



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 02:27 PM UTC

PDB ID : 8PEY / pdb_00008pey
EMDB ID : EMD-17641
Title : Rho P167L-ATPgS-Psu complex II locked
Authors : Gjorgjevikj, D.; Wahl, M.C.; Hilal, T.; Loll, B.
Deposited on : 2023-06-15
Resolution : 3.00 Å (reported)
Based on initial models : 1PV4, 3RX6

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 EMD 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

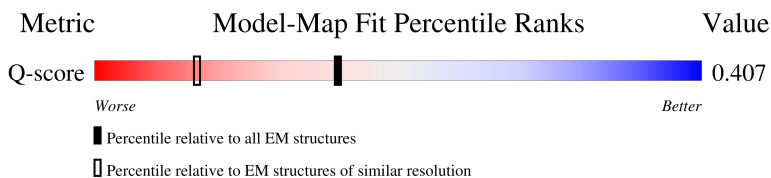
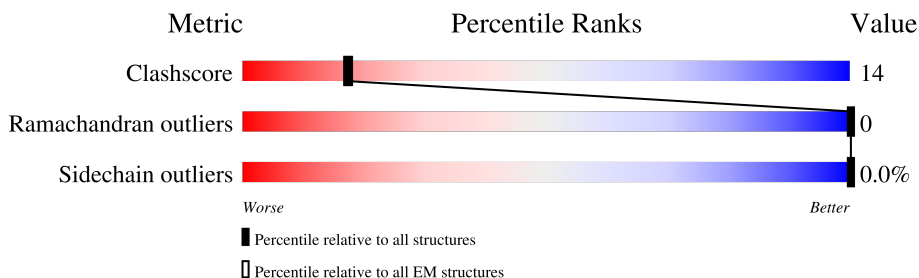
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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.



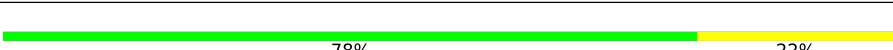
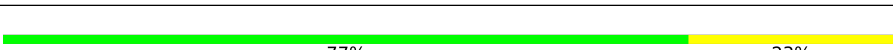
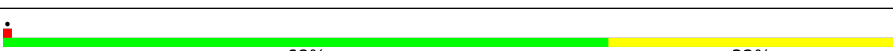
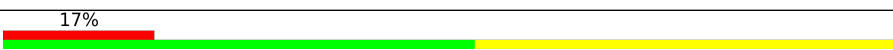
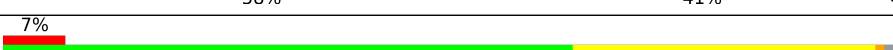
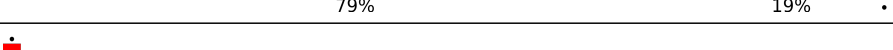
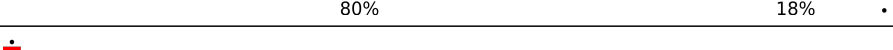
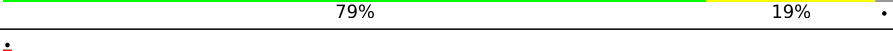
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	419	11% 33% 24% 43%
1	B	419	8% 66% 34%
1	C	419	72% 28%
1	D	419	72% 28%

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Mol	Chain	Length	Quality of chain
1	E	419	
1	F	419	
1	G	419	
1	I	419	
1	J	419	
1	K	419	
1	L	419	
1	M	419	
1	N	419	
2	a	190	
2	b	190	
2	c	190	
2	d	190	
2	e	190	
2	f	190	
2	g	190	
2	h	190	
2	i	190	
2	j	190	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 55957 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 Transcription termination factor Rho.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	240	Total	C	N	O	S	0	0
			1875	1185	332	348	10		
1	B	419	Total	C	N	O	S	0	0
			3299	2075	586	621	17		
1	C	419	Total	C	N	O	S	0	0
			3299	2075	586	621	17		
1	D	419	Total	C	N	O	S	0	0
			3299	2075	586	621	17		
1	E	419	Total	C	N	O	S	0	0
			3299	2075	586	621	17		
1	F	419	Total	C	N	O	S	0	0
			3299	2075	586	621	17		
1	G	374	Total	C	N	O	S	0	0
			2944	1852	523	555	14		
1	I	380	Total	C	N	O	S	0	0
			2984	1886	526	559	13		
1	J	419	Total	C	N	O	S	0	0
			3299	2075	586	621	17		
1	K	419	Total	C	N	O	S	0	0
			3299	2075	586	621	17		
1	L	419	Total	C	N	O	S	0	0
			3299	2075	586	621	17		
1	M	419	Total	C	N	O	S	0	0
			3299	2075	586	621	17		
1	N	419	Total	C	N	O	S	0	0
			3299	2075	586	621	17		

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	167	LEU	PRO	engineered mutation	UNP P0AG30
B	167	LEU	PRO	engineered mutation	UNP P0AG30
C	167	LEU	PRO	engineered mutation	UNP P0AG30
D	167	LEU	PRO	engineered mutation	UNP P0AG30

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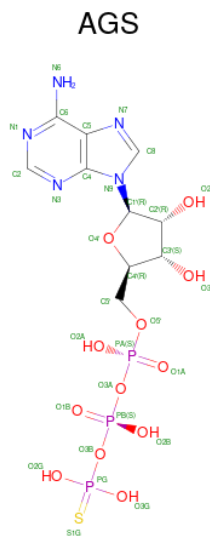
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Chain	Residue	Modelled	Actual	Comment	Reference
E	167	LEU	PRO	engineered mutation	UNP P0AG30
F	167	LEU	PRO	engineered mutation	UNP P0AG30
G	167	LEU	PRO	engineered mutation	UNP P0AG30
I	167	LEU	PRO	engineered mutation	UNP P0AG30
J	167	LEU	PRO	engineered mutation	UNP P0AG30
K	167	LEU	PRO	engineered mutation	UNP P0AG30
L	167	LEU	PRO	engineered mutation	UNP P0AG30
M	167	LEU	PRO	engineered mutation	UNP P0AG30
N	167	LEU	PRO	engineered mutation	UNP P0AG30

- Molecule 2 is a protein called Polarity suppression protein.

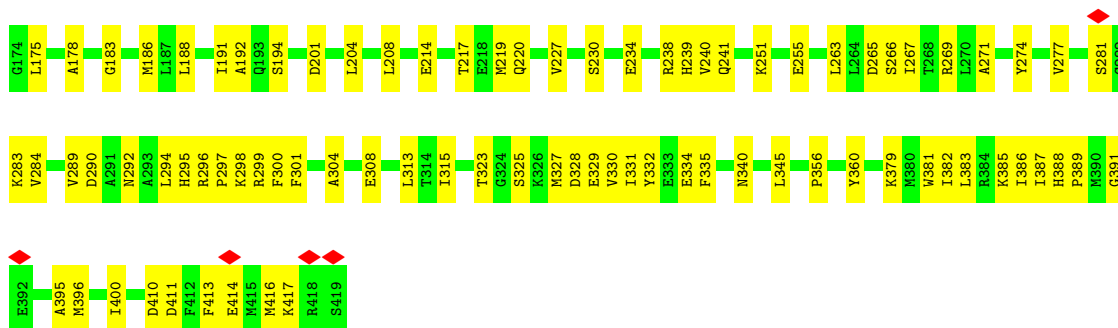
Mol	Chain	Residues	Atoms					AltConf	Trace
2	a	187	Total	C	N	O	S	0	0
			1478	911	279	283	5		
2	b	187	Total	C	N	O	S	0	0
			1478	911	279	283	5		
2	c	187	Total	C	N	O	S	0	0
			1478	911	279	283	5		
2	d	187	Total	C	N	O	S	0	0
			1478	911	279	283	5		
2	e	187	Total	C	N	O	S	0	0
			1478	911	279	283	5		
2	f	187	Total	C	N	O	S	0	0
			1478	911	279	283	5		
2	g	187	Total	C	N	O	S	0	0
			1478	911	279	283	5		
2	h	187	Total	C	N	O	S	0	0
			1478	911	279	283	5		
2	i	187	Total	C	N	O	S	0	0
			1478	911	279	283	5		
2	j	187	Total	C	N	O	S	0	0
			1478	911	279	283	5		

- Molecule 3 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).

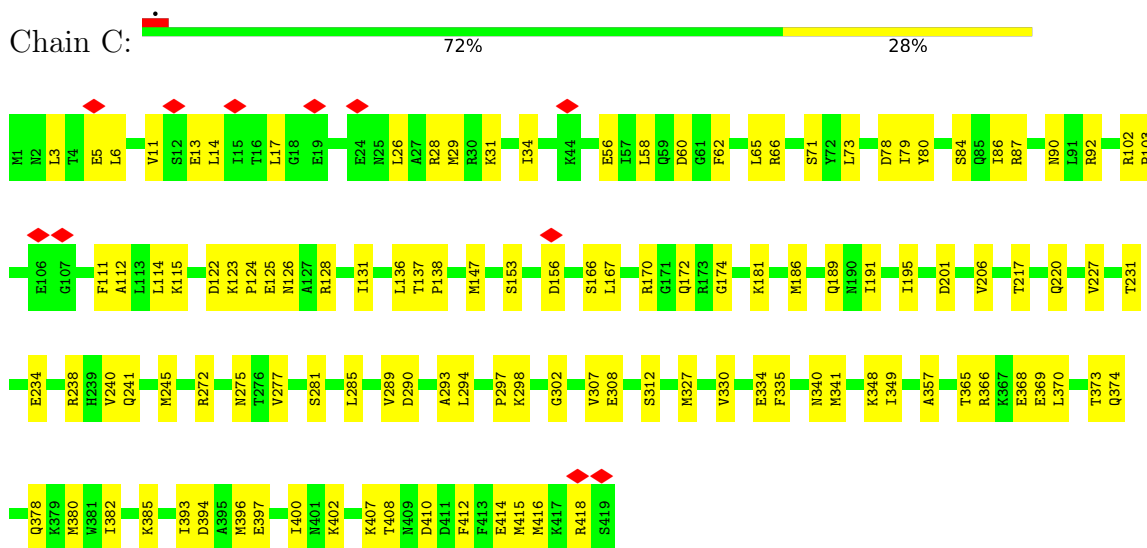


- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

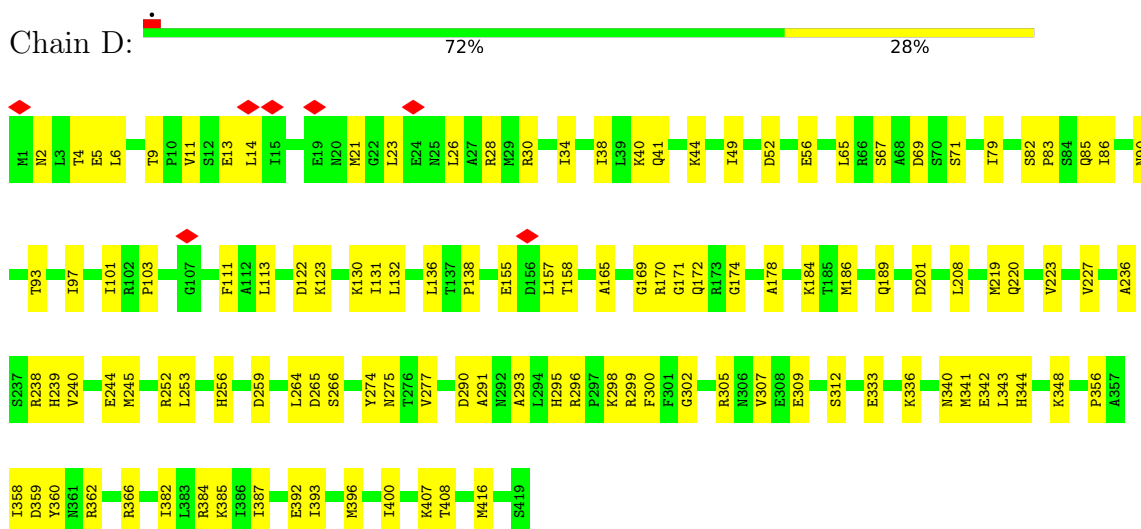
Mol	Chain	Residues	Atoms		AltConf
4	B	1	Total 1	Mg 1	0
4	C	1	Total 1	Mg 1	0
4	D	1	Total 1	Mg 1	0
4	E	1	Total 1	Mg 1	0
4	F	1	Total 1	Mg 1	0
4	G	1	Total 1	Mg 1	0
4	I	1	Total 1	Mg 1	0
4	J	1	Total 1	Mg 1	0
4	K	1	Total 1	Mg 1	0
4	L	1	Total 1	Mg 1	0
4	M	1	Total 1	Mg 1	0
4	N	1	Total 1	Mg 1	0



