



wwPDB EM Validation Summary Report ⓘ

Mar 24, 2026 – 03:47 PM UTC

PDB ID : 5FTN / pdb_00005ftn
EMDB ID : EMD-3299
Title : Cryo-EM structure of human p97 bound to ATPgS (Conformation III)
Authors : Banerjee, S.; Bartesaghi, A.; Merk, A.; Rao, P.; Bulfer, S.L.; Yan, Y.; Green, N.; Mroczkowski, B.; Neitz, R.J.; Wipf, P.; Falconieri, V.; Deshaies, R.J.; Milne, J.L.S.; Huryn, D.; Arkin, M.; Subramaniam, S.
Deposited on : 2016-01-14
Resolution : 3.30 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

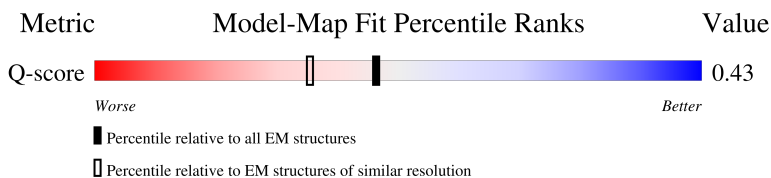
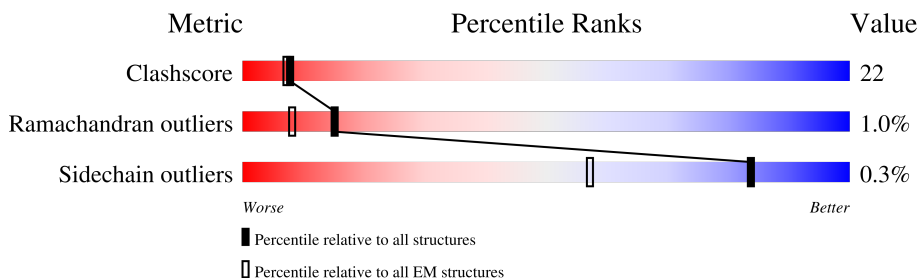
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.30 Å.

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



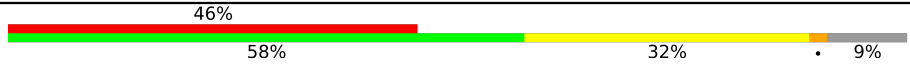
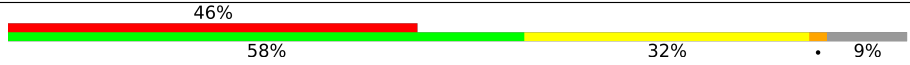
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	806	<p>46% (poor fit), 58% (outliers), 32% (outliers), 9% (not modelled)</p>
1	B	806	<p>46% (poor fit), 58% (outliers), 32% (outliers), 9% (not modelled)</p>
1	C	806	<p>46% (poor fit), 58% (outliers), 32% (outliers), 9% (not modelled)</p>
1	D	806	<p>46% (poor fit), 58% (outliers), 32% (outliers), 9% (not modelled)</p>

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Mol	Chain	Length	Quality of chain
1	E	806	
1	F	806	

2 Entry composition [i](#)

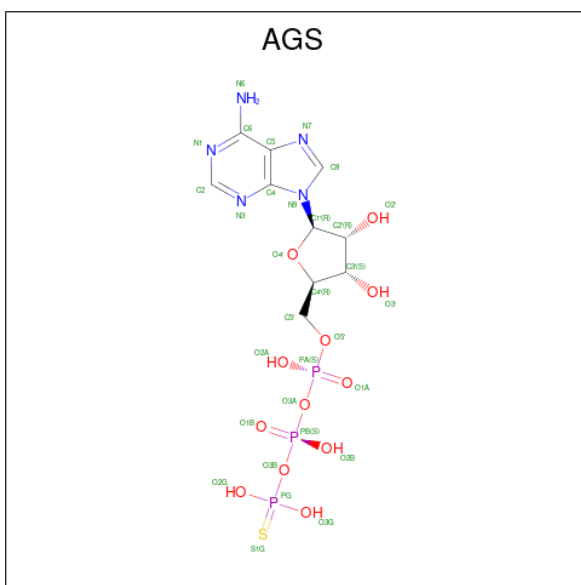
There are 3 unique types of molecules in this entry. The entry contains 34956 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called TRANSITIONAL ENDOPLASMIC RETICULUM ATPASE.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	737	Total 5762	C 3627	N 1014	O 1091	S 30	0	0
1	B	737	Total 5762	C 3627	N 1014	O 1091	S 30	0	0
1	C	737	Total 5762	C 3627	N 1014	O 1091	S 30	0	0
1	D	737	Total 5762	C 3627	N 1014	O 1091	S 30	0	0
1	E	737	Total 5762	C 3627	N 1014	O 1091	S 30	0	0
1	F	737	Total 5762	C 3627	N 1014	O 1091	S 30	0	0

- Molecule 2 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



Mol	Chain	Residues	Atoms					AltConf	
2	A	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	A	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	B	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	B	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	C	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	C	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	D	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	D	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	E	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	E	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	F	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	F	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
3	A	2	Total	Mg	0
			2	2	
3	B	2	Total	Mg	0
			2	2	
3	C	2	Total	Mg	0
			2	2	
3	D	2	Total	Mg	0
			2	2	
3	E	2	Total	Mg	0
			2	2	
3	F	2	Total	Mg	0
			2	2	

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: TRANSITIONAL ENDOPLASMIC RETICULUM ATPASE



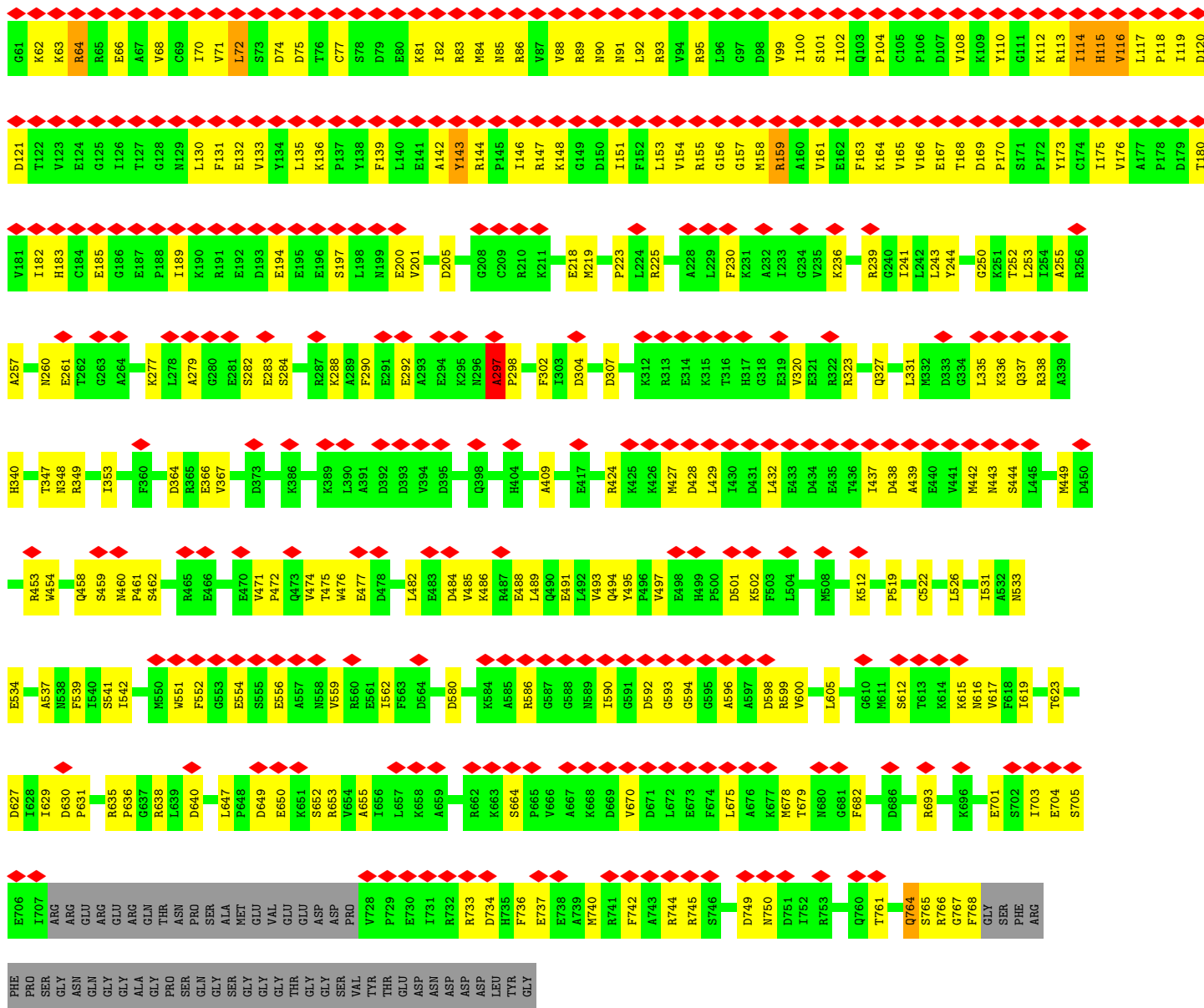


MET	ALA	SER	GLY	ALA	ASP	SER	LYS	GLY	ASP	L12	L13	S13	T14	A15	I16	L17	K18	Q19	K20	N21	R22	P23	N24	R25	L26	I27	V28	D29	E30	A31	I32	N33	E34	D35	N36	S37	V38	V39	S40	L41	S42	Q43	P44	K45	M46	D47	E48	L49	Q50	L51	F52	R53	G54	D55	T56	V57	L58	L59	K60								
G61	K62	K63	R64	R65	E66	A67	V68	C69	I70	V71	L72	S73	D74	D75	T76	C77	S78	D79	E80	K81	R82	R83	M84	N85	R86	V87	V88	R89	N90	N91	L92	R93	R94	L95	V96	R97	L96	G97	M98	D98	V99	I100	S101	I102	Q103	P104	C105	E106	D107	V108	L109	L110	F111	G112	K113	I114	H115	V116	L117	P118	I119	D120					
D121	T122	V123	E124	G125	I126	T127	G128	M129	L130	F131	E132	V133	L134	L135	K136	F137	F138	F139	L140	E141	A142	Y143	R144	F145	L146	R147	K148	G149	I150	I151	F152	L153	V154	R155	G156	G157	M158	R159	A160	V161	E162	F163	K164	V165	V166	D167	T168	D169	P170	S171	P172	Y173	G174	I175	A176	P177	D178	T180									
V181	I182	H183	C184	E185	G186	E187	P188	I189	K190	R191	E192	D193	E194	E195	E196	S197	L198	N199	E200	V201	D205	C209	R210	K211	E218	M219	P223	L224	R225	A228	L229	F230	K231	A232	L233	G234	V235	K236	R239	G240	L241	L242	L243	Y244	G250	K251	T252	L253	L254	A255	R256	A257															
M260	E261	T262	G263	A264	K277	L278	A279	G280	E281	S282	E283	S284	R287	K288	A289	F290	E291	E292	A293	E294	K295	N296	A297	P298	F302	I303	D304	D307	K312	R313	E314	K315	T316	H317	G318	E319	V320	E321	R322	R323	Q327	L331	K332	D333	G334	L335	K336	Q337	R338	A339	H340																
T347	R348	R349	L353	F360	D364	R365	E366	V367	D373	K386	K389	L390	A391	D392	D393	V394	D395	G398	H404	A409	E417	R424	K425	K426	M427	D428	L429	I430	D431	L432	E433	D434	E435	T436	L437	D438	A439	E440	V441	M442	S444	L445	M449	D450																							
R453	W454	Q458	S459	M460	P461	S462	R465	E466	E470	V471	P472	V474	T475	W476	E477	D478	L482	E483	D484	Y485	K486	R487	E488	L489	E491	L492	V493	Q494	Y495	F496	V497	E498	H499	F500	D501	K502	F503	L504	K505	M508	T509	K512	P519	C522	L526	M443	S444	L445	M449	D450																	
N533	E534	A537	N538	F539	S541	I542	M550	W551	F552	G553	E554	S555	E556	A557	M558	V559	R560	D561	I562	D590	K594	A595	R596	G597	G598	N599	I590	G591	D592	G593	G594	G595	A596	A597	D598	R599	V600	L605	G610	M611	S612	T613	K614	K615	M616	V617	F618	L619	T623	D627																	
I628	I629	P631	R635	P636	G637	R638	L639	D640	L647	P648	D649	E650	R651	S652	R653	V654	A655	F656	L657	K658	A659	R662	K663	S664	P665	V666	A667	K668	D669	V670	D671	R743	K744	R745	D749	N750	D751	I752	R753	G760	T761	Q764	S765	R766	G767	F768	GLY	SER	PHE	ARG	PHE	PRO															
I707	ARG	ASN	ARG	GLU	ARG	GLU	ARG	GLU	ASN	PRO	GLN	SER	ALA	MET	GLU	VAL	GLU	GLU	GLY	ASP	ASP	VAL	TYR	THR	THR	THR	GLU	GLU	ASP	ASN	R728	F729	E730	I731	R732	R733	D734	H735	F736	E737	E738	A739	M740	E741	F742	R743	R744	R745	D749	N750	D751	I752	R753	G760	T761	Q764	S765	R766	G767	F768	GLY	SER	PHE	ARG	PHE	PRO	
SER	GLY	ASN	GLN	GLY	ALA	ASP	SER	LYS	GLY	ASP	GLN	GLY	SER	ALA	MET	GLU	VAL	GLU	GLU	GLY	ASP	ASP	VAL	TYR	THR	THR	THR	GLU	GLU	ASP	ASN	R728	F729	E730	I731	R732	R733	D734	H735	F736	E737	E738	A739	M740	E741	F742	R743	R744	R745	D749	N750	D751	I752	R753	G760	T761	Q764	S765	R766	G767	F768	GLY	SER	PHE	ARG	PHE	PRO

