, 39% 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	 0.3870	 0.2580
A	 0.5050	 0.2980
B	 0.5170	 0.3080
C	 0.5110	 0.3130
D	 0.6570	 0.3600
E	 0.6100	 0.3350
F	 0.4030	 0.2470
G	 0.0510	 0.1590
H	 0.0130	 0.1510
I	 0.0570	 0.1540
J	 0.0210	 0.1410
K	 0.0000	 0.0990
L	 0.0080	 0.1170
M	 0.0200	 0.1230
N	 0.0040	 0.1170
O	 0.5080	 0.4410