• Molecule 1: Transcription termination factor Rho

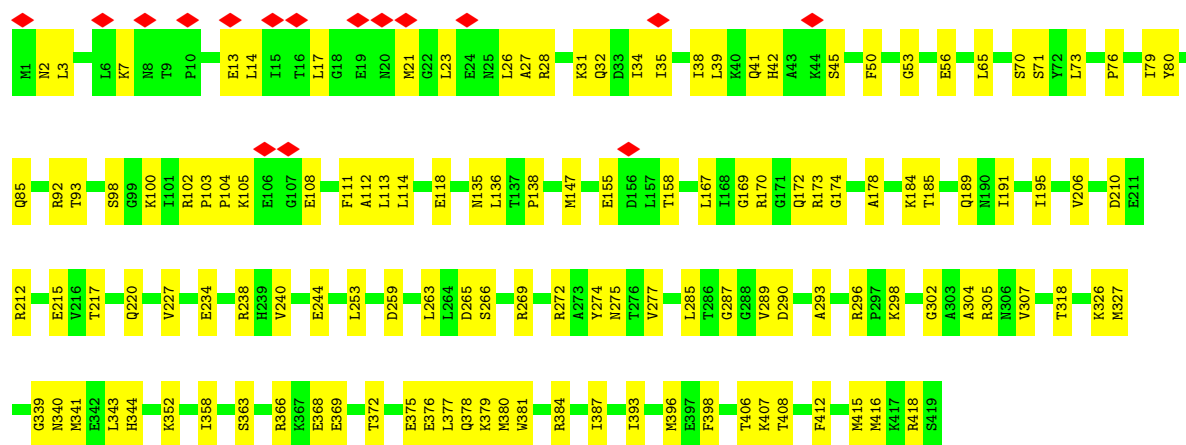


• Molecule 1: Transcription termination factor Rho

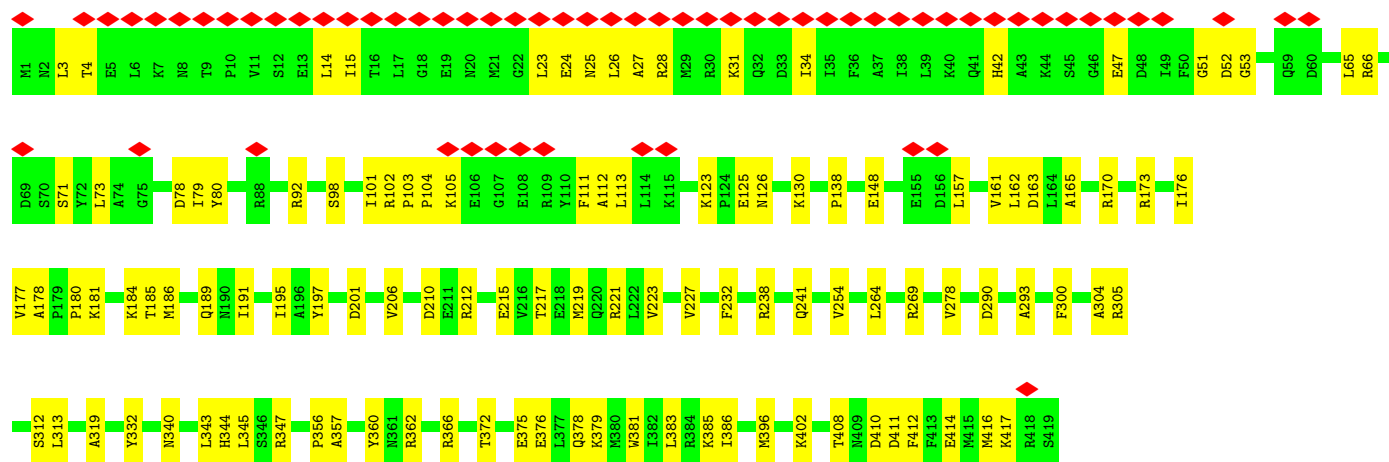
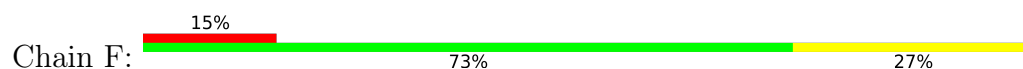