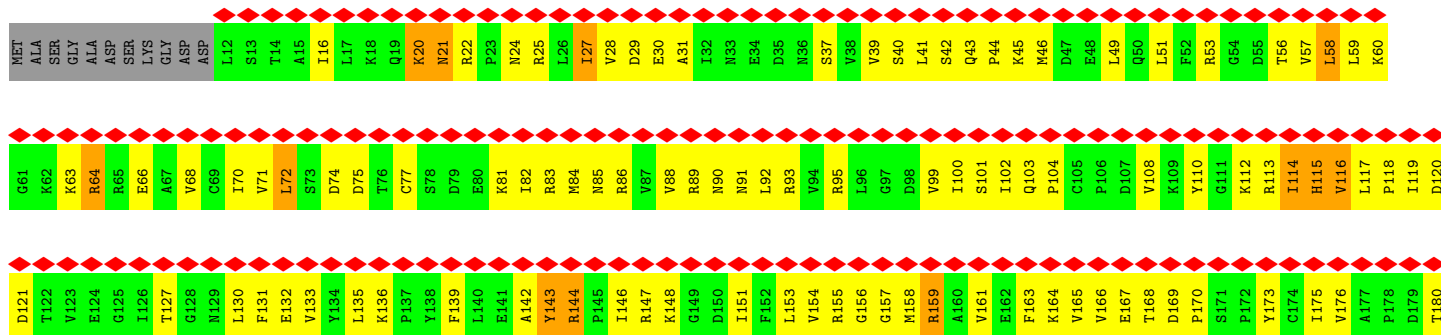
• Molecule 1: TRANSITIONAL ENDOPLASMIC RETICULUM ATPASE

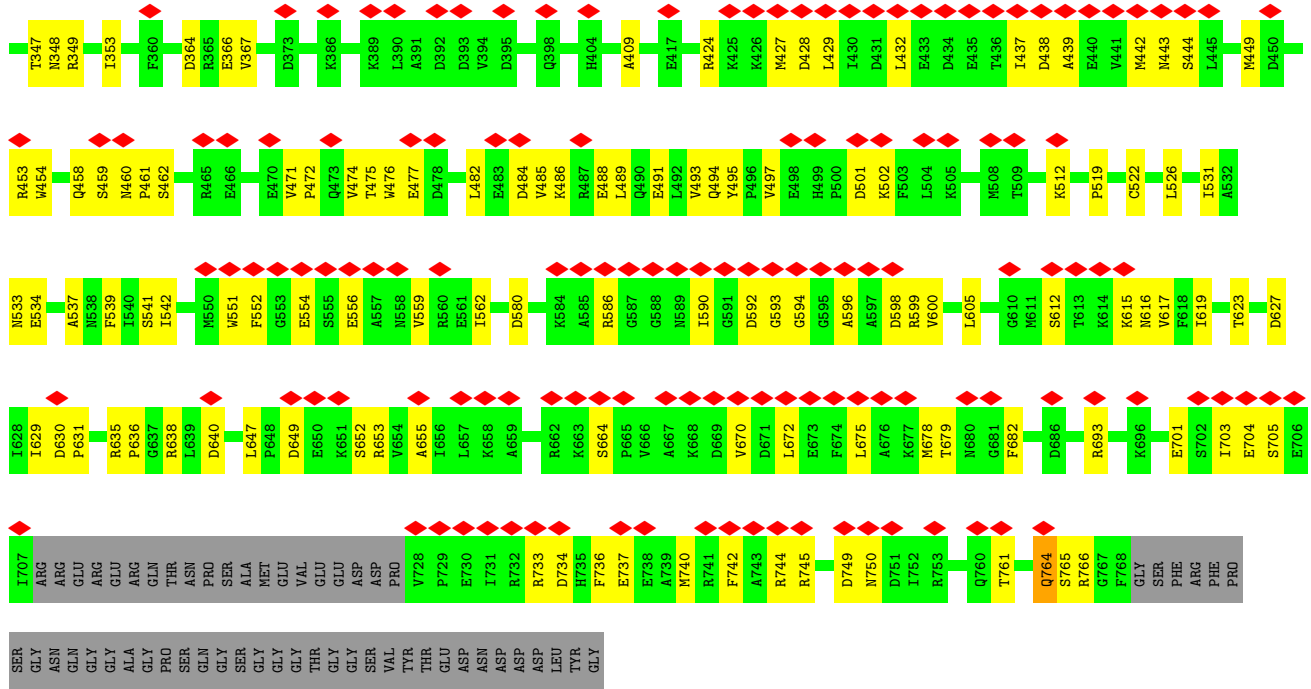


MET	ALA	SER	GLY	ALA	ASP	SER	LYS	GLY	ASP	L12	L13	S13	T14	A15	I16	L17	K18	Q19	K20	N21	R22	P23	N24	R25	L26	I27	V28	D29	E30	A31	I32	N33	E34	D35	N36	S37	V38	V39	S40	L41	S42	Q43	P44	K45	M46	D47	E48	L49	Q50	L51	F52	R53	G54	D55	T56	V57	L58	L59	K60
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● Molecule 1: TRANSITIONAL ENDOPLASMIC RETICULUM ATPASE





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	23306	Depositor
Resolution determination method	Not provided	
CTF correction method	EACH PARTICLE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	950	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	36980	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.072	Depositor
Minimum map value	-0.034	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0199	Depositor
Map size (\AA)	186.576, 186.576, 186.576	wwPDB
Map dimensions	276, 276, 276	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.676, 0.676, 0.676	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MG, AGS

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	0.49	1/5855 (0.0%)	0.73	10/7905 (0.1%)
1	B	0.49	1/5855 (0.0%)	0.73	10/7905 (0.1%)
1	C	0.49	1/5855 (0.0%)	0.73	10/7905 (0.1%)
1	D	0.49	1/5855 (0.0%)	0.73	10/7905 (0.1%)
1	E	0.49	1/5855 (0.0%)	0.73	10/7905 (0.1%)
1	F	0.49	1/5855 (0.0%)	0.73	10/7905 (0.1%)
All	All	0.49	6/35130 (0.0%)	0.73	60/47430 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	6
1	C	0	6
1	D	0	6
1	E	0	6
1	F	0	6
All	All	0	36

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	297	ALA	C-N	5.19	1.40	1.33
1	C	297	ALA	C-N	5.15	1.40	1.33
1	A	297	ALA	C-N	5.13	1.40	1.33
1	D	297	ALA	C-N	5.13	1.40	1.33
1	B	297	ALA	C-N	5.12	1.40	1.33

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	20	LYS	N-CA-C	9.41	122.95	110.53
1	F	20	LYS	N-CA-C	9.40	122.94	110.53
1	A	20	LYS	N-CA-C	9.40	122.94	110.53
1	B	20	LYS	N-CA-C	9.40	122.93	110.53
1	D	20	LYS	N-CA-C	9.38	122.92	110.53

There are no chirality outliers.

5 of 36 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	142	ALA	Peptide
1	A	144	ARG	Peptide
1	A	156	GLY	Peptide
1	A	64	ARG	Peptide
1	A	72	LEU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5762	0	5841	269	0
1	B	5762	0	5841	268	0
1	C	5762	0	5841	270	0
1	D	5762	0	5841	272	0
1	E	5762	0	5841	268	0
1	F	5762	0	5841	273	0
2	A	62	0	24	10	0
2	B	62	0	24	10	0
2	C	62	0	24	10	0
2	D	62	0	24	9	0
2	E	62	0	24	10	0
2	F	62	0	24	10	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	2	0	0	0	0
3	F	2	0	0	0	0
All	All	34956	0	35190	1575	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 22.

The worst 5 of 1575 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:B:113:ARG:NH2	1:B:131:PHE:CE2	2.26	1.03
1:C:113:ARG:NH2	1:C:131:PHE:CE2	2.26	1.03
1:D:113:ARG:NH2	1:D:131:PHE:CE2	2.26	1.03
1:A:113:ARG:NH2	1:A:131:PHE:CE2	2.26	1.03
1:F:113:ARG:NH2	1:F:131:PHE:CE2	2.26	1.02

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	733/806 (91%)	672 (92%)	54 (7%)	7 (1%)	12	40
1	B	733/806 (91%)	671 (92%)	55 (8%)	7 (1%)	12	40
1	C	733/806 (91%)	672 (92%)	54 (7%)	7 (1%)	12	40
1	D	733/806 (91%)	672 (92%)	54 (7%)	7 (1%)	12	40
1	E	733/806 (91%)	672 (92%)	54 (7%)	7 (1%)	12	40
1	F	733/806 (91%)	672 (92%)	54 (7%)	7 (1%)	12	40
All	All	4398/4836 (91%)	4031 (92%)	325 (7%)	42 (1%)	15	40

5 of 42 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	297	ALA
1	B	297	ALA
1	C	297	ALA
1	D	297	ALA
1	E	297	ALA

5.3.2 Protein sidechains [i](#)

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	626/678 (92%)	624 (100%)	2 (0%)	86	86
1	B	626/678 (92%)	624 (100%)	2 (0%)	86	86
1	C	626/678 (92%)	624 (100%)	2 (0%)	86	86
1	D	626/678 (92%)	624 (100%)	2 (0%)	86	86
1	E	626/678 (92%)	624 (100%)	2 (0%)	86	86
1	F	626/678 (92%)	624 (100%)	2 (0%)	86	86
All	All	3756/4068 (92%)	3744 (100%)	12 (0%)	84	86

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	474	VAL
1	E	58	LEU
1	F	474	VAL
1	E	474	VAL
1	B	474	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	91	ASN
1	F	91	ASN

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Mol	Chain	Res	Type
1	E	285	ASN
1	E	337	GLN
1	F	317	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](#)

Of 24 ligands modelled in this entry, 12 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	AGS	D	902	-	32,33,33	1.99	7 (21%)	45,52,52	1.88	10 (22%)
2	AGS	C	902	-	32,33,33	1.99	6 (18%)	45,52,52	1.89	10 (22%)
2	AGS	F	901	-	32,33,33	2.01	6 (18%)	45,52,52	1.88	10 (22%)
2	AGS	A	901	-	32,33,33	2.00	6 (18%)	45,52,52	1.87	10 (22%)
2	AGS	B	901	-	32,33,33	1.99	6 (18%)	45,52,52	1.87	10 (22%)
2	AGS	A	902	-	32,33,33	1.99	6 (18%)	45,52,52	1.88	10 (22%)
2	AGS	B	902	-	32,33,33	1.99	6 (18%)	45,52,52	1.88	10 (22%)
2	AGS	E	902	-	32,33,33	1.99	6 (18%)	45,52,52	1.87	10 (22%)
2	AGS	D	901	-	32,33,33	2.00	6 (18%)	45,52,52	1.87	10 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	AGS	E	901	-	32,33,33	2.01	6 (18%)	45,52,52	1.87	10 (22%)
2	AGS	F	902	-	32,33,33	1.99	7 (21%)	45,52,52	1.87	10 (22%)
2	AGS	C	901	-	32,33,33	2.01	6 (18%)	45,52,52	1.87	10 (22%)

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
2	AGS	D	902	-	-	1/21/38/38	0/3/3/3
2	AGS	C	902	-	-	1/21/38/38	0/3/3/3
2	AGS	F	901	-	-	3/21/38/38	0/3/3/3
2	AGS	A	901	-	-	3/21/38/38	0/3/3/3
2	AGS	B	901	-	-	3/21/38/38	0/3/3/3
2	AGS	A	902	-	-	1/21/38/38	0/3/3/3
2	AGS	B	902	-	-	1/21/38/38	0/3/3/3
2	AGS	E	902	-	-	1/21/38/38	0/3/3/3
2	AGS	D	901	-	-	3/21/38/38	0/3/3/3
2	AGS	E	901	-	-	3/21/38/38	0/3/3/3
2	AGS	F	902	-	-	1/21/38/38	0/3/3/3
2	AGS	C	901	-	-	3/21/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	902	AGS	PG-S1G	7.83	2.07	1.90
2	D	902	AGS	PG-S1G	7.83	2.07	1.90
2	C	901	AGS	PG-S1G	7.82	2.07	1.90
2	C	902	AGS	PG-S1G	7.81	2.07	1.90
2	E	901	AGS	PG-S1G	7.80	2.07	1.90

The worst 5 of 120 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	901	AGS	C5-C4-N3	-5.90	118.60	126.72
2	C	901	AGS	C5-C4-N3	-5.87	118.63	126.72
2	C	902	AGS	C5-C4-N3	-5.86	118.64	126.72
2	A	901	AGS	C5-C4-N3	-5.86	118.65	126.72
2	D	901	AGS	C5-C4-N3	-5.86	118.65	126.72

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

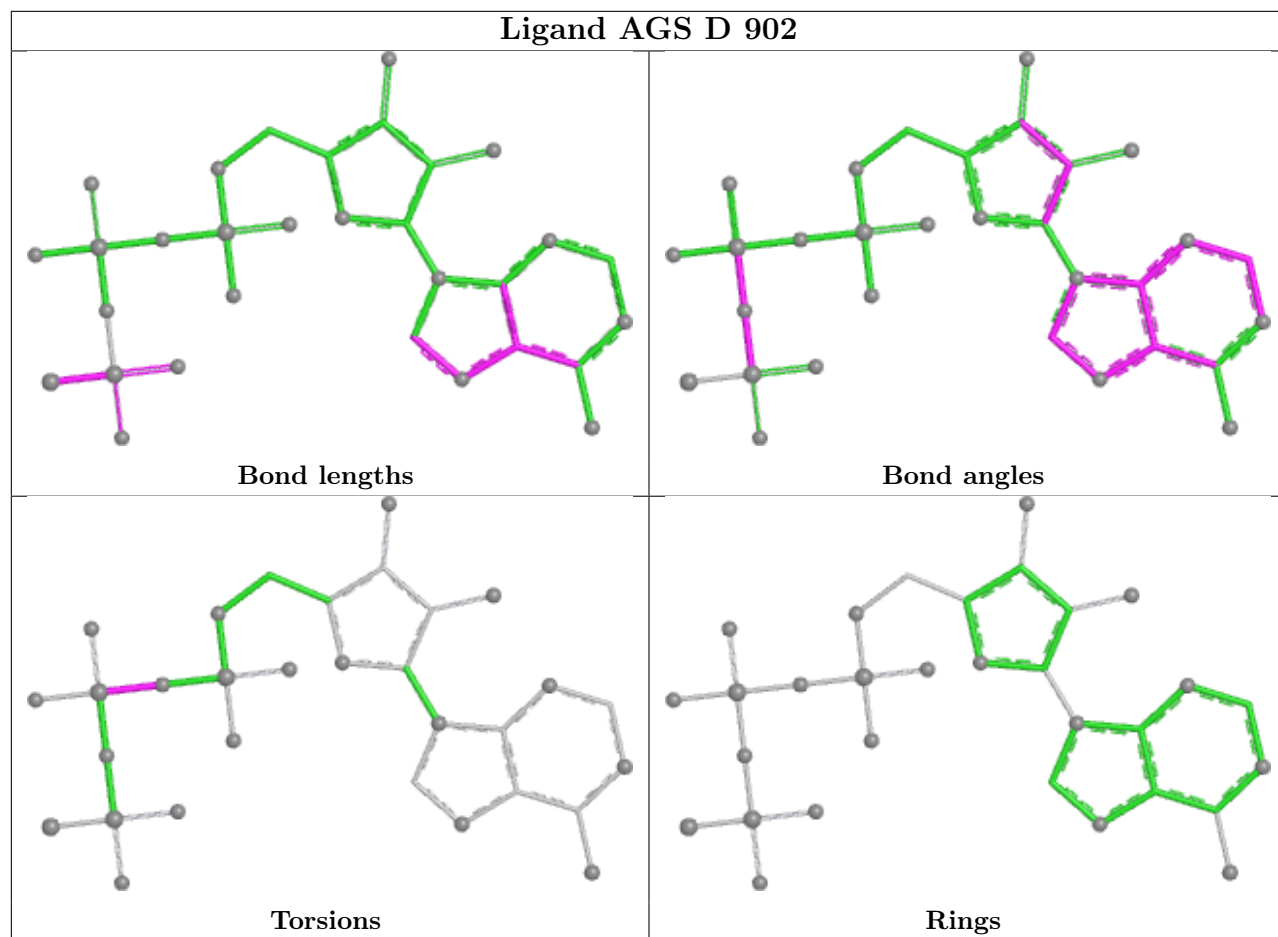
Mol	Chain	Res	Type	Atoms
2	A	901	AGS	C5'-O5'-PA-O1A
2	A	901	AGS	C5'-O5'-PA-O2A
2	A	901	AGS	C5'-O5'-PA-O3A
2	B	901	AGS	C5'-O5'-PA-O1A
2	B	901	AGS	C5'-O5'-PA-O2A

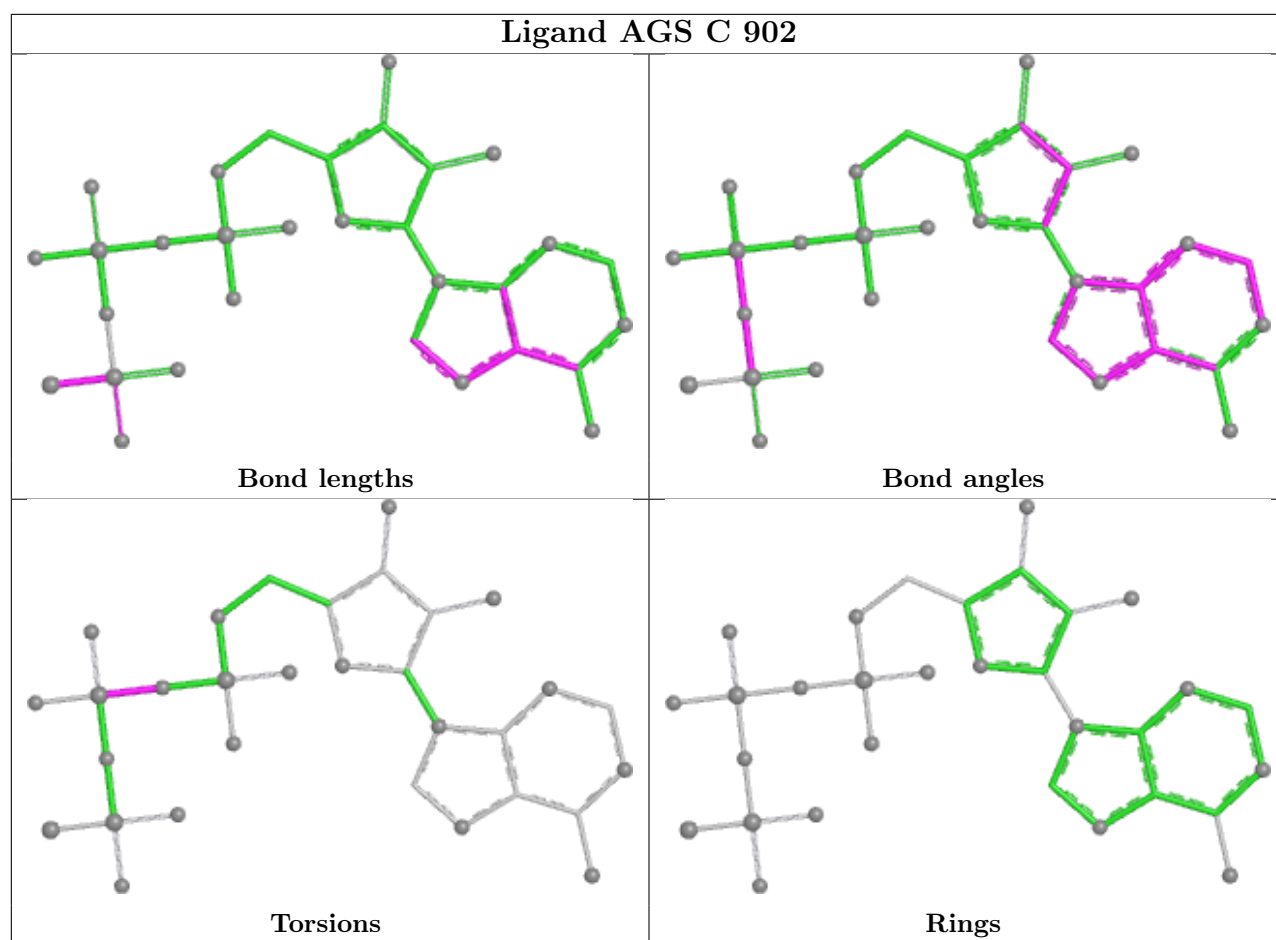
There are no ring outliers.

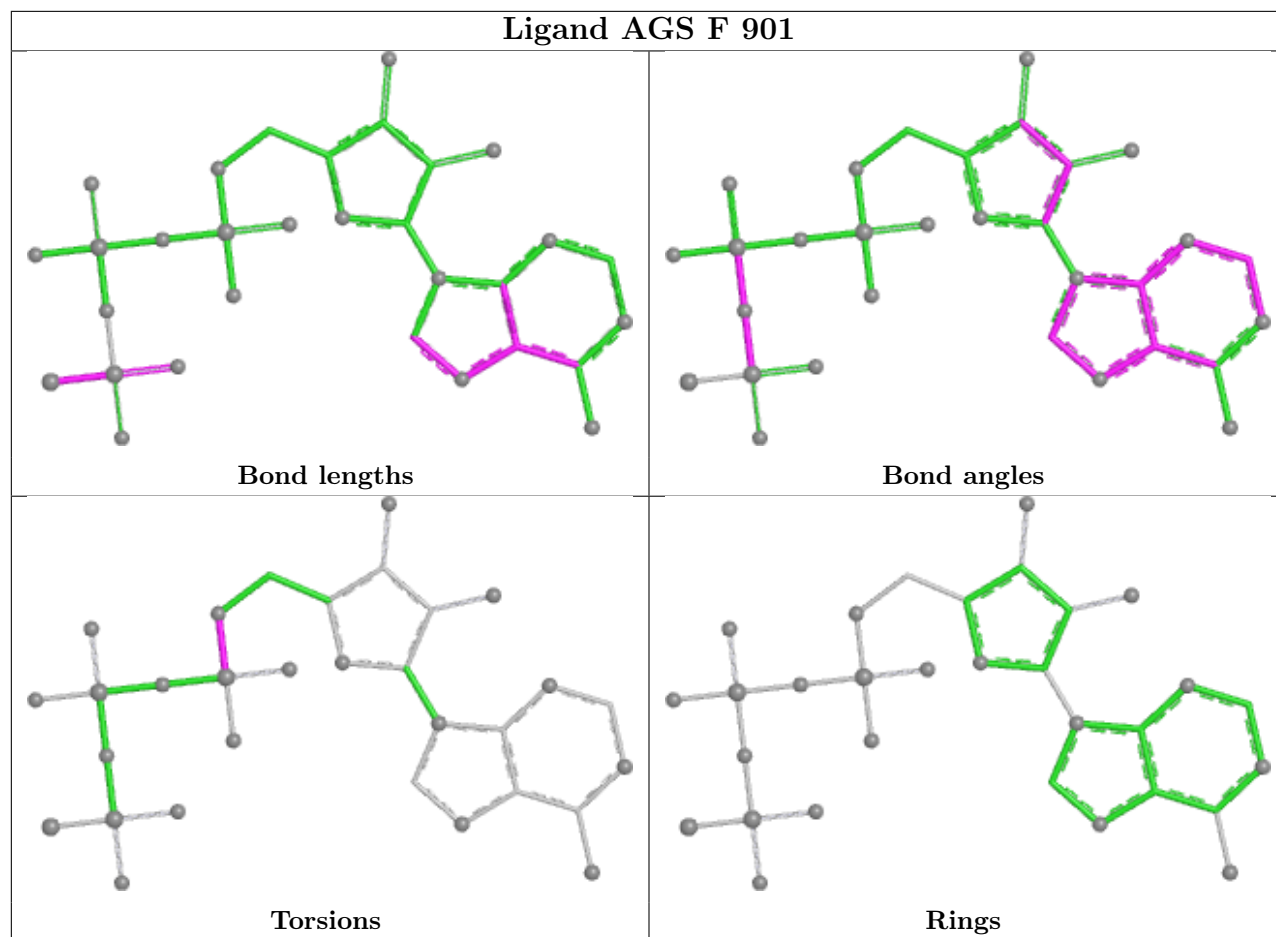
12 monomers are involved in 59 short contacts:

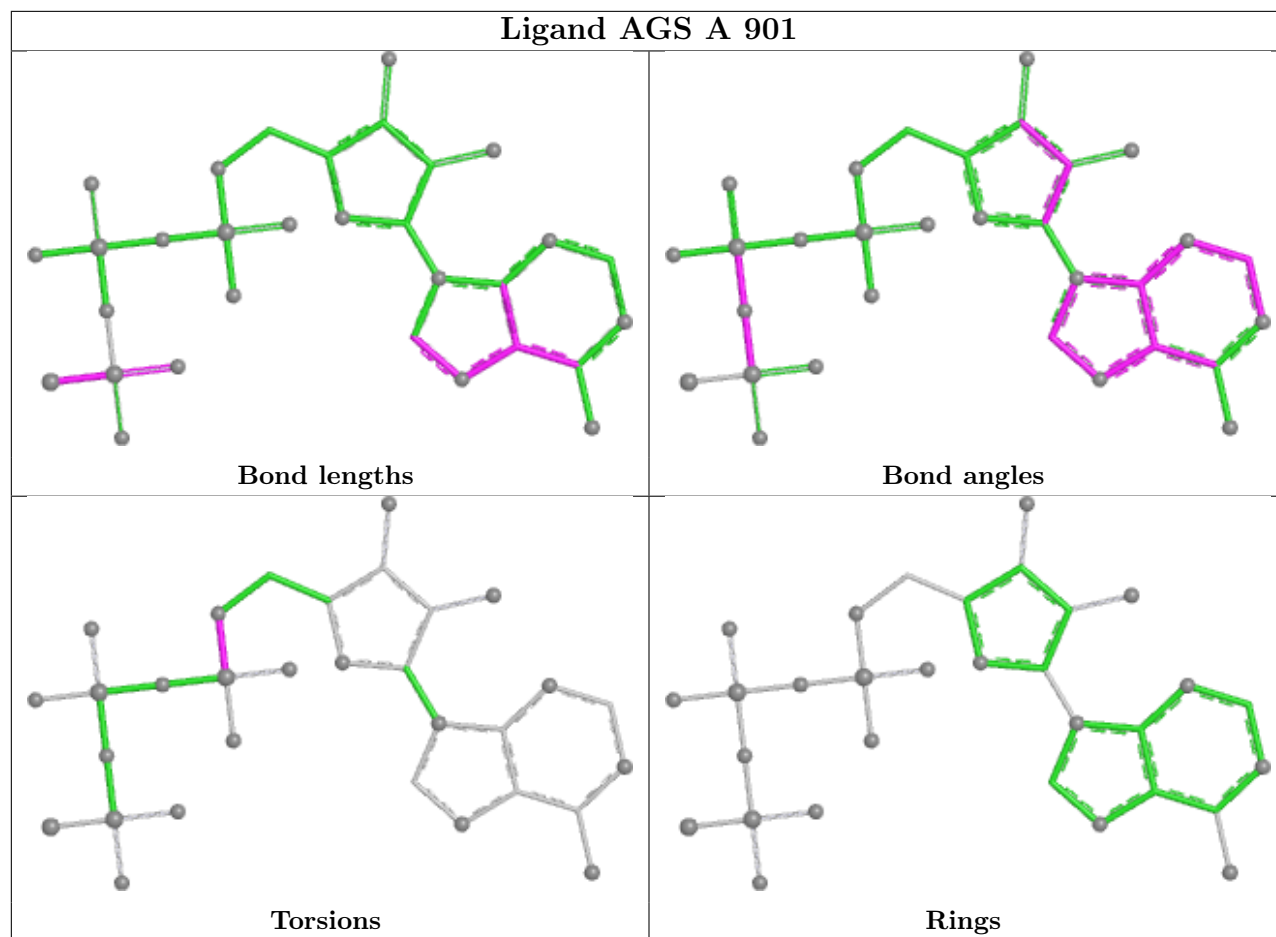
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	902	AGS	2	0
2	C	902	AGS	3	0
2	F	901	AGS	8	0
2	A	901	AGS	8	0
2	B	901	AGS	8	0
2	A	902	AGS	2	0
2	B	902	AGS	2	0
2	E	902	AGS	3	0
2	D	901	AGS	7	0
2	E	901	AGS	7	0
2	F	902	AGS	2	0
2	C	901	AGS	7	0

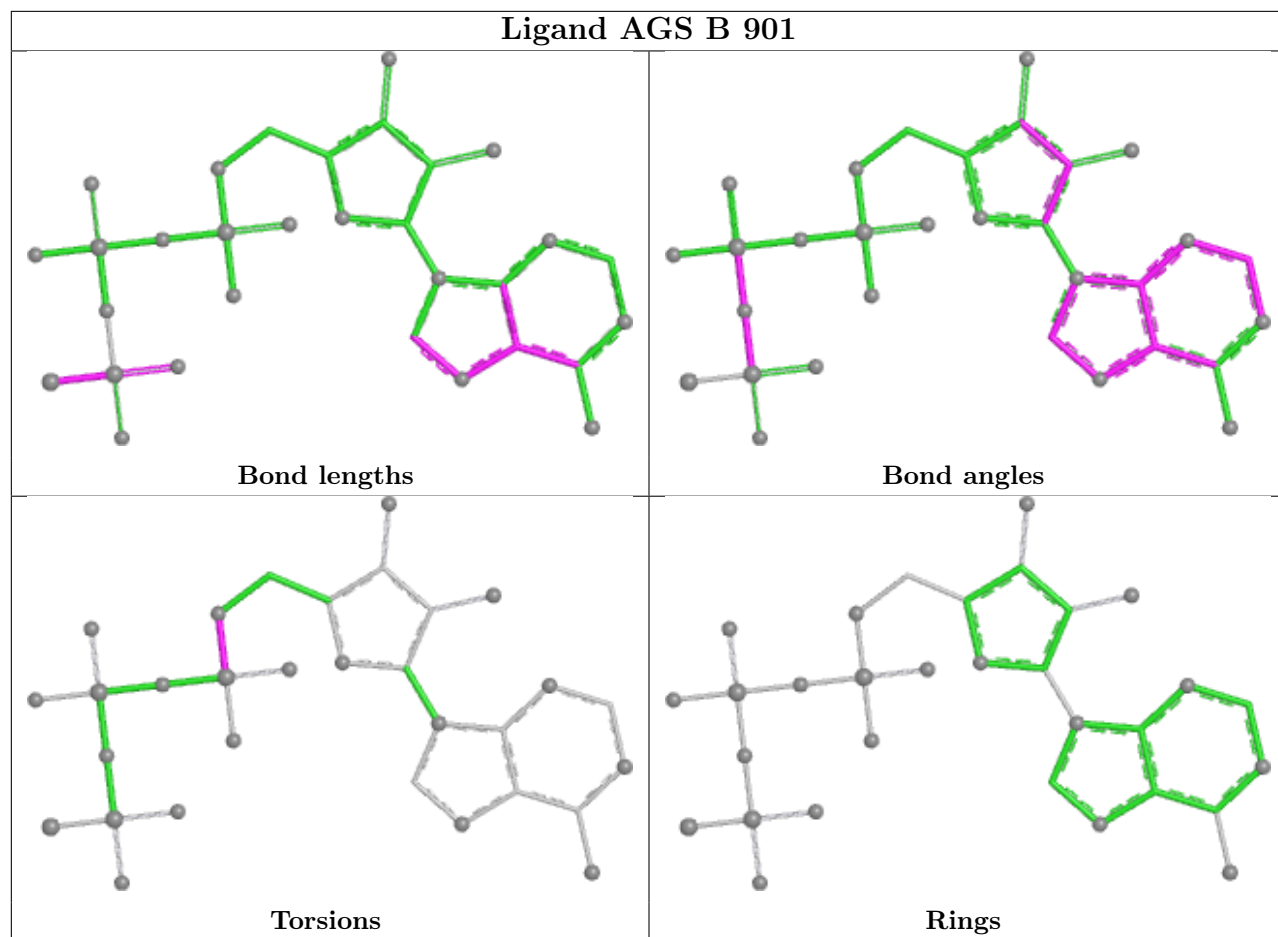
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