• Molecule 1: Transcription termination factor Rho

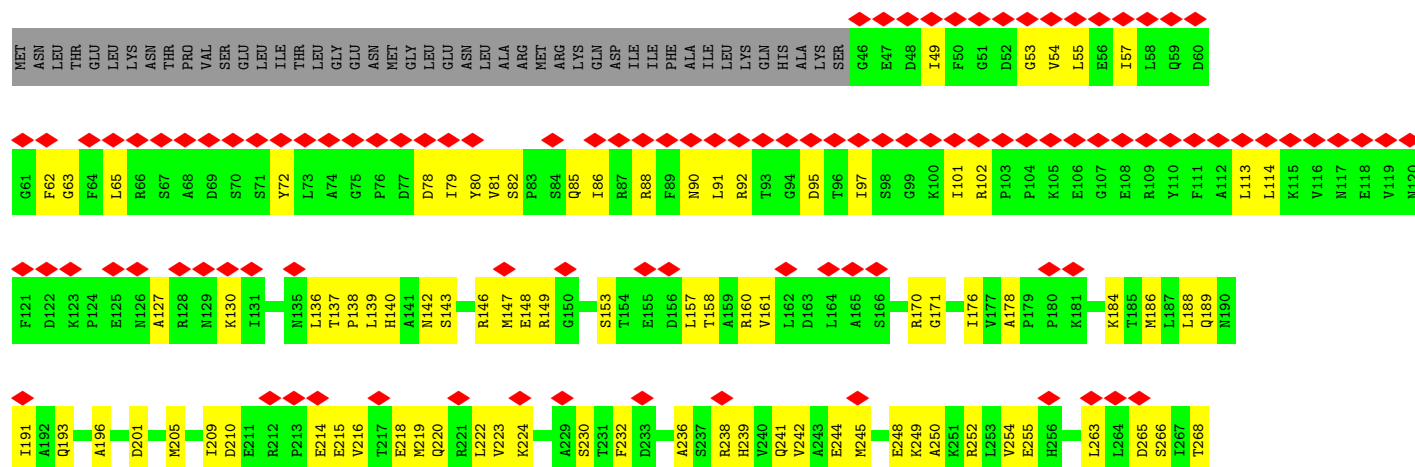


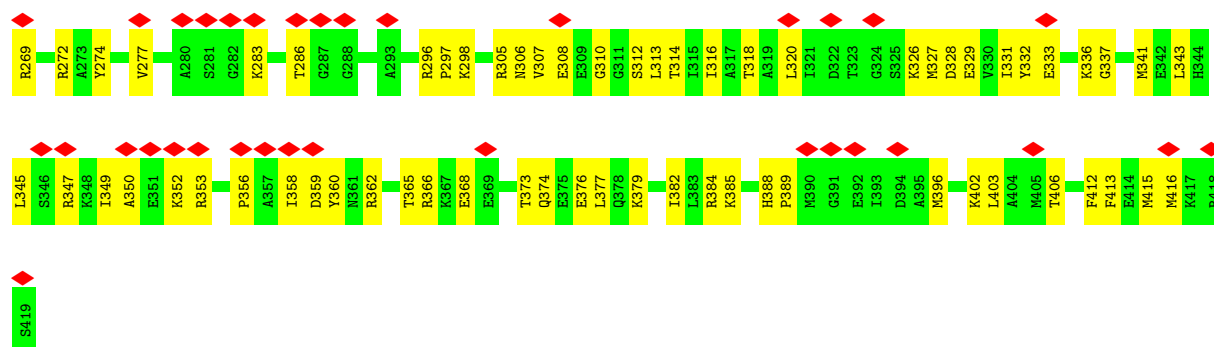


• Molecule 1: Transcription termination factor Rho

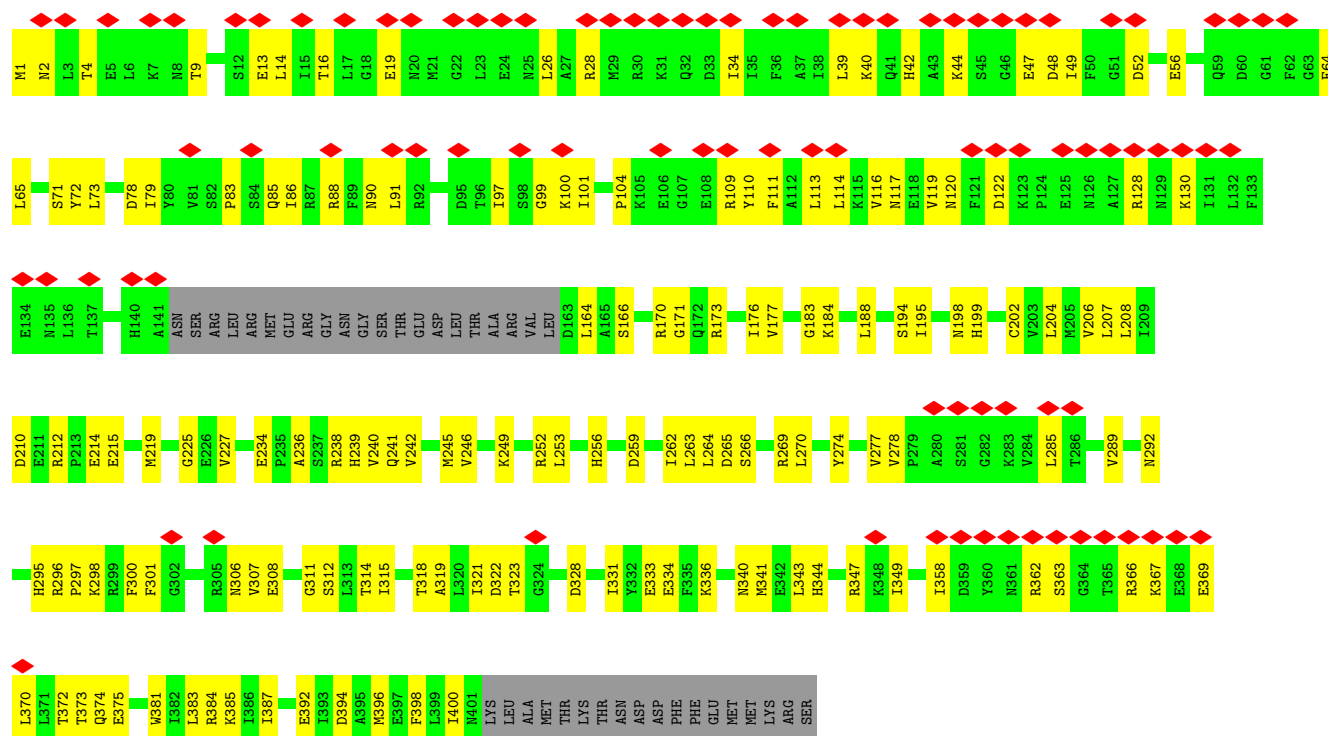


• Molecule 1: Transcription termination factor Rho

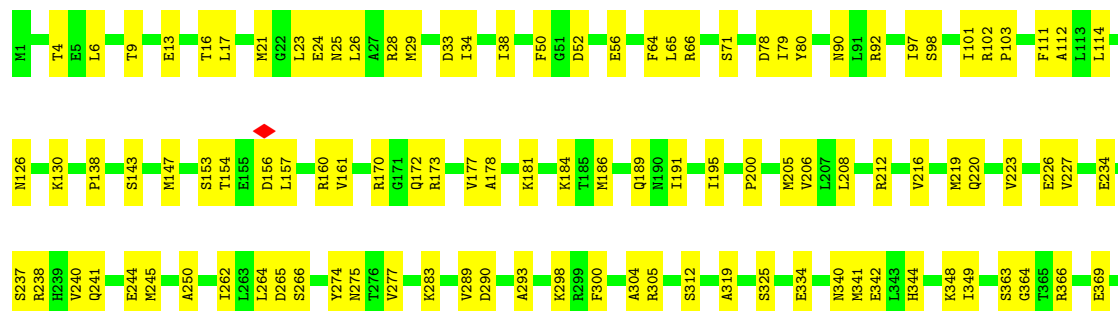


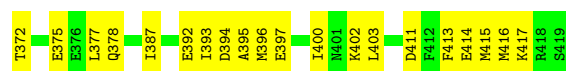


• Molecule 1: Transcription termination factor Rho

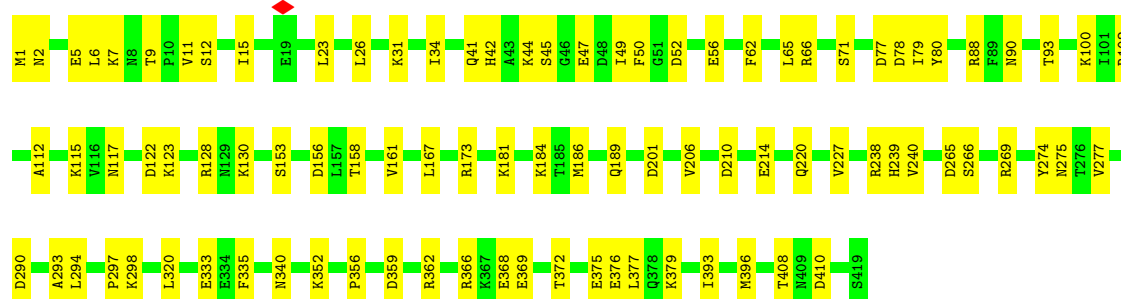
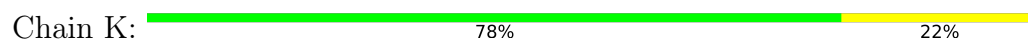


• Molecule 1: Transcription termination factor Rho

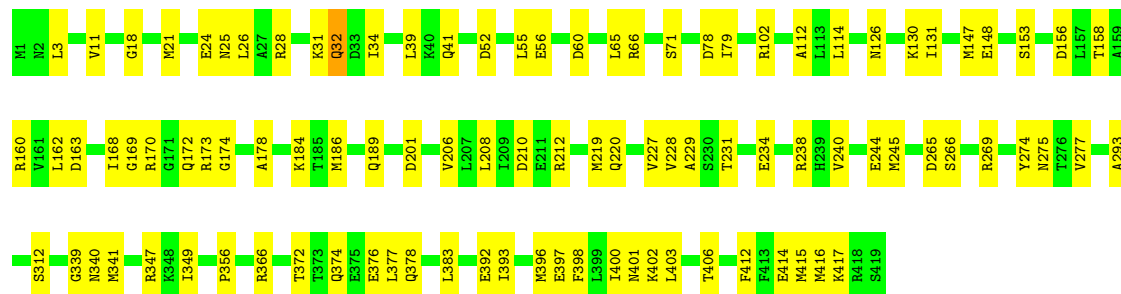




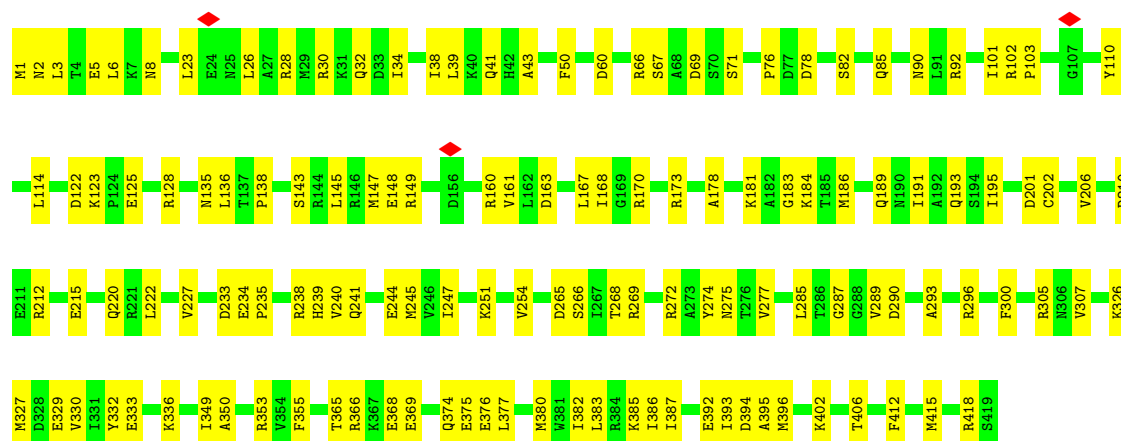
• Molecule 1: Transcription termination factor Rho



• Molecule 1: Transcription termination factor Rho



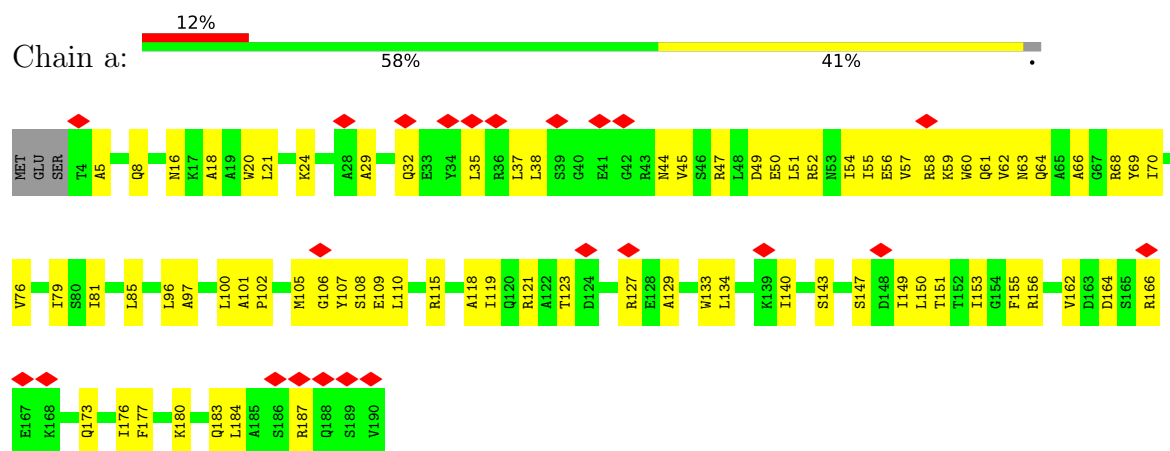
• Molecule 1: Transcription termination factor Rho



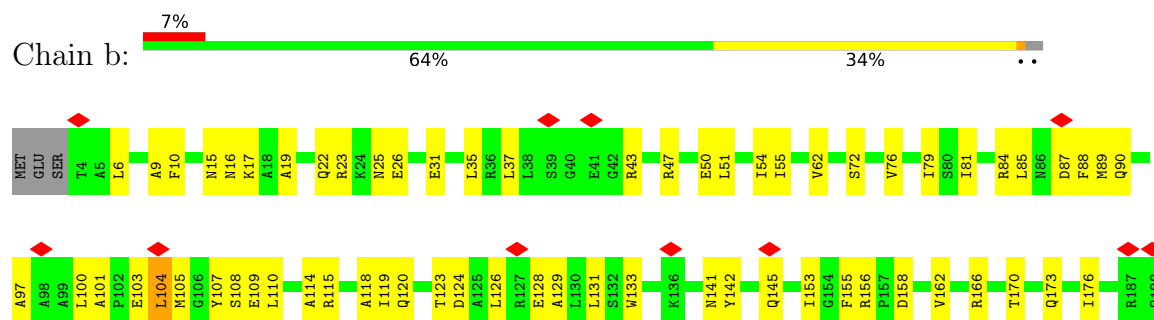
• Molecule 1: Transcription termination factor Rho



• Molecule 2: Polarity suppression protein

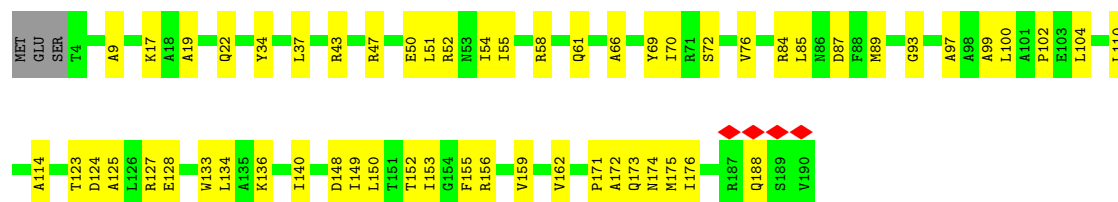


• Molecule 2: Polarity suppression protein

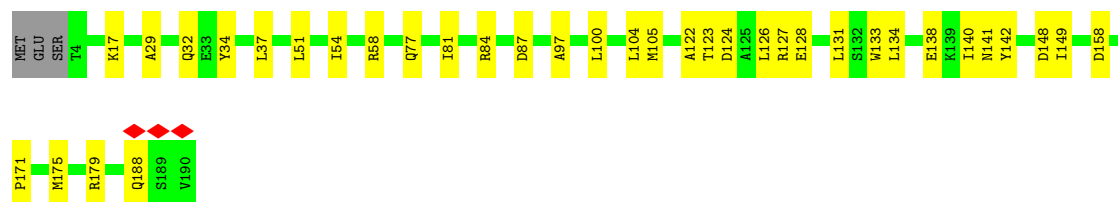
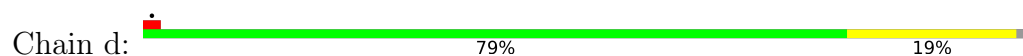




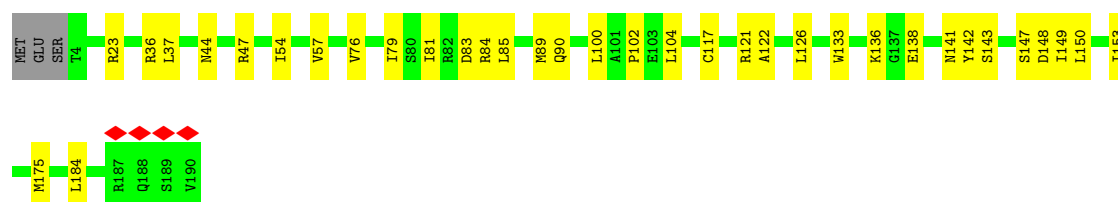
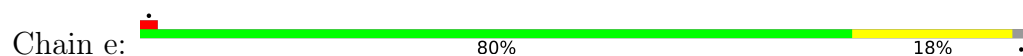
- Molecule 2: Polarity suppression protein



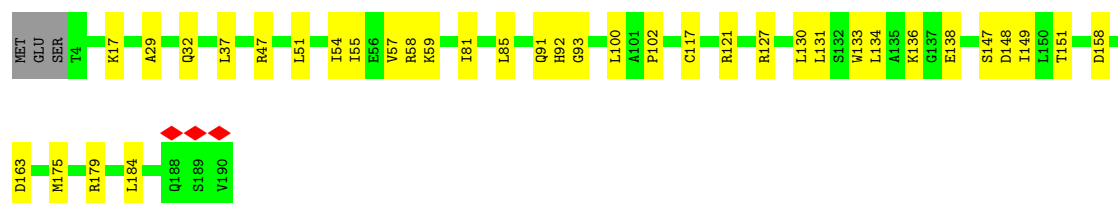
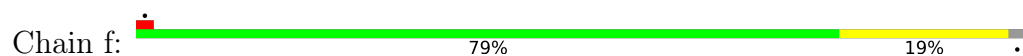
- Molecule 2: Polarity suppression protein



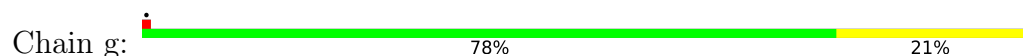
- Molecule 2: Polarity suppression protein



- Molecule 2: Polarity suppression protein

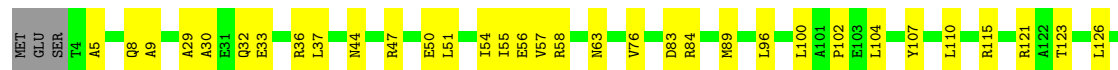


- Molecule 2: Polarity suppression protein

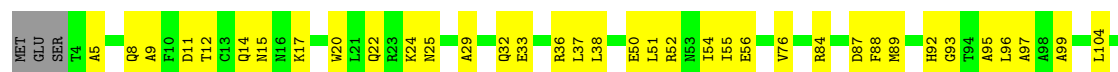




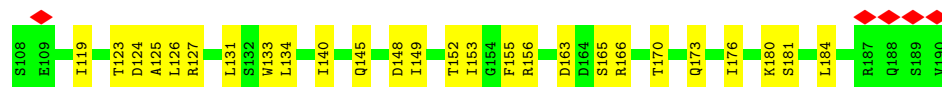
- Molecule 2: Polarity suppression protein



- Molecule 2: Polarity suppression protein



- Molecule 2: Polarity suppression protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	317635	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	2.245	Depositor
Minimum map value	-0.000	Depositor
Average map value	0.010	Depositor
Map value standard deviation	0.059	Depositor
Recommended contour level	0.25	Depositor
Map size ($\text{\AA}$)	372.73602, 372.73602, 372.73602	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.8320001, 0.8320001, 0.8320001	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: AGS, MG

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	0.15	0/1901	0.44	0/2563
1	B	0.14	0/3347	0.39	0/4504
1	C	0.12	0/3347	0.33	0/4504
1	D	0.12	0/3347	0.32	0/4504
1	E	0.10	0/3347	0.28	0/4504
1	F	0.10	0/3347	0.32	0/4504
1	G	0.13	0/2989	0.42	0/4024
1	I	0.13	0/3029	0.38	0/4082
1	J	0.11	0/3347	0.34	0/4504
1	K	0.10	0/3347	0.31	0/4504
1	L	0.11	0/3347	0.31	0/4504
1	M	0.13	0/3347	0.35	0/4504
1	N	0.13	0/3347	0.39	0/4504
2	a	0.13	0/1498	0.38	0/2020
2	b	0.14	0/1498	0.43	2/2020 (0.1%)
2	c	0.16	0/1498	0.42	0/2020
2	d	0.13	0/1498	0.33	0/2020
2	e	0.12	0/1498	0.29	0/2020
2	f	0.13	0/1498	0.31	0/2020
2	g	0.12	0/1498	0.32	0/2020
2	h	0.13	0/1498	0.31	0/2020
2	i	0.14	0/1498	0.35	0/2020
2	j	0.12	0/1498	0.32	0/2020
All	All	0.12	0/56369	0.35	2/75909 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	104	LEU	CA-C-N	-5.21	112.96	122.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	104	LEU	C-N-CA	-5.21	112.96	122.38

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	1875	0	1946	80	0
1	B	3299	0	3380	110	0
1	C	3299	0	3380	92	0
1	D	3299	0	3380	82	0
1	E	3299	0	3380	88	0
1	F	3299	0	3380	89	0
1	G	2944	0	2999	114	0
1	I	2984	0	3061	128	0
1	J	3299	0	3380	93	0
1	K	3299	0	3380	64	0
1	L	3299	0	3380	69	0
1	M	3299	0	3380	103	0
1	N	3299	0	3380	150	0
2	a	1478	0	1468	58	0
2	b	1478	0	1468	49	0
2	c	1478	0	1468	45	0
2	d	1478	0	1468	35	0
2	e	1478	0	1468	31	0
2	f	1478	0	1468	28	0
2	g	1478	0	1468	32	0
2	h	1478	0	1468	40	0
2	i	1478	0	1468	62	0
2	j	1478	0	1468	48	0
3	B	31	0	12	2	0
3	C	31	0	12	0	0
3	D	31	0	12	3	0
3	E	31	0	12	2	0
3	F	31	0	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	31	0	12	2	0
3	I	31	0	12	3	0
3	J	31	0	12	2	0
3	K	31	0	12	1	0
3	L	31	0	12	2	0
3	M	31	0	12	2	0
3	N	31	0	12	2	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
4	M	1	0	0	0	0
4	N	1	0	0	0	0
All	All	55957	0	56630	1538	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 14.

The worst 5 of 1538 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:F:65:LEU:HB3	1:F:79:ILE:HB	1.55	0.89
1:G:347:ARG:O	1:G:347:ARG:NH1	2.05	0.88
1:N:85:GLN:HA	1:N:88:ARG:HG3	1.58	0.84
1:G:65:LEU:O	1:G:78:ASP:HA	1.76	0.84
1:C:298:LYS:NZ	1:C:334:GLU:OE2	2.11	0.84

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	238/419 (57%)	225 (94%)	13 (6%)	0	100	100
1	B	417/419 (100%)	403 (97%)	14 (3%)	0	100	100
1	C	417/419 (100%)	410 (98%)	7 (2%)	0	100	100
1	D	417/419 (100%)	413 (99%)	4 (1%)	0	100	100
1	E	417/419 (100%)	407 (98%)	10 (2%)	0	100	100
1	F	417/419 (100%)	407 (98%)	10 (2%)	0	100	100
1	G	372/419 (89%)	362 (97%)	10 (3%)	0	100	100
1	I	376/419 (90%)	359 (96%)	17 (4%)	0	100	100
1	J	417/419 (100%)	410 (98%)	7 (2%)	0	100	100
1	K	417/419 (100%)	407 (98%)	10 (2%)	0	100	100
1	L	417/419 (100%)	407 (98%)	10 (2%)	0	100	100
1	M	417/419 (100%)	409 (98%)	8 (2%)	0	100	100
1	N	417/419 (100%)	402 (96%)	15 (4%)	0	100	100
2	a	185/190 (97%)	179 (97%)	6 (3%)	0	100	100
2	b	185/190 (97%)	182 (98%)	3 (2%)	0	100	100
2	c	185/190 (97%)	183 (99%)	2 (1%)	0	100	100
2	d	185/190 (97%)	183 (99%)	2 (1%)	0	100	100
2	e	185/190 (97%)	184 (100%)	1 (0%)	0	100	100
2	f	185/190 (97%)	185 (100%)	0	0	100	100
2	g	185/190 (97%)	183 (99%)	2 (1%)	0	100	100
2	h	185/190 (97%)	184 (100%)	1 (0%)	0	100	100
2	i	185/190 (97%)	182 (98%)	3 (2%)	0	100	100
2	j	185/190 (97%)	183 (99%)	2 (1%)	0	100	100
All	All	7006/7347 (95%)	6849 (98%)	157 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	203/359 (56%)	203 (100%)	0	100	100
1	B	359/359 (100%)	359 (100%)	0	100	100
1	C	359/359 (100%)	359 (100%)	0	100	100
1	D	359/359 (100%)	359 (100%)	0	100	100
1	E	359/359 (100%)	359 (100%)	0	100	100
1	F	359/359 (100%)	359 (100%)	0	100	100
1	G	319/359 (89%)	319 (100%)	0	100	100
1	I	324/359 (90%)	324 (100%)	0	100	100
1	J	359/359 (100%)	359 (100%)	0	100	100
1	K	359/359 (100%)	359 (100%)	0	100	100
1	L	359/359 (100%)	358 (100%)	1 (0%)	86	91
1	M	359/359 (100%)	359 (100%)	0	100	100
1	N	359/359 (100%)	359 (100%)	0	100	100
2	a	153/156 (98%)	153 (100%)	0	100	100
2	b	153/156 (98%)	153 (100%)	0	100	100
2	c	153/156 (98%)	153 (100%)	0	100	100
2	d	153/156 (98%)	153 (100%)	0	100	100
2	e	153/156 (98%)	153 (100%)	0	100	100
2	f	153/156 (98%)	153 (100%)	0	100	100
2	g	153/156 (98%)	153 (100%)	0	100	100
2	h	153/156 (98%)	153 (100%)	0	100	100
2	i	153/156 (98%)	153 (100%)	0	100	100
2	j	153/156 (98%)	153 (100%)	0	100	100
All	All	5966/6227 (96%)	5965 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	32	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 70 such sidechains are listed below:

Mol	Chain	Res	Type
2	a	63	ASN
2	b	61	GLN
2	h	64	GLN
1	G	306	ASN
1	G	275	ASN

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	$\# Z > 2$
3	AGS	C	501	4	32,33,33	0.48	1 (3%)	45,52,52	0.67	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AGS	E	501	4	32,33,33	0.48	1 (3%)	45,52,52	0.67	1 (2%)
3	AGS	M	501	4	32,33,33	0.48	1 (3%)	45,52,52	0.66	1 (2%)
3	AGS	B	501	4	32,33,33	0.46	1 (3%)	45,52,52	0.71	1 (2%)
3	AGS	F	501	4	32,33,33	0.48	1 (3%)	45,52,52	0.69	1 (2%)
3	AGS	G	501	4	32,33,33	0.48	1 (3%)	45,52,52	0.71	1 (2%)
3	AGS	L	501	4	32,33,33	0.49	1 (3%)	45,52,52	0.66	1 (2%)
3	AGS	J	501	4	32,33,33	0.48	1 (3%)	45,52,52	0.69	1 (2%)
3	AGS	K	501	4	32,33,33	0.49	1 (3%)	45,52,52	0.67	1 (2%)
3	AGS	N	501	4	32,33,33	0.48	1 (3%)	45,52,52	0.71	1 (2%)
3	AGS	D	501	4	32,33,33	0.49	1 (3%)	45,52,52	0.66	1 (2%)
3	AGS	I	501	4	32,33,33	0.55	1 (3%)	45,52,52	0.79	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AGS	C	501	4	-	3/21/38/38	0/3/3/3
3	AGS	E	501	4	-	3/21/38/38	0/3/3/3
3	AGS	M	501	4	-	4/21/38/38	0/3/3/3
3	AGS	B	501	4	-	2/21/38/38	0/3/3/3
3	AGS	F	501	4	-	3/21/38/38	0/3/3/3
3	AGS	G	501	4	-	2/21/38/38	0/3/3/3
3	AGS	L	501	4	-	2/21/38/38	0/3/3/3
3	AGS	J	501	4	-	4/21/38/38	0/3/3/3
3	AGS	K	501	4	-	0/21/38/38	0/3/3/3
3	AGS	N	501	4	-	2/21/38/38	0/3/3/3
3	AGS	D	501	4	-	2/21/38/38	0/3/3/3
3	AGS	I	501	4	-	4/21/38/38	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	501	AGS	PG-S1G	2.26	1.95	1.90
3	N	501	AGS	PG-S1G	2.14	1.95	1.90
3	G	501	AGS	PG-S1G	2.14	1.95	1.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	501	AGS	PG-S1G	2.12	1.95	1.90
3	B	501	AGS	PG-S1G	2.12	1.95	1.90