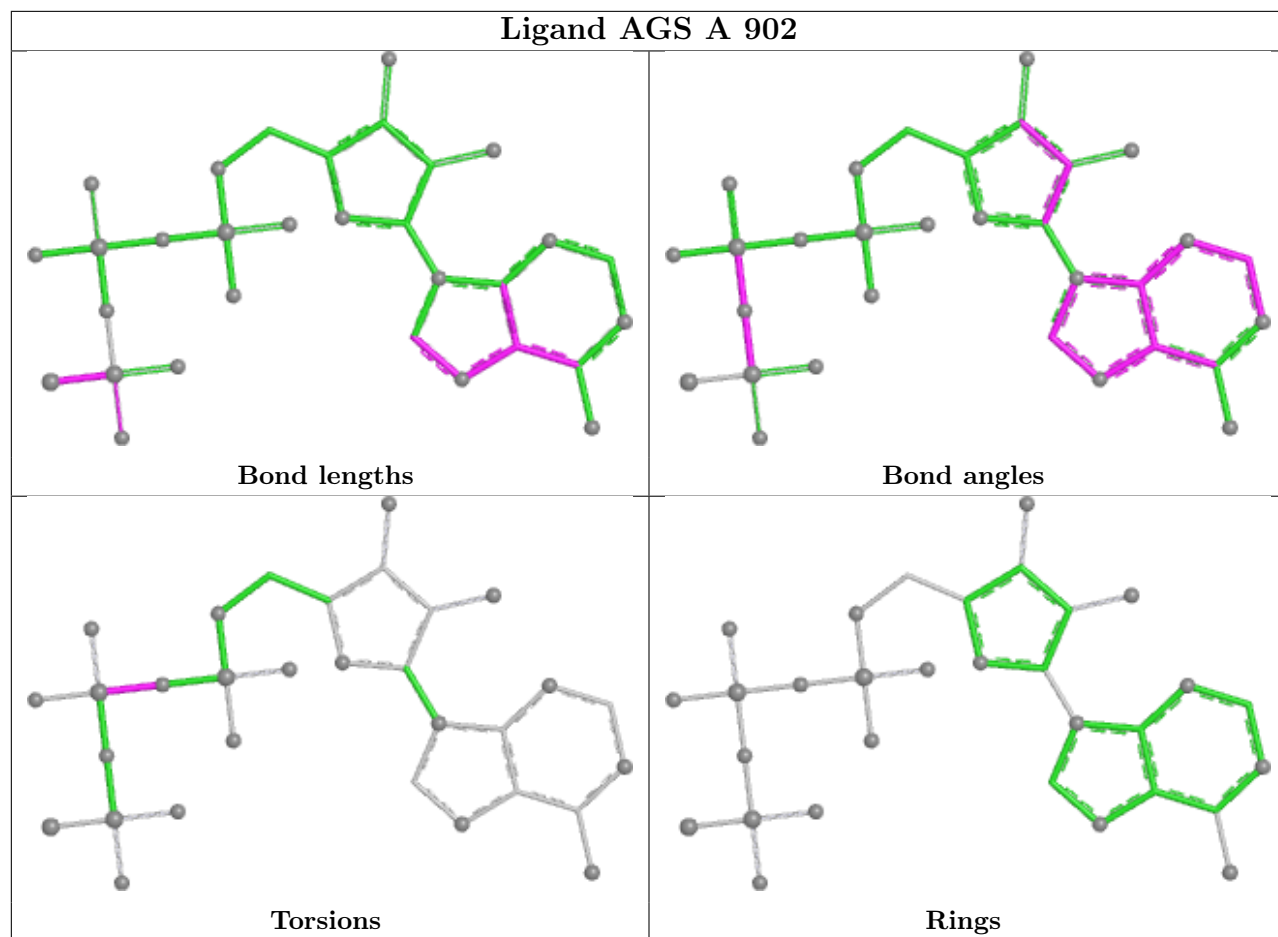


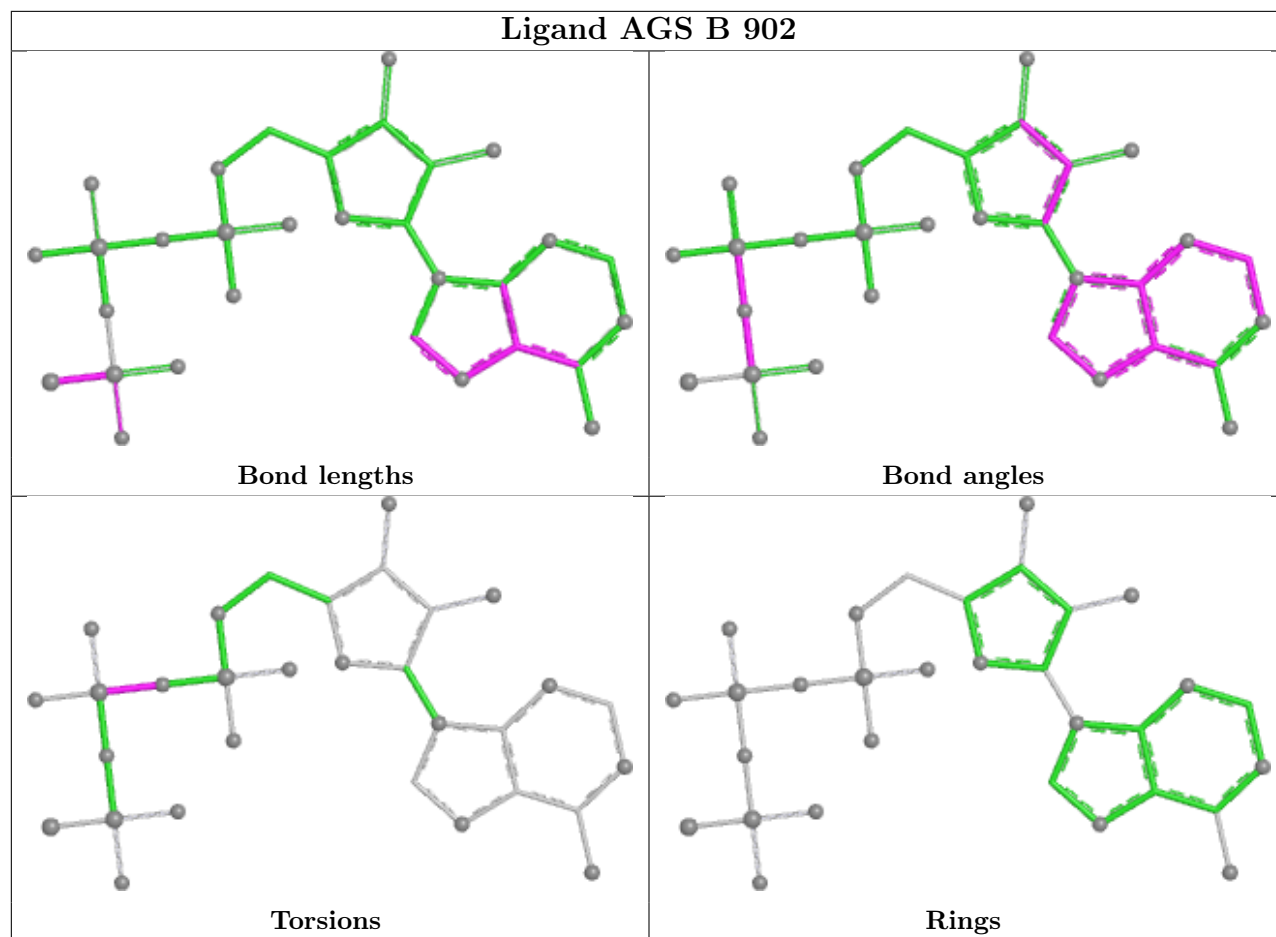


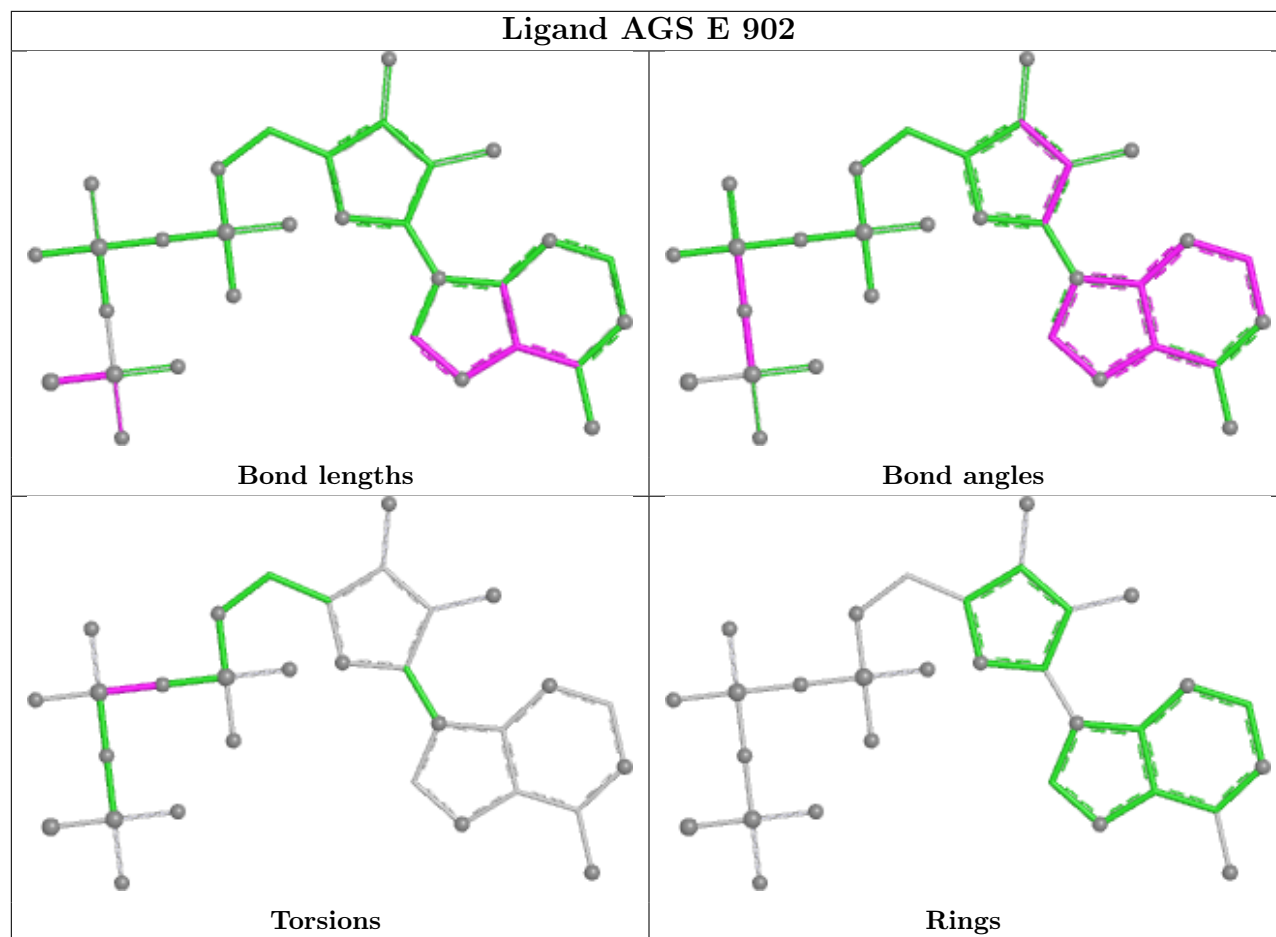


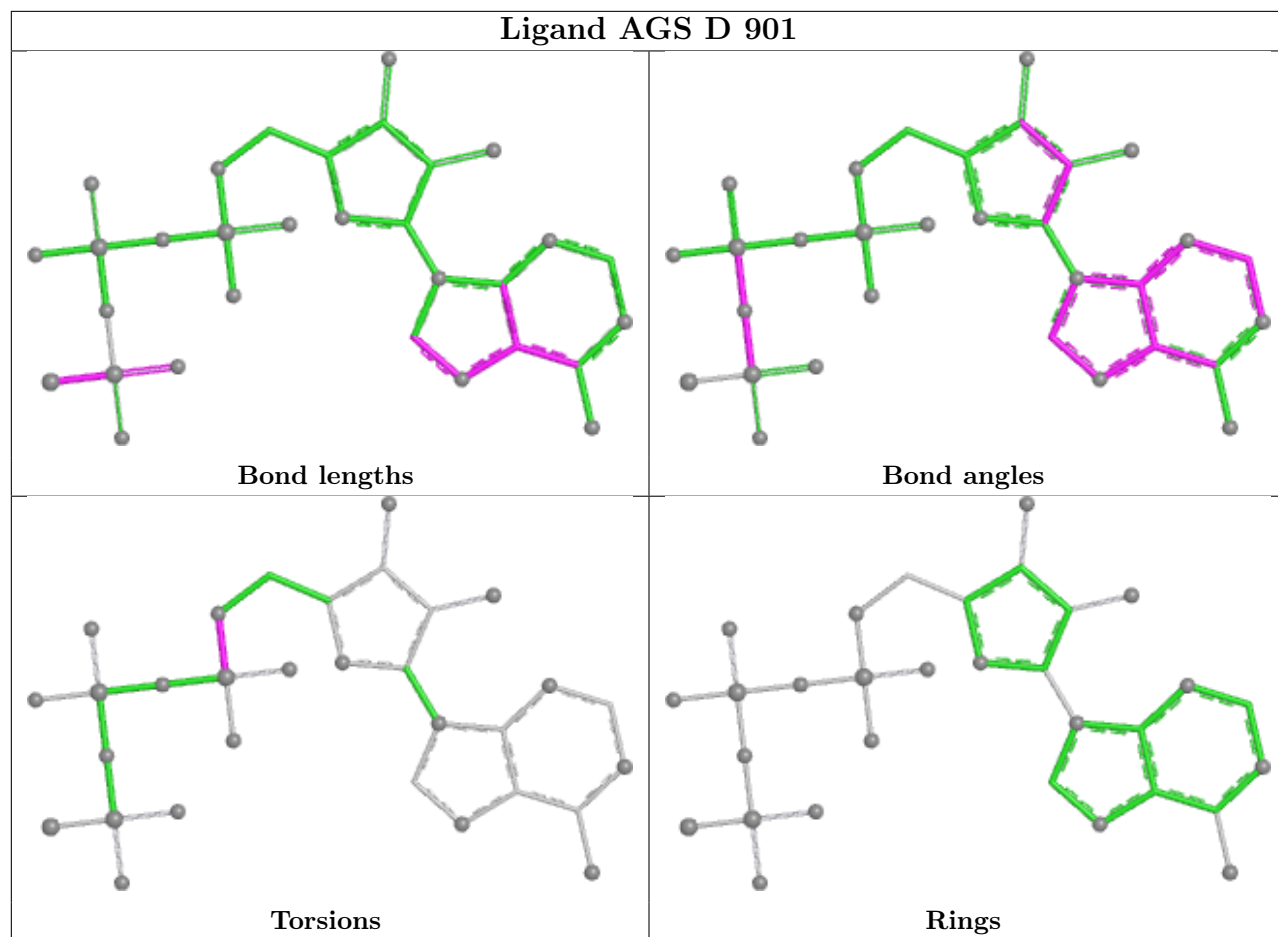


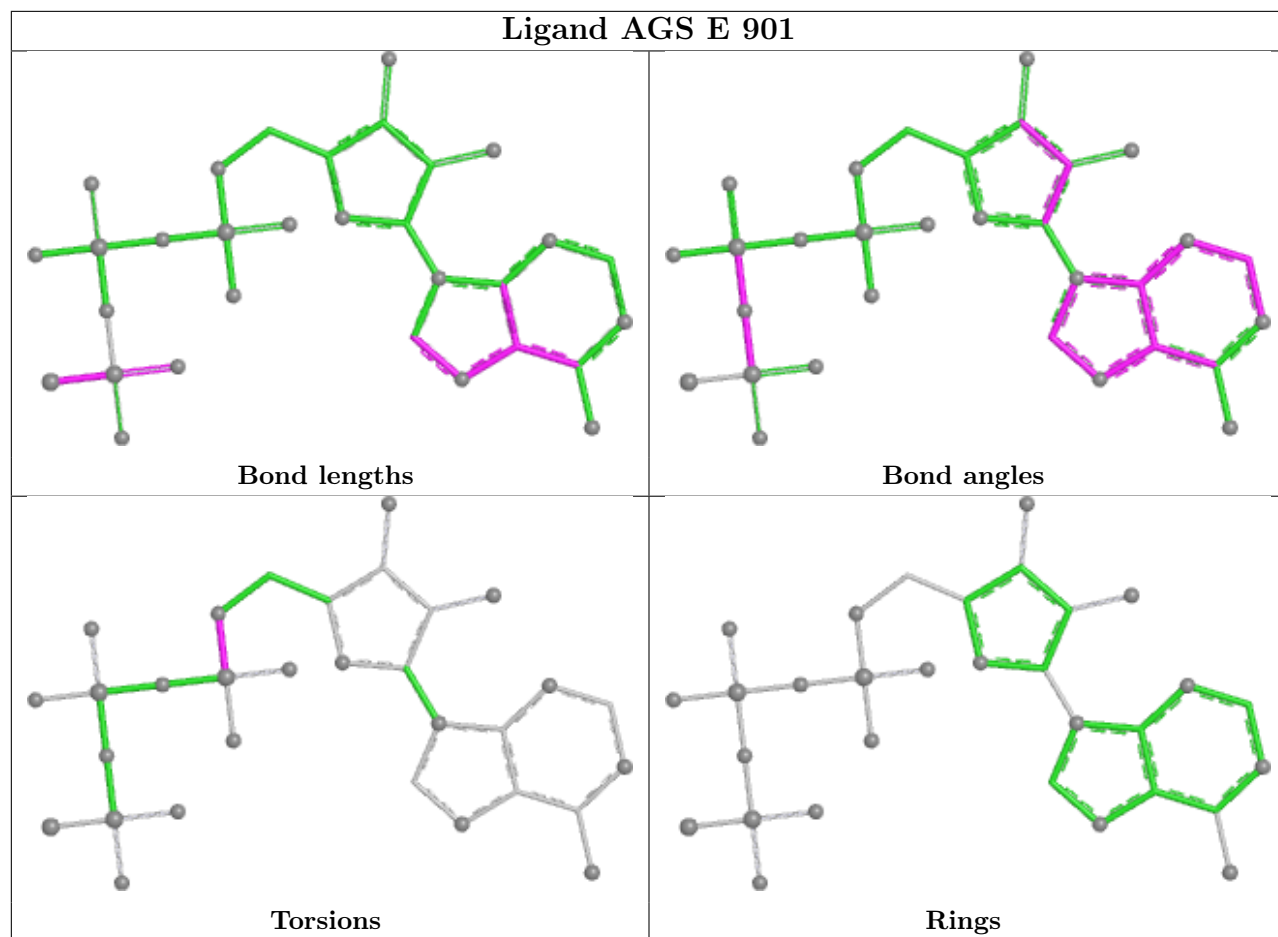


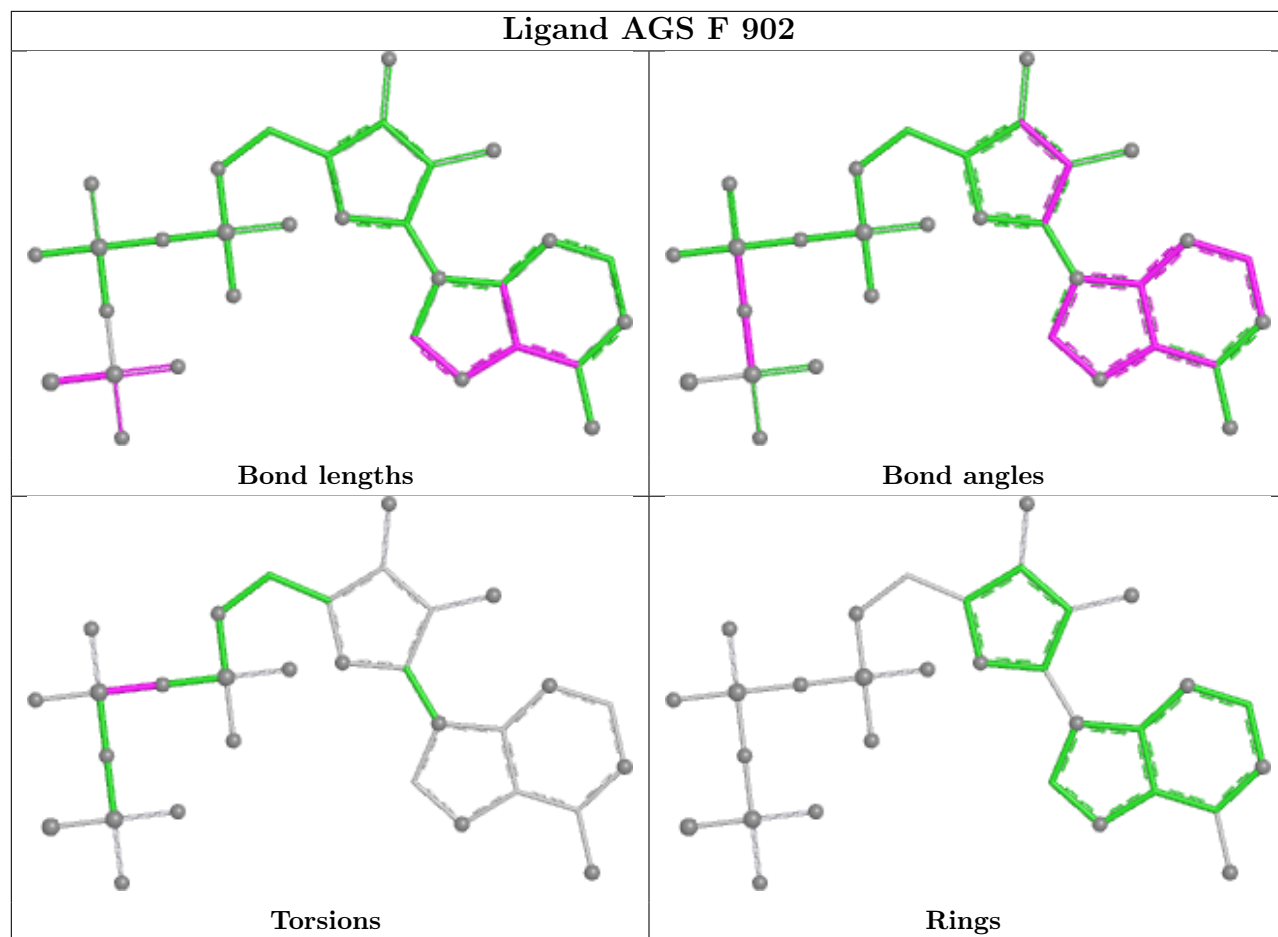


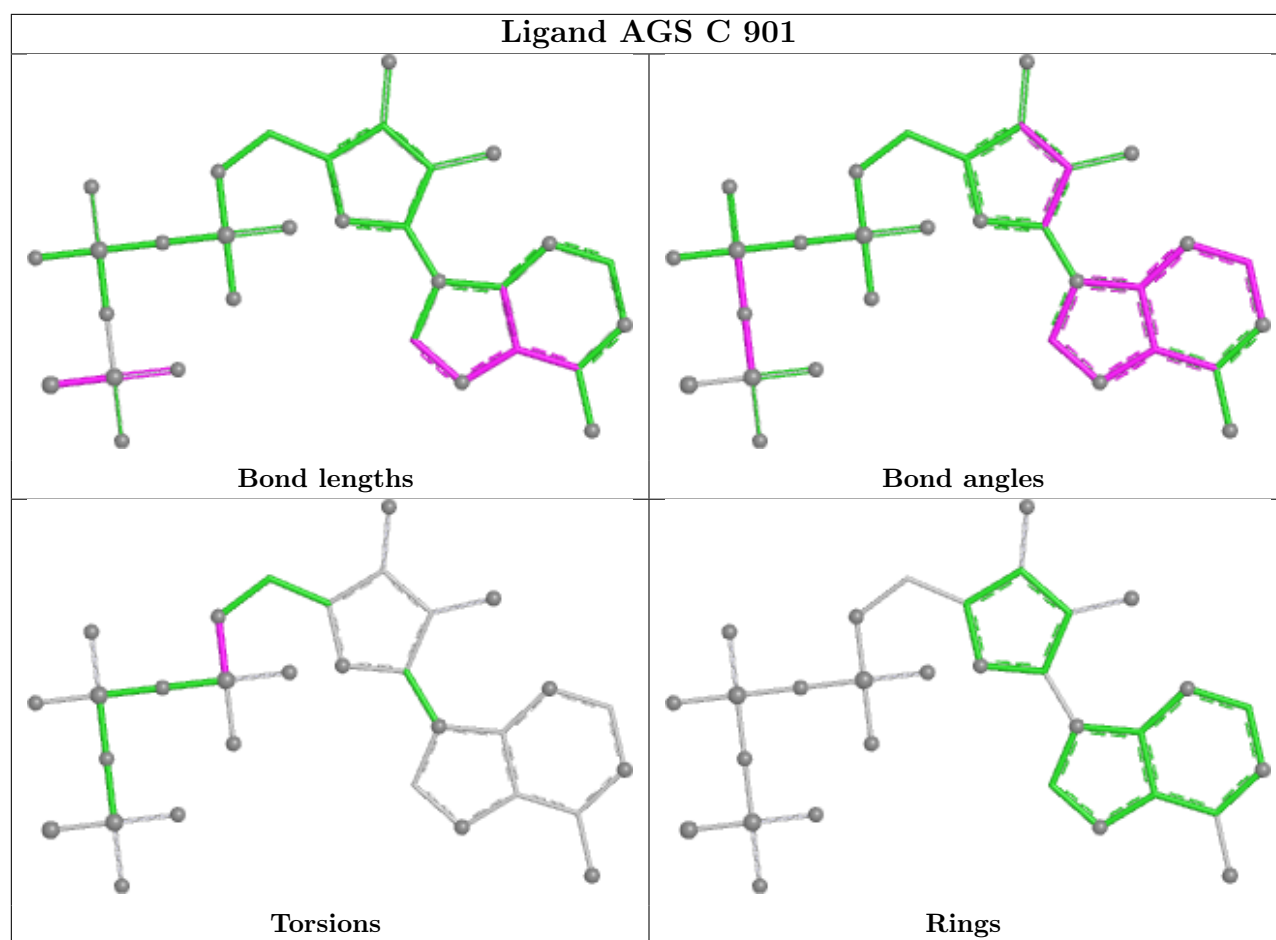












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

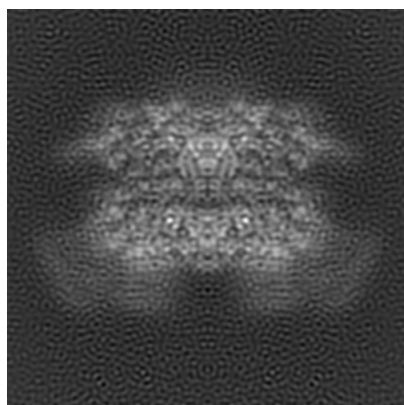
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3299. These allow visual inspection of the internal detail of the map and identification of artifacts.