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	501	AGS	PB-O3B-PG	-4.17	117.91	133.17
3	J	501	AGS	PB-O3B-PG	-3.75	119.43	133.17
3	G	501	AGS	PB-O3B-PG	-3.74	119.49	133.17
3	M	501	AGS	PB-O3B-PG	-3.62	119.94	133.17
3	D	501	AGS	PB-O3B-PG	-3.60	120.00	133.17

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	501	AGS	O4'-C4'-C5'-O5'
3	L	501	AGS	O4'-C4'-C5'-O5'
3	M	501	AGS	O4'-C4'-C5'-O5'
3	B	501	AGS	PA-O3A-PB-O1B
3	J	501	AGS	PA-O3A-PB-O1B

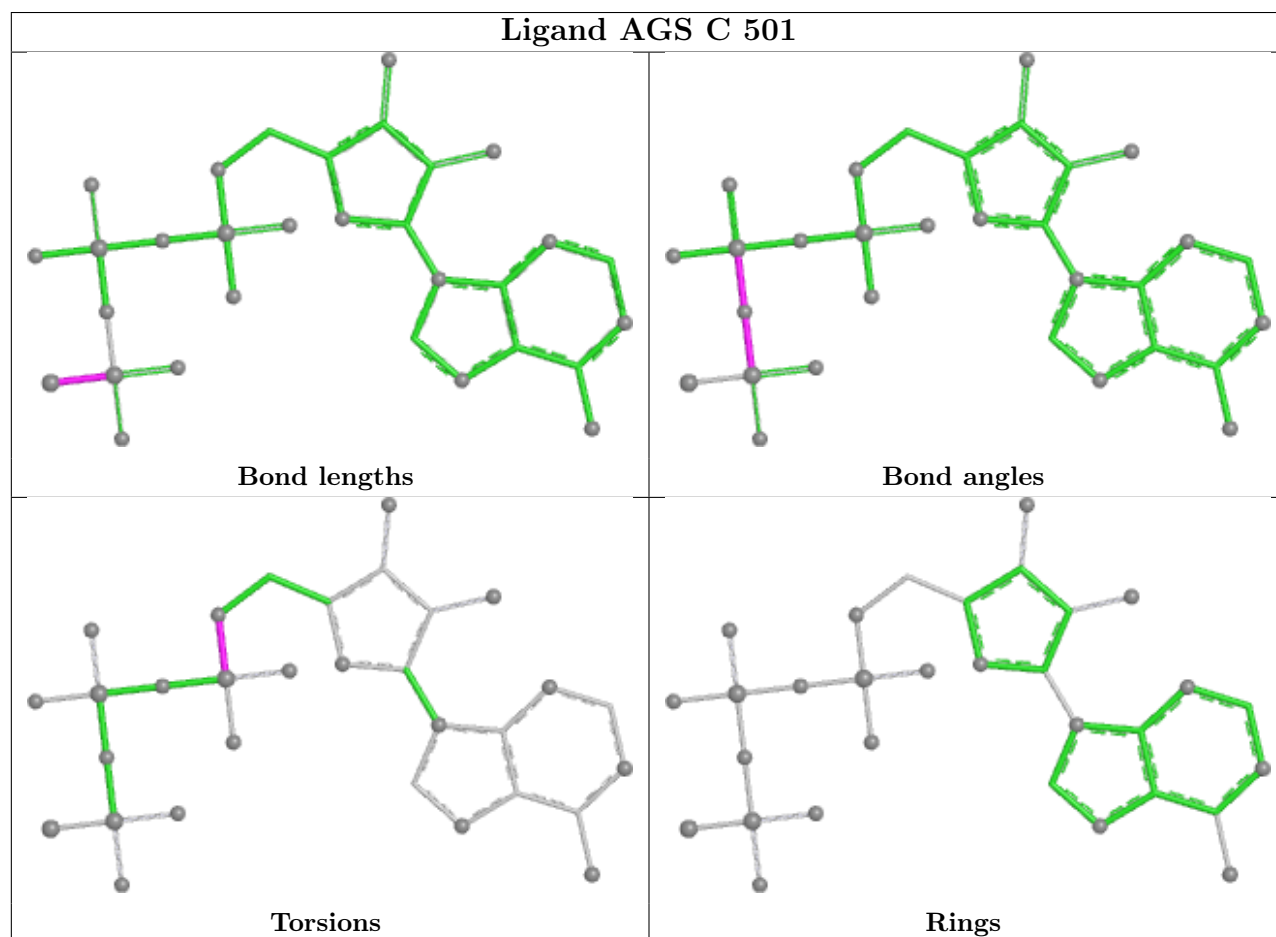
There are no ring outliers.

11 monomers are involved in 24 short contacts:

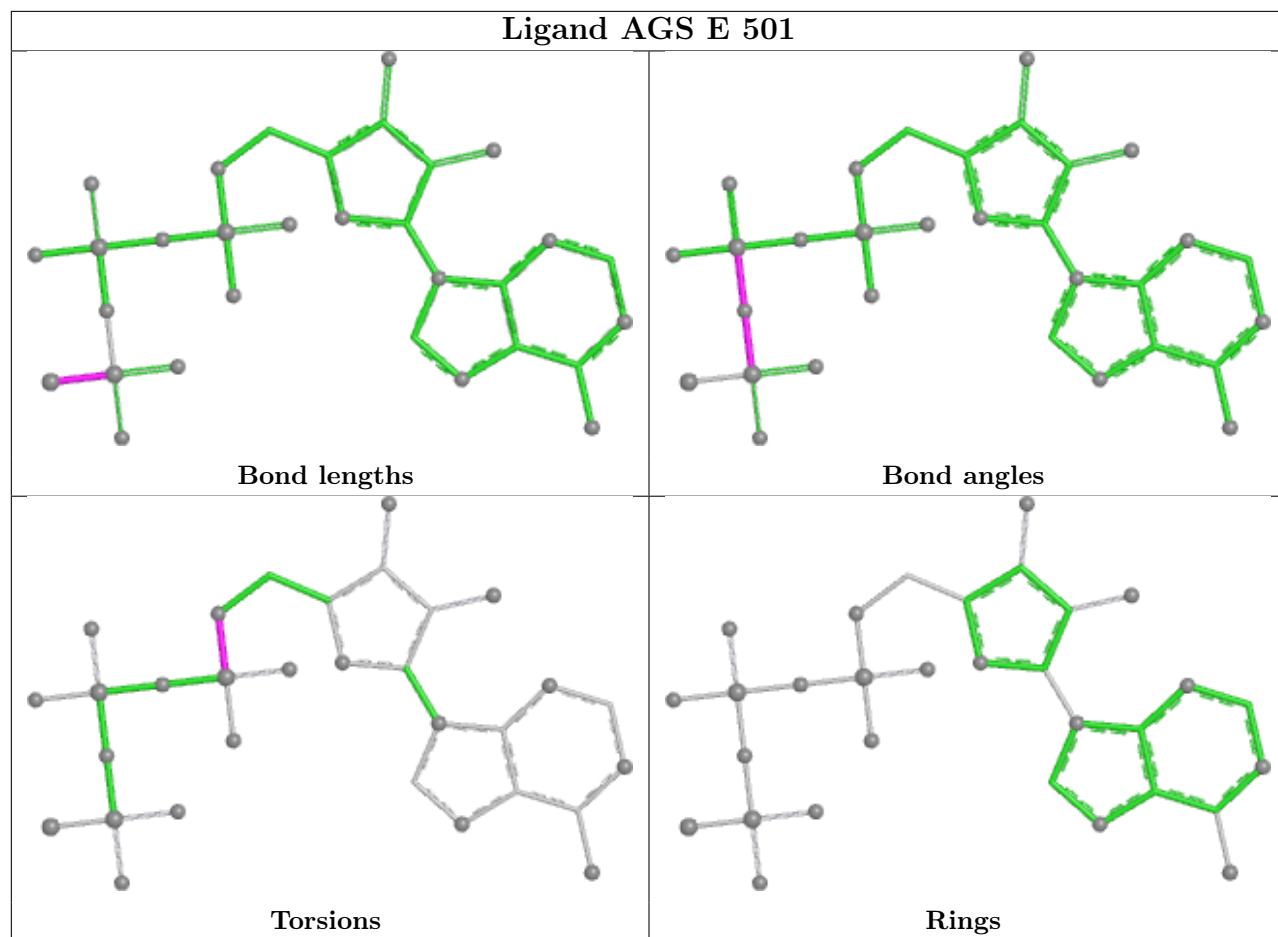
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	501	AGS	2	0
3	M	501	AGS	2	0
3	B	501	AGS	2	0
3	F	501	AGS	3	0
3	G	501	AGS	2	0
3	L	501	AGS	2	0
3	J	501	AGS	2	0
3	K	501	AGS	1	0
3	N	501	AGS	2	0
3	D	501	AGS	3	0
3	I	501	AGS	3	0

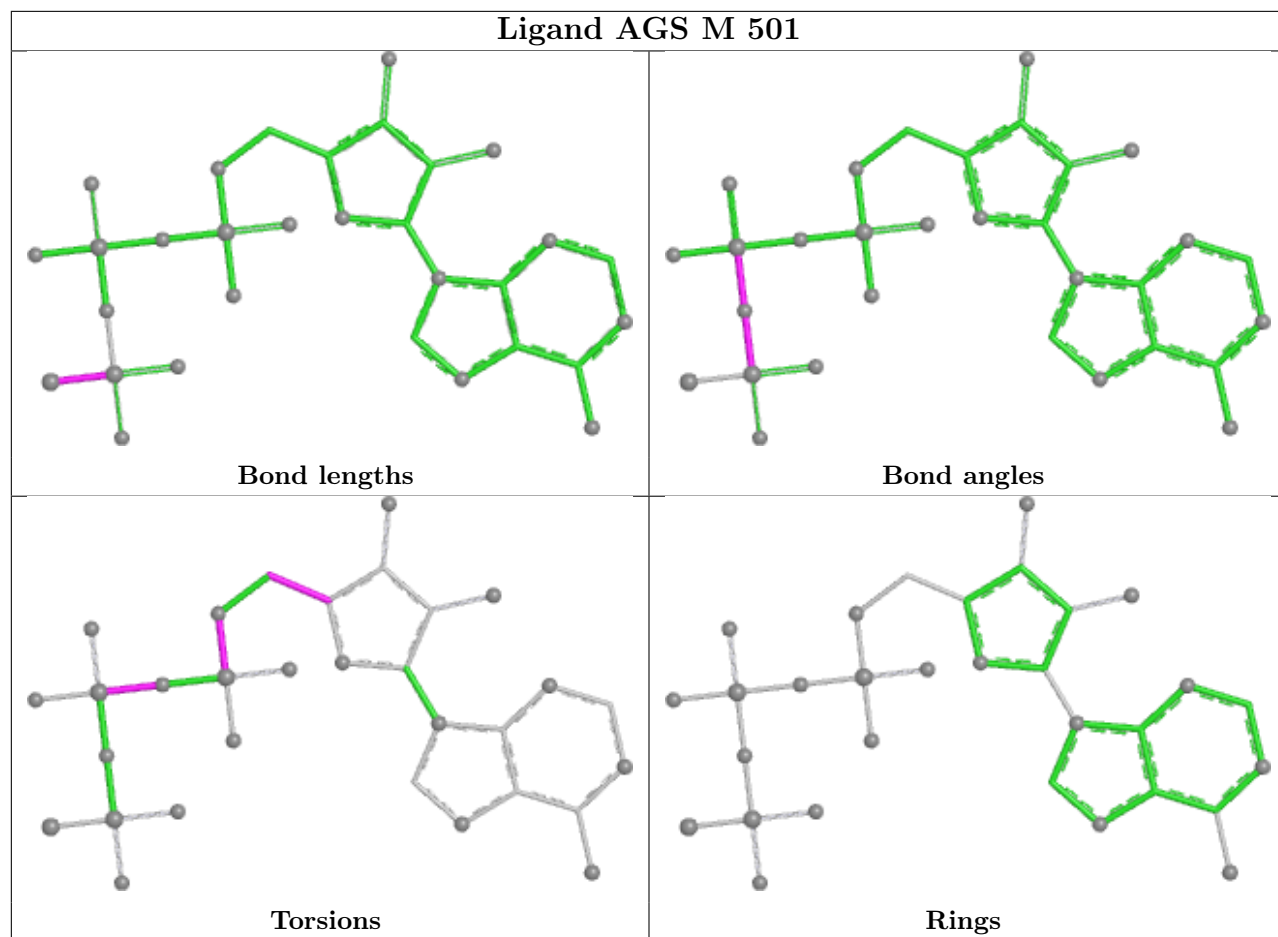
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