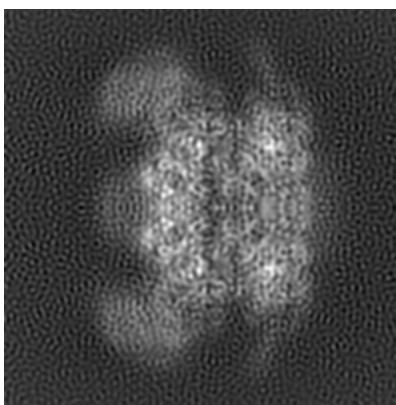
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

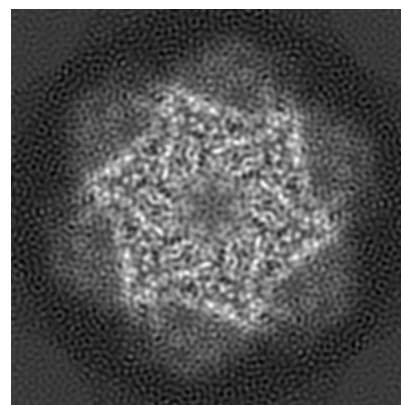
6.1.1 Primary map



X



Y

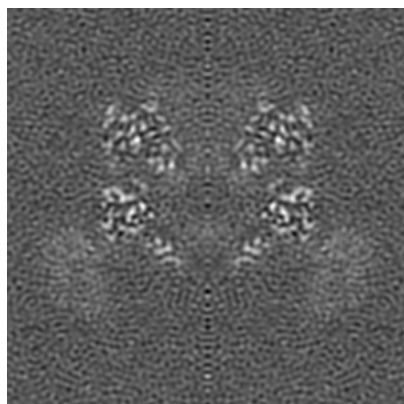


Z

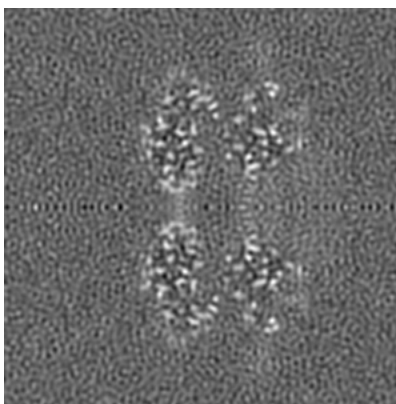
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

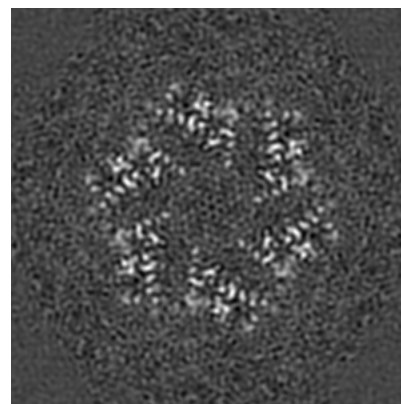
6.2.1 Primary map



X Index: 138



Y Index: 138

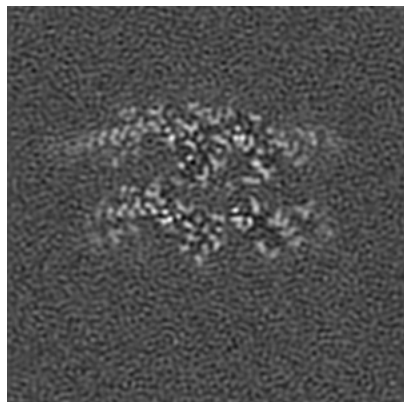


Z Index: 138

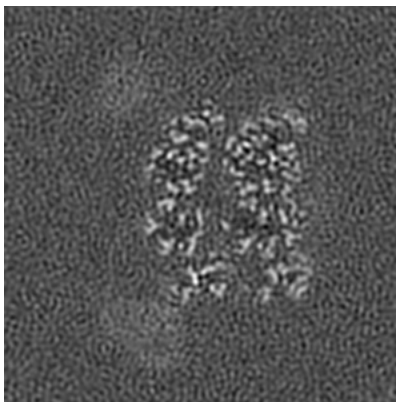
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

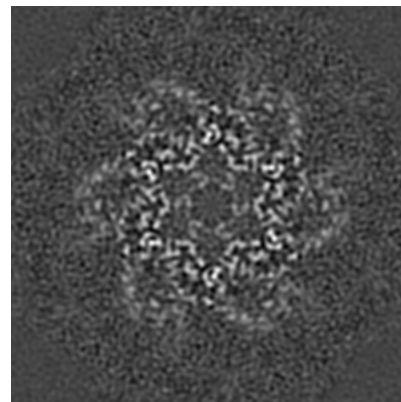
6.3.1 Primary map



X Index: 96



Y Index: 104

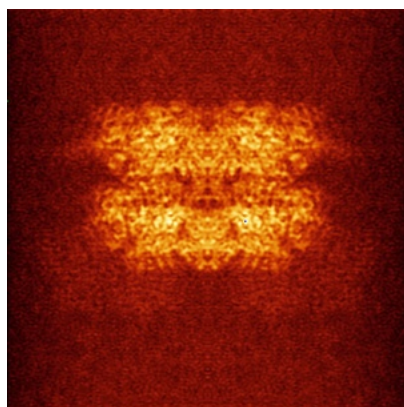


Z Index: 129

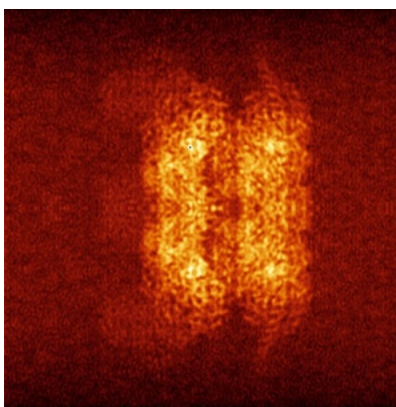
The images above show the largest variance slices of the map in three orthogonal directions.

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

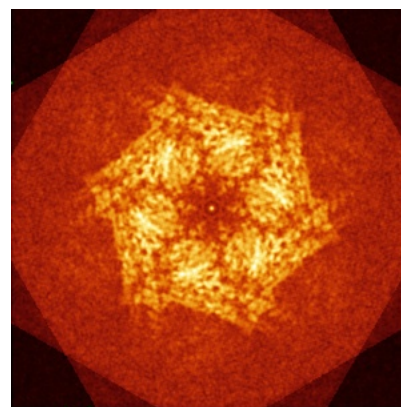
6.4.1 Primary map



X



Y

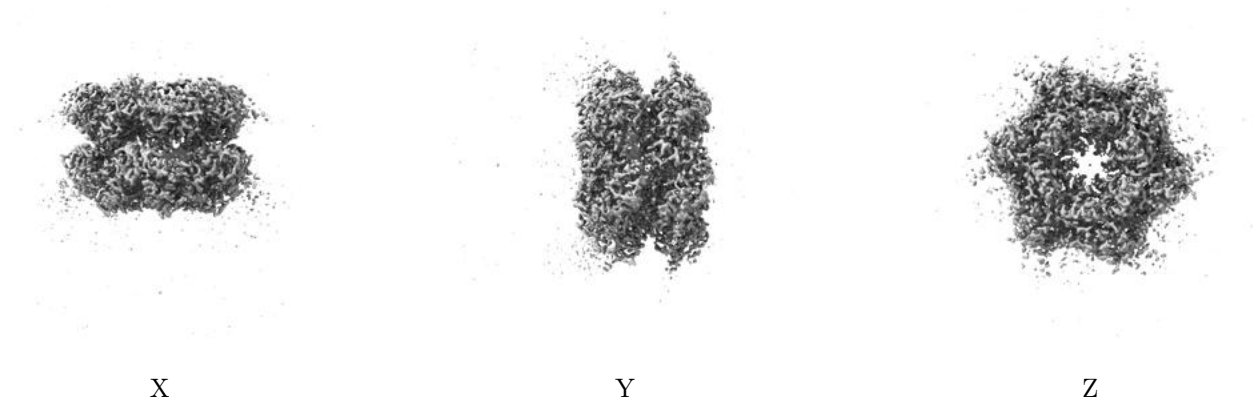


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0199. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

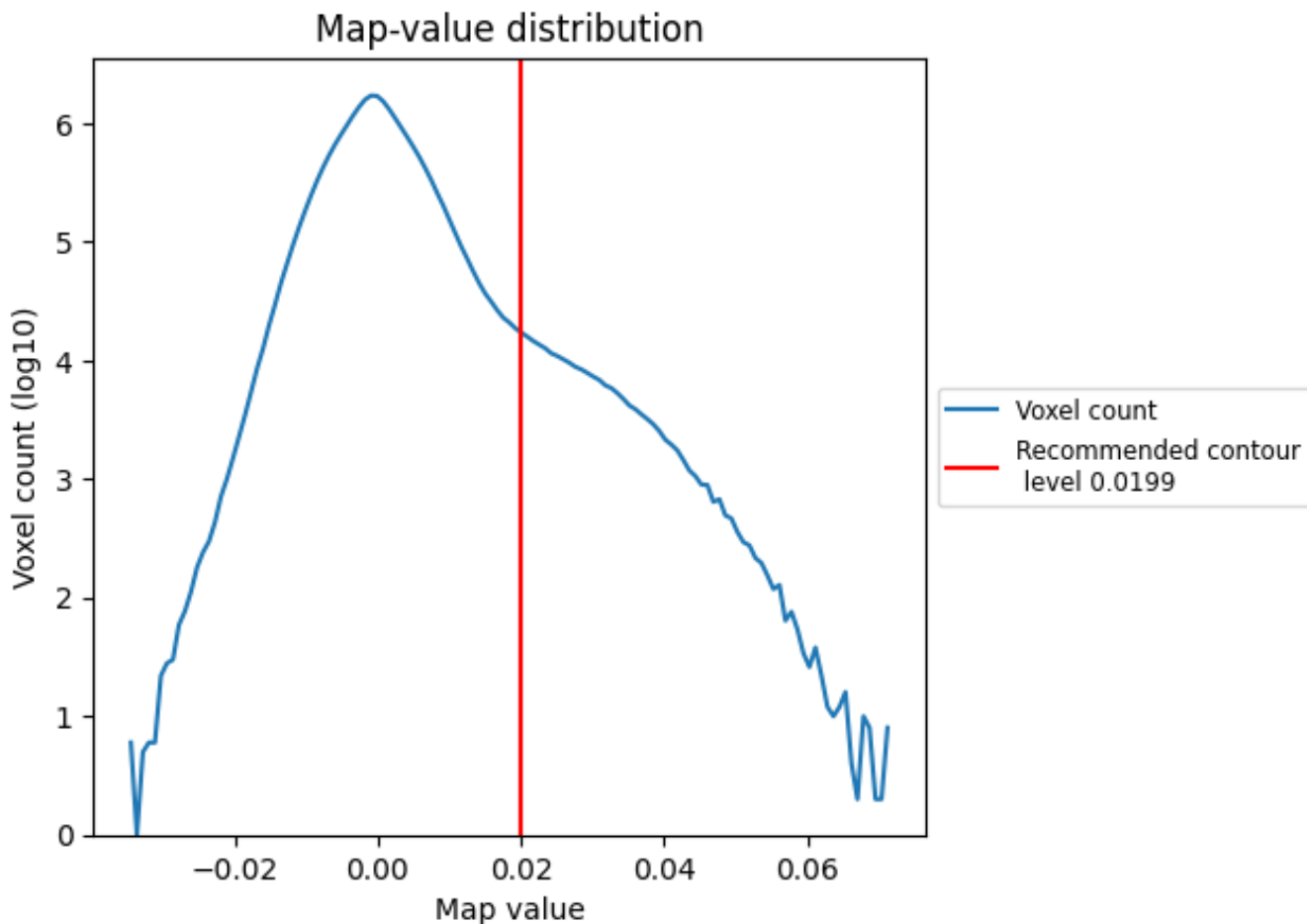
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

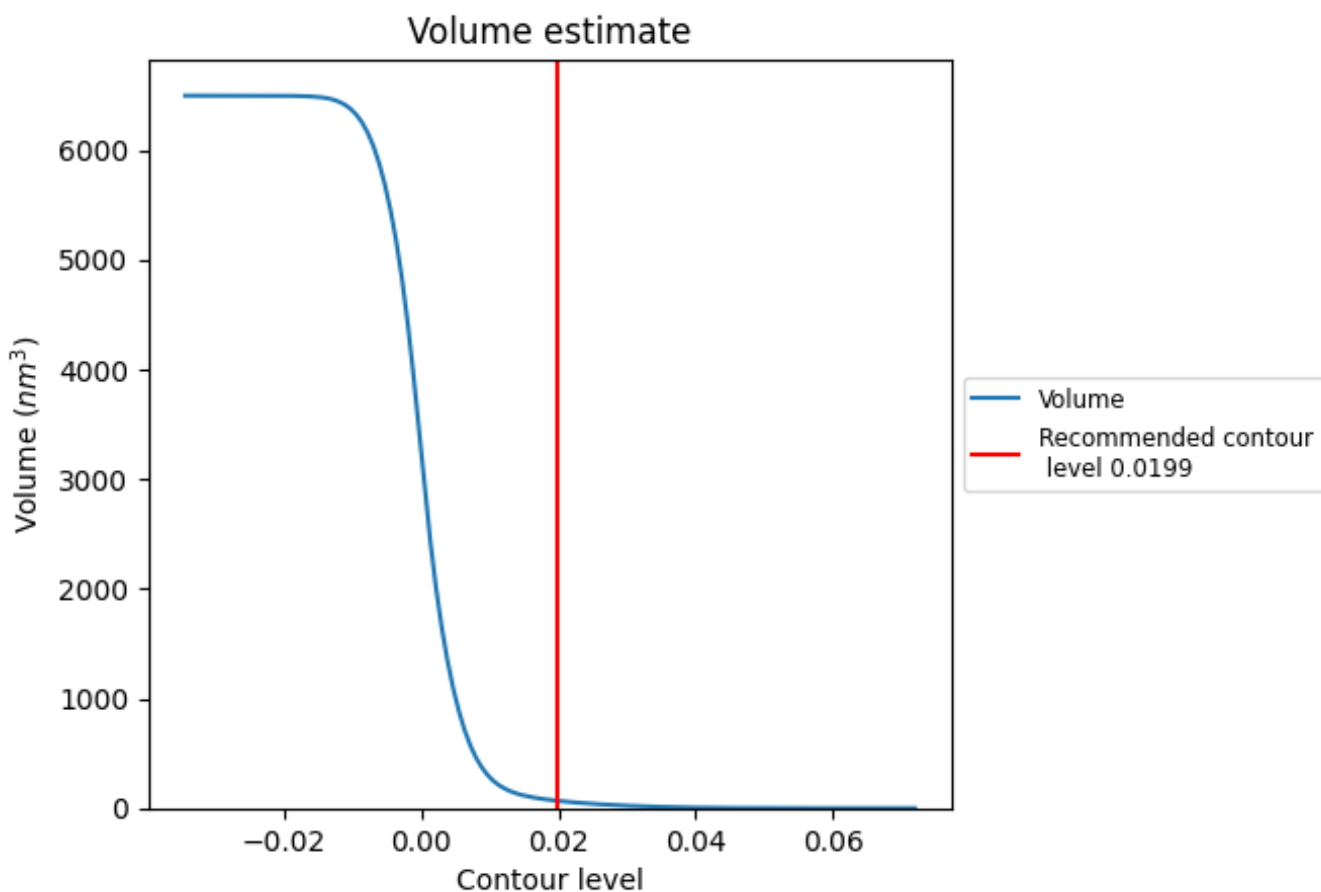
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