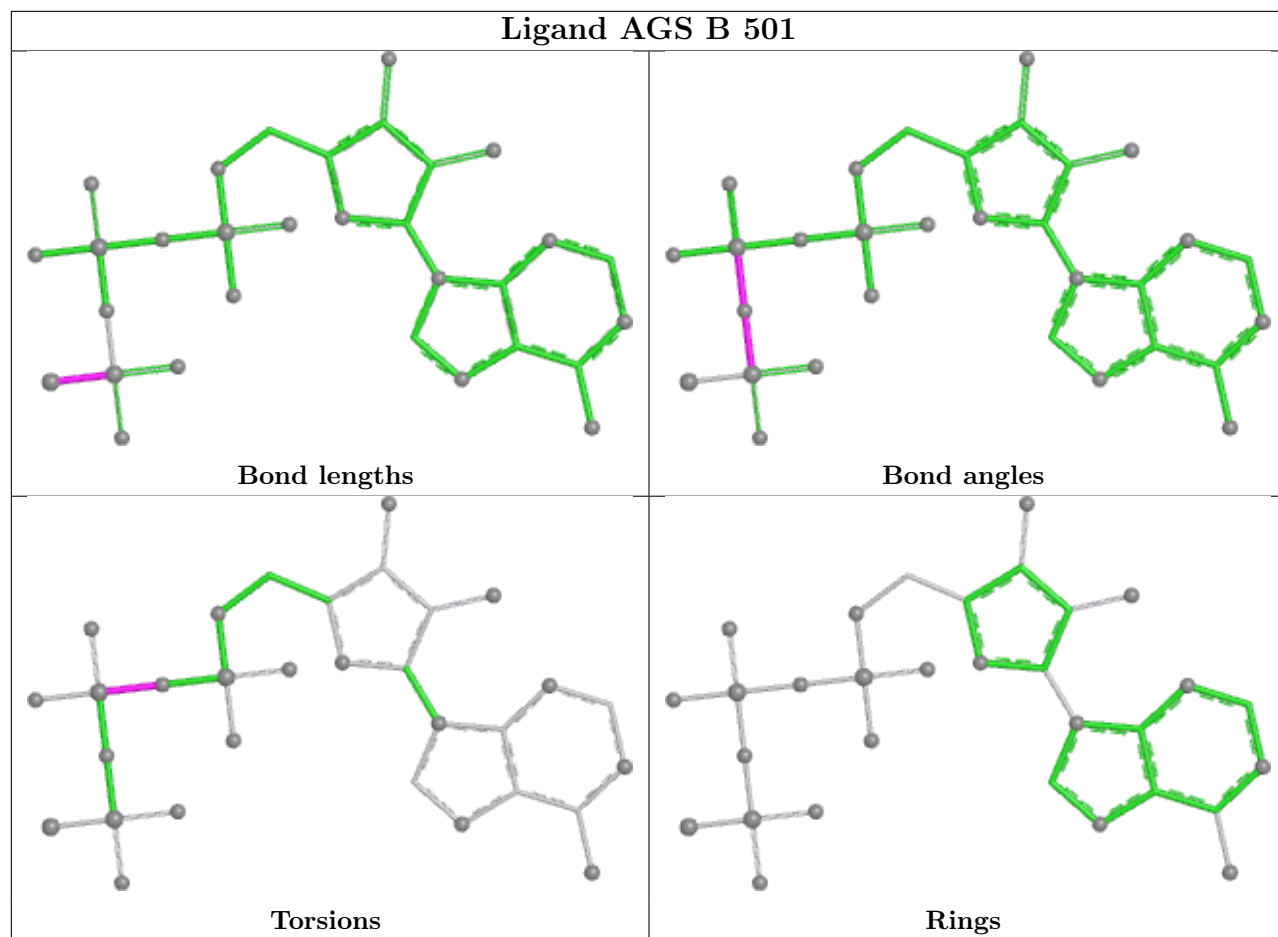
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.



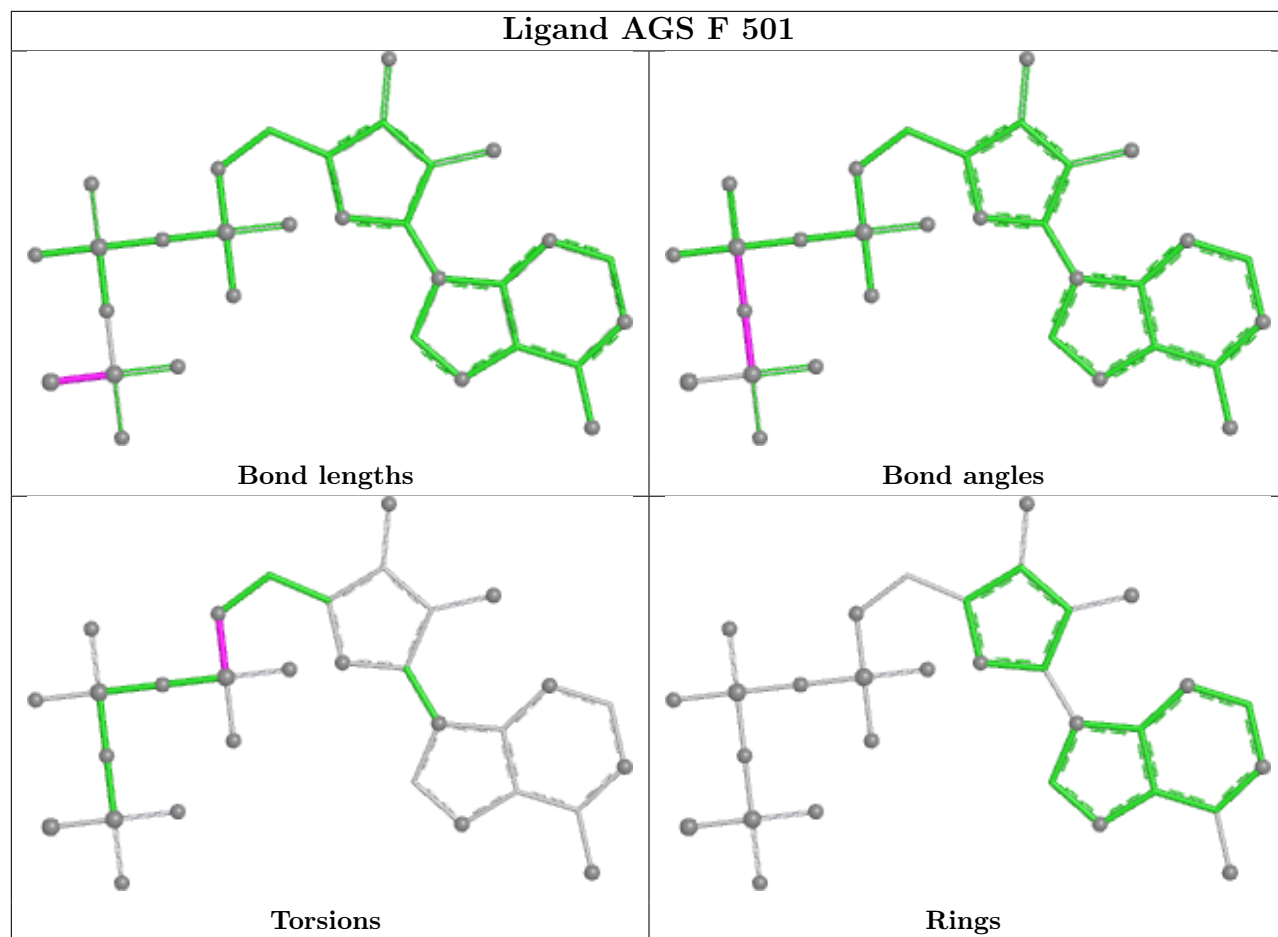
Ligand AGS E 501

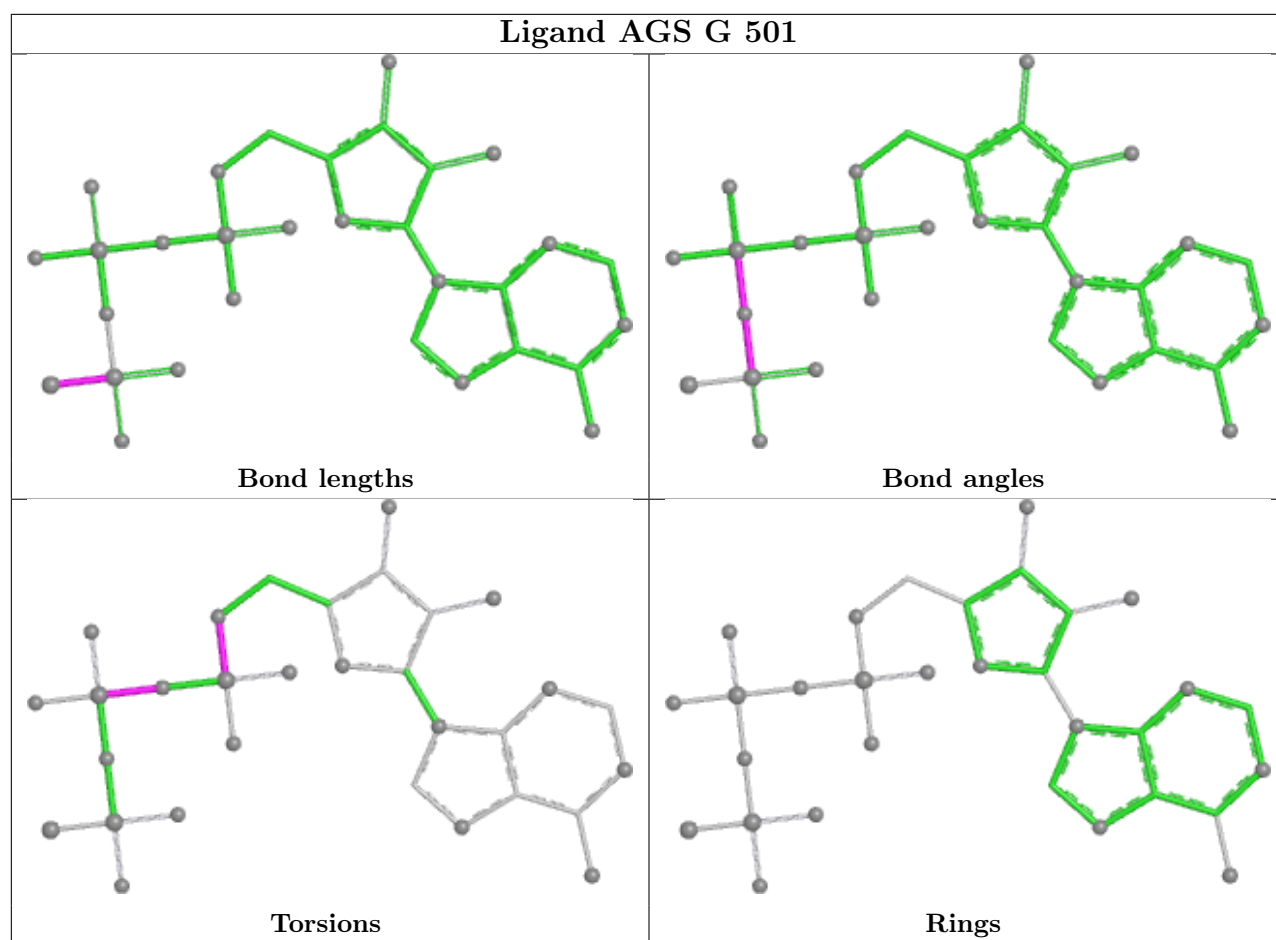


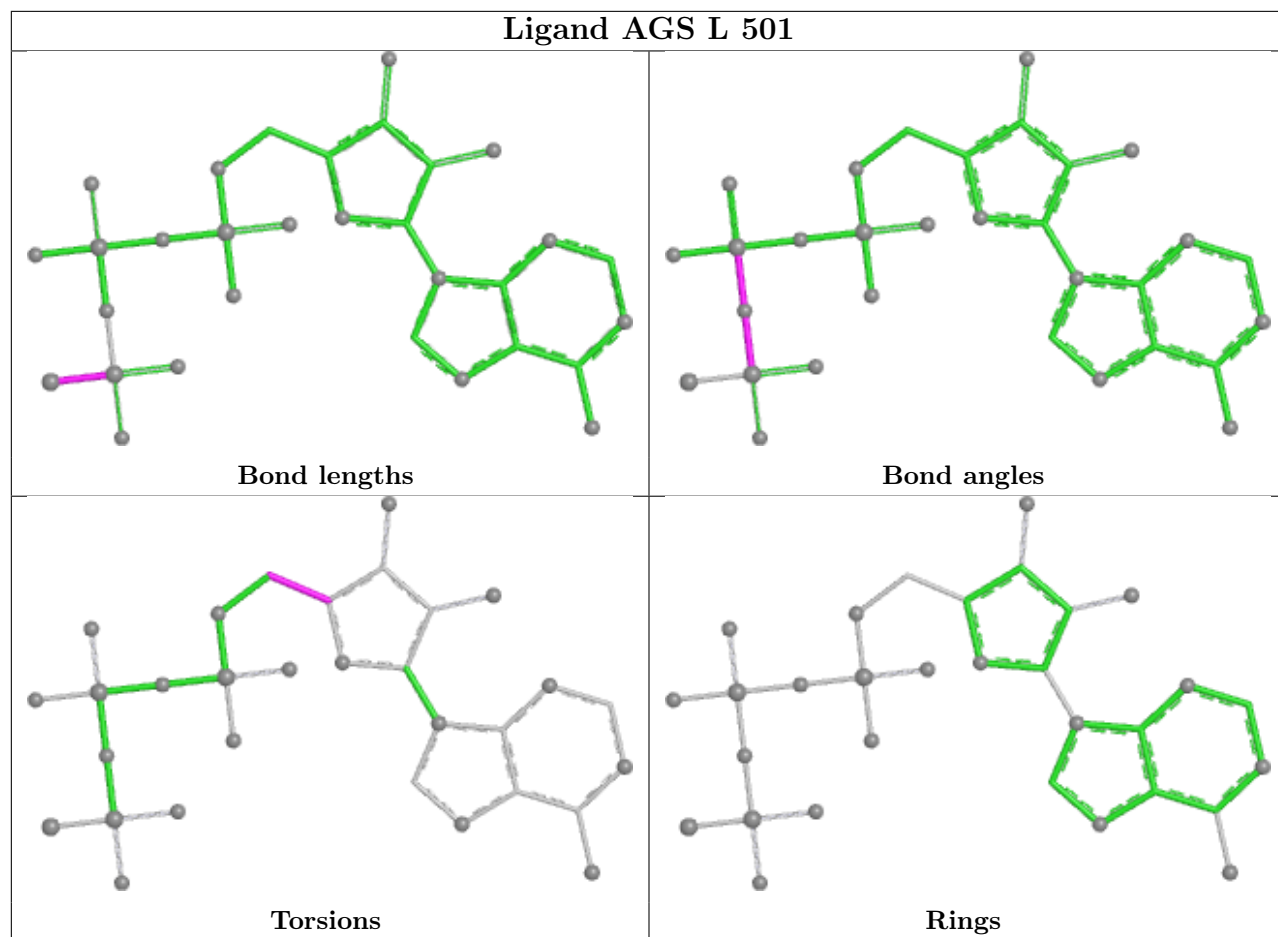




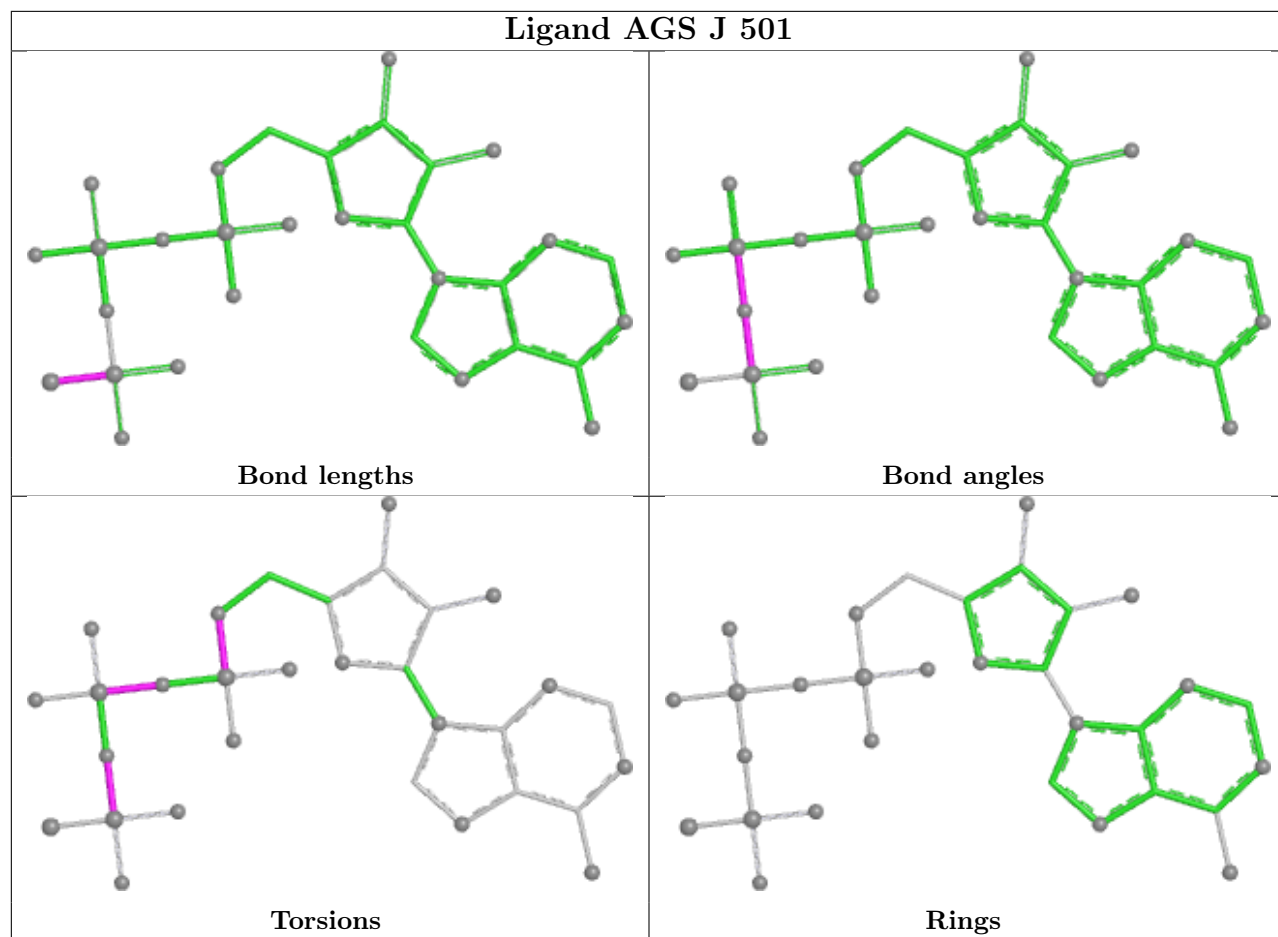
Ligand AGS F 501

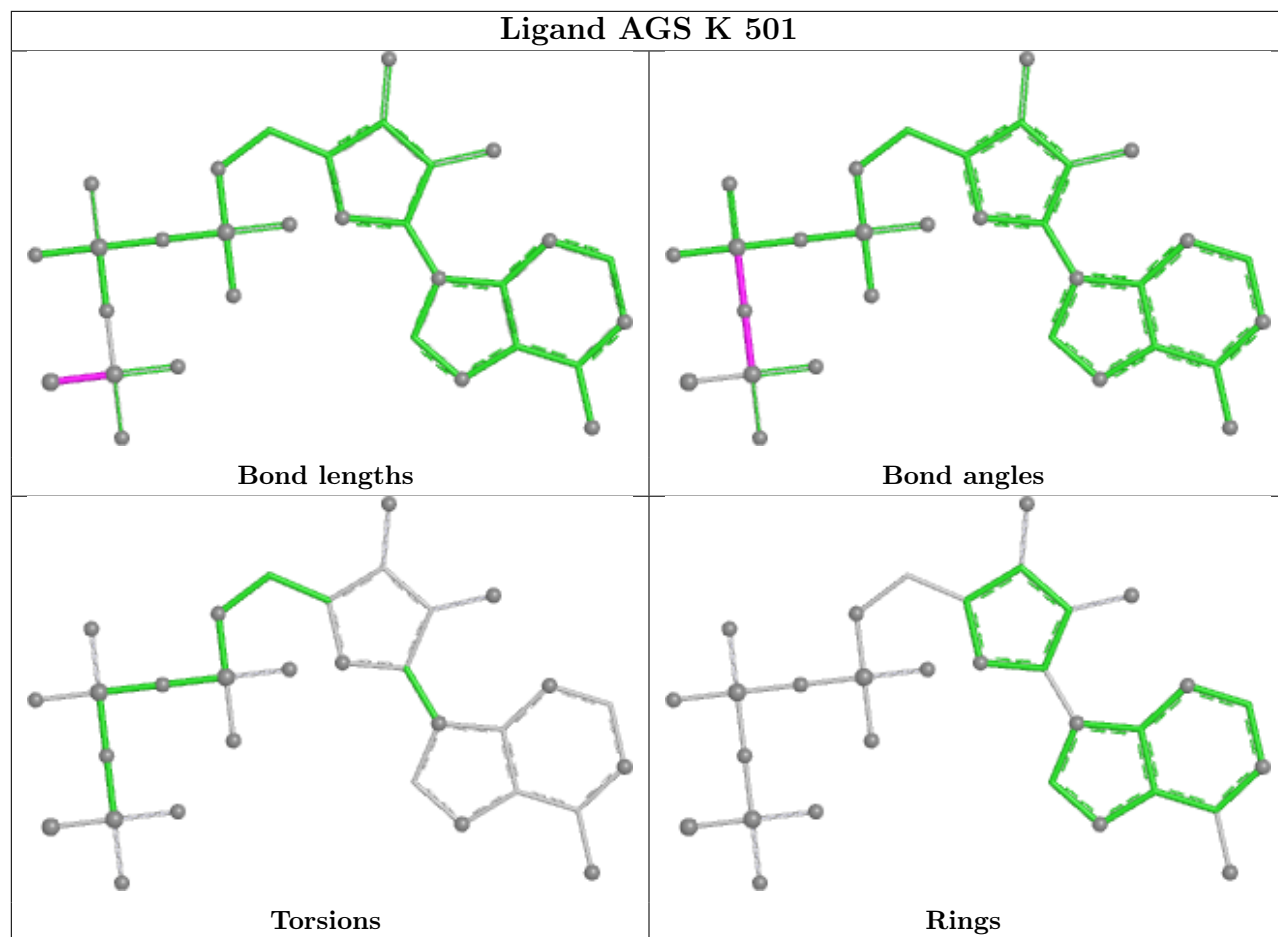


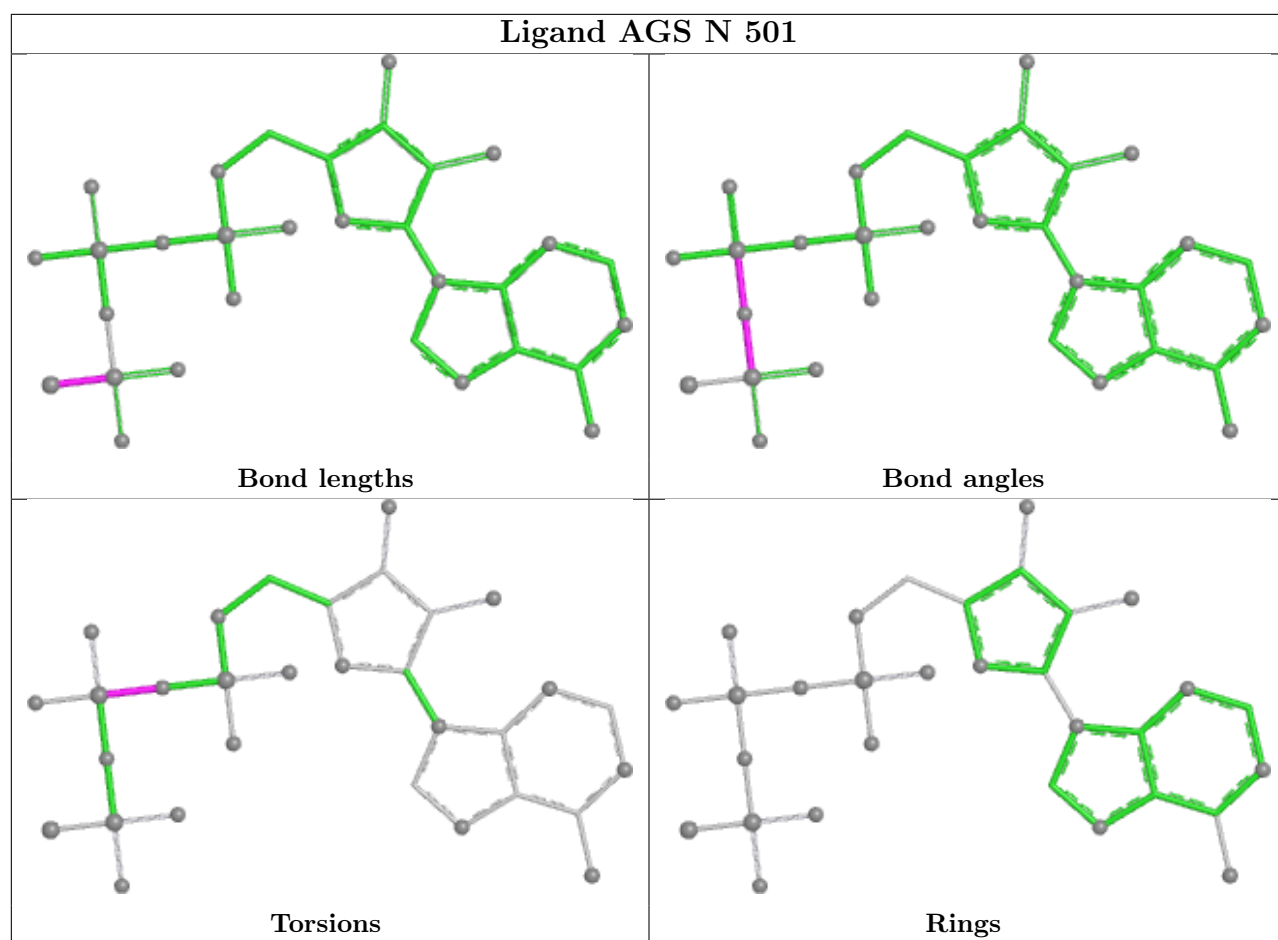


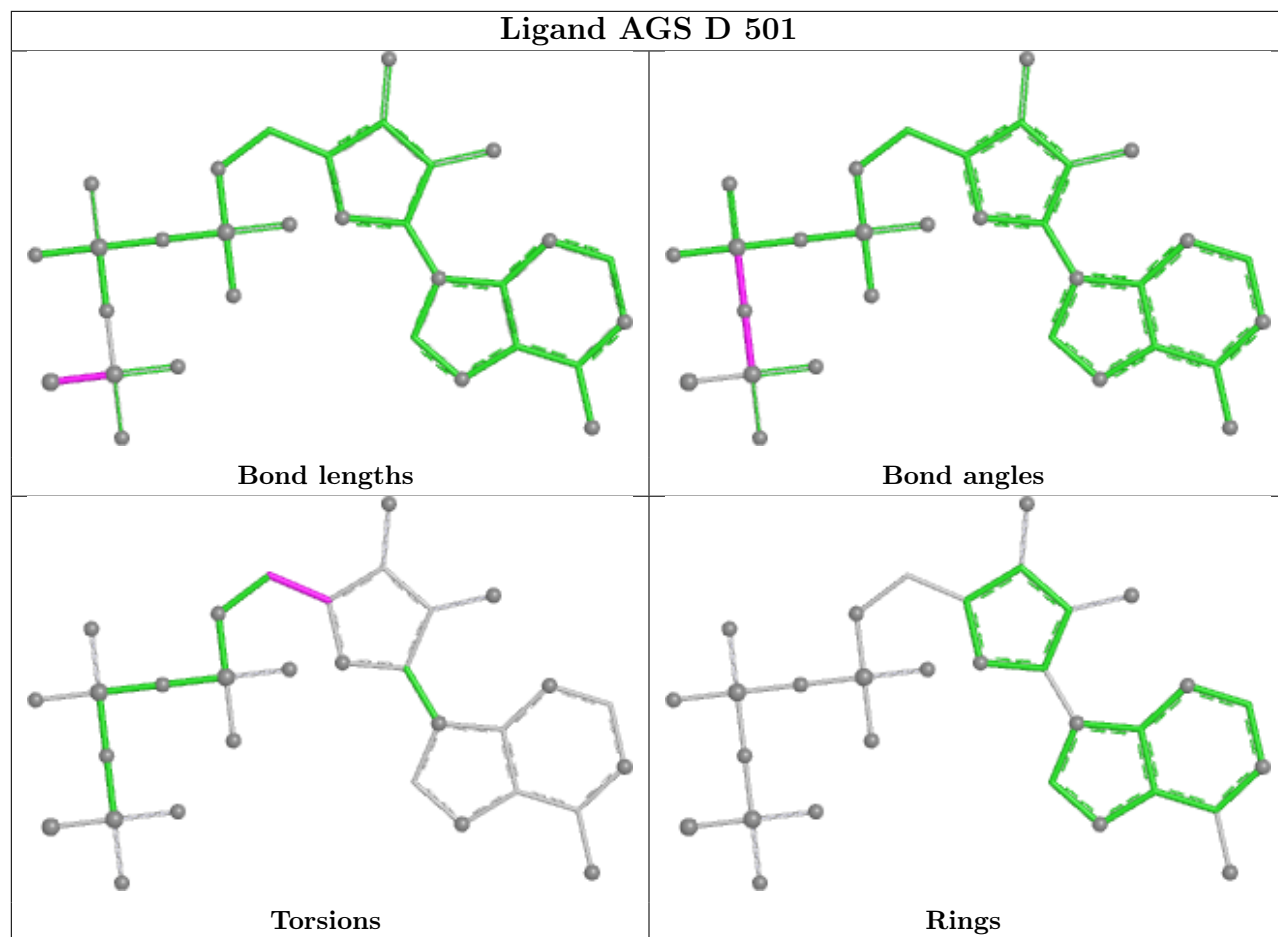