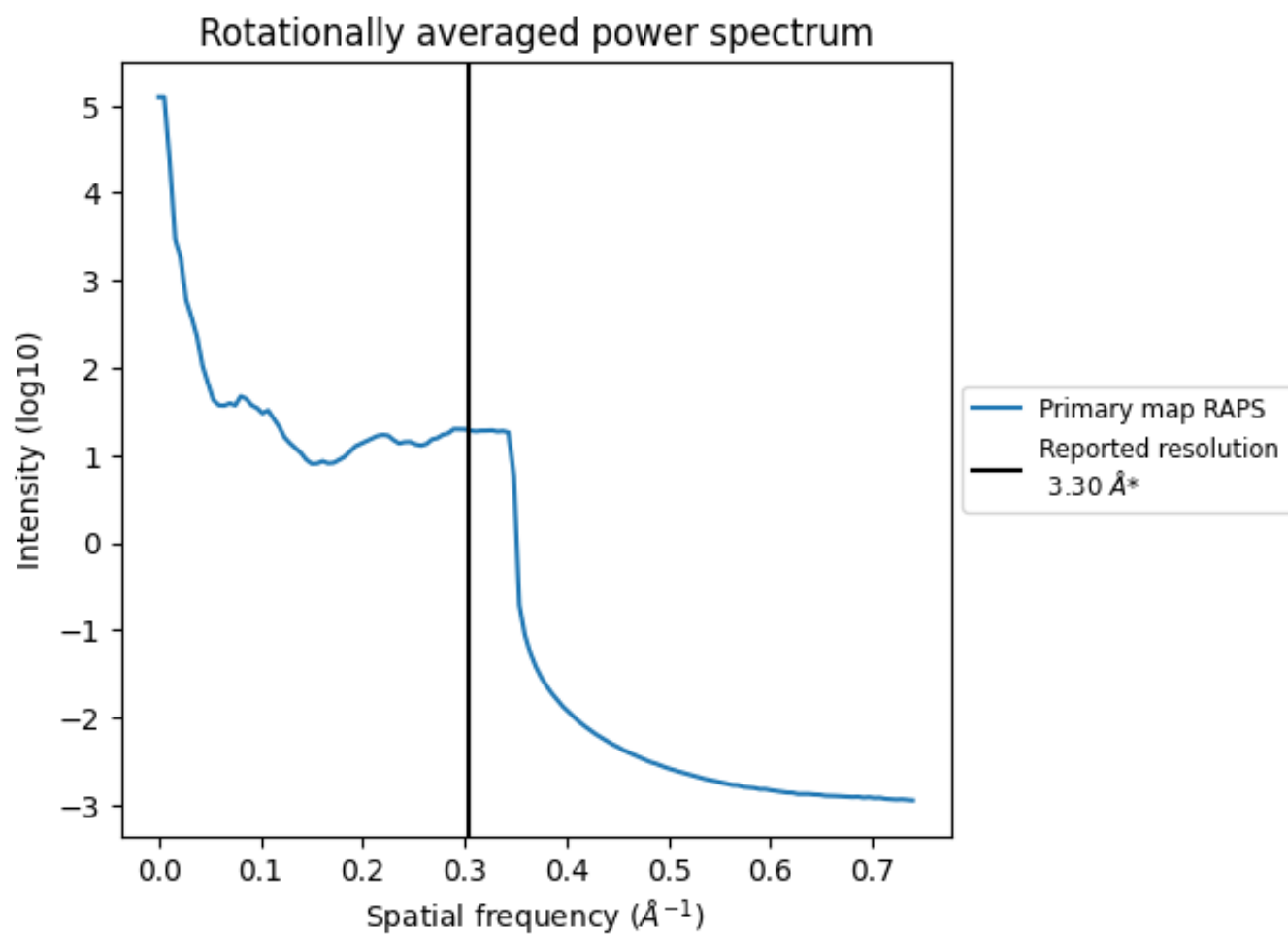
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 67 nm^3 ; this corresponds to an approximate mass of 60 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 i



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

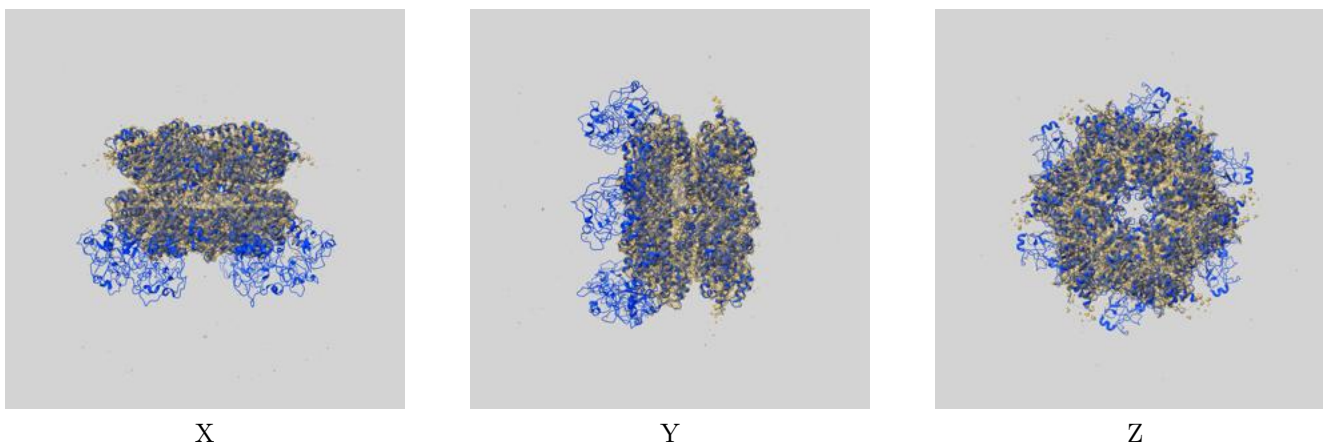
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

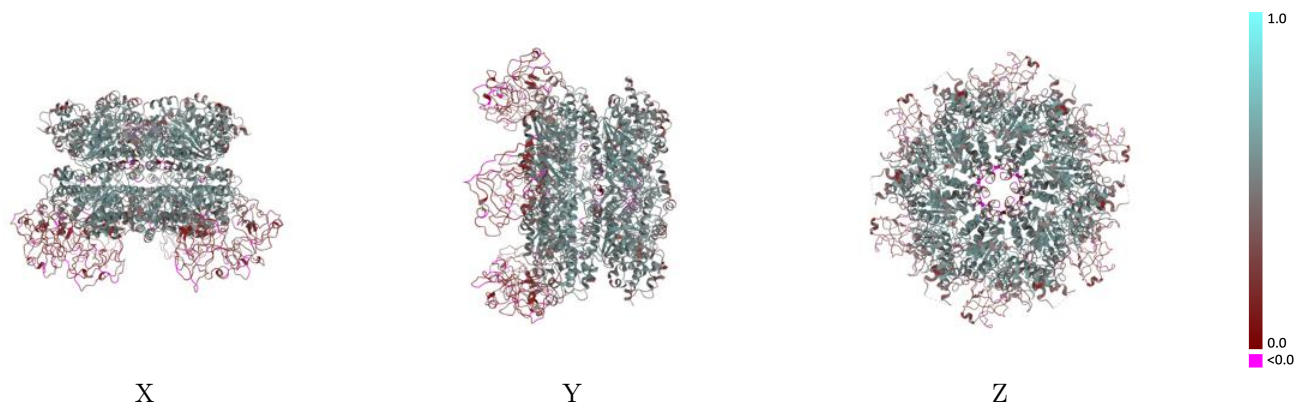
This section contains information regarding the fit between EMDB map EMD-3299 and PDB model 5FTN. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



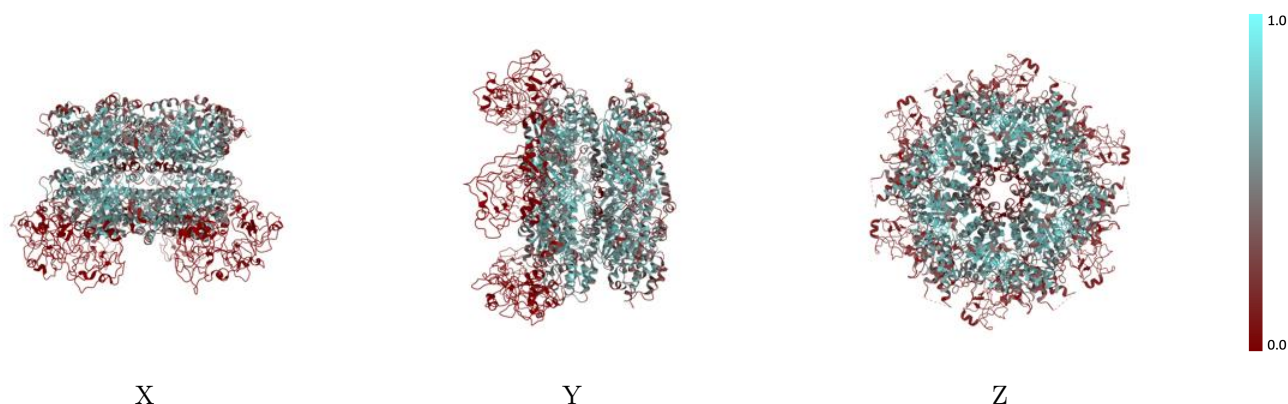
The images above show the 3D surface view of the map at the recommended contour level 0.0199 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



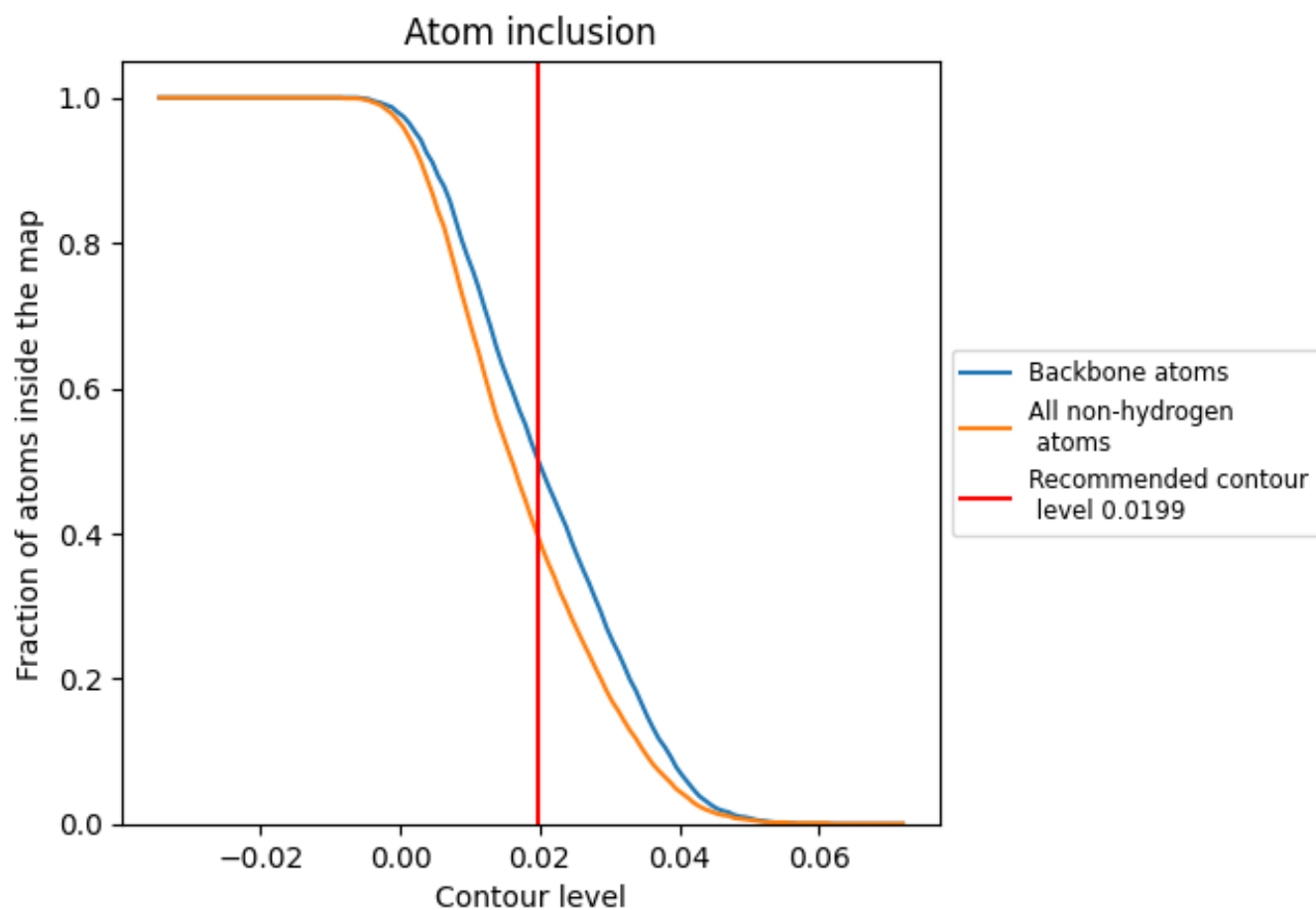
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0199).















9.4 Atom inclusion [i](#)



At the recommended contour level, 50% of all backbone atoms, 39% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.0199) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3920	 0.4300
A	 0.3910	 0.4300
B	 0.3930	 0.4300
C	 0.3910	 0.4300
D	 0.3900	 0.4290
E	 0.3920	 0.4300
F	 0.3920	 0.4300