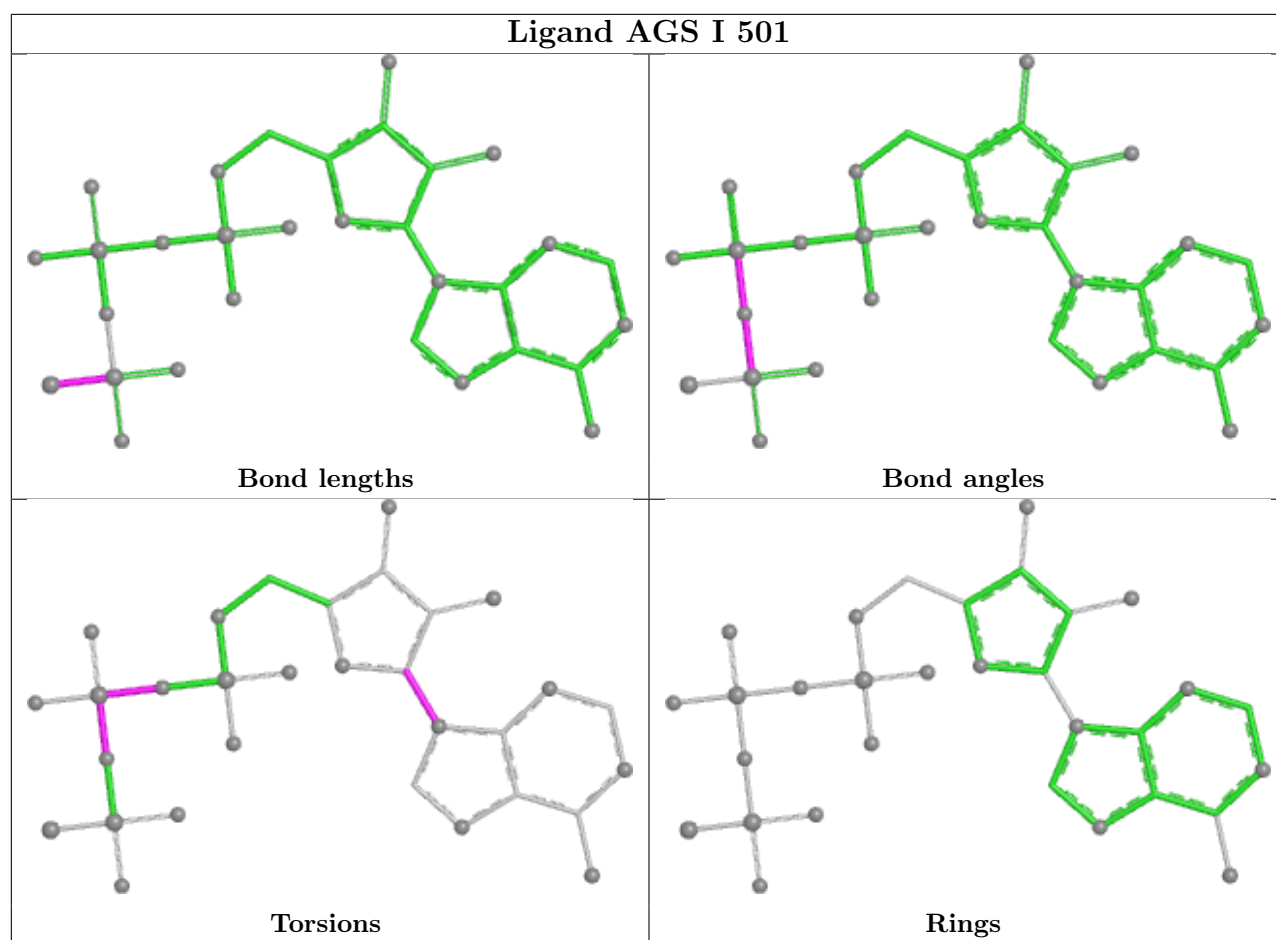
Ligand AGS J 501











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.

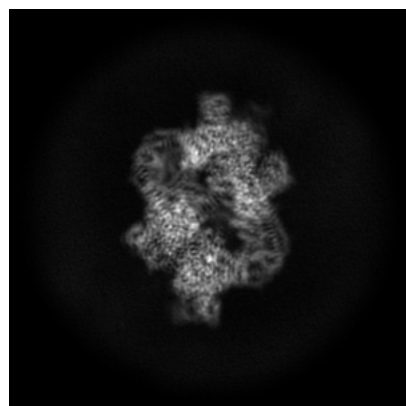
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17641. These allow visual inspection of the internal detail of the map and identification of artifacts.

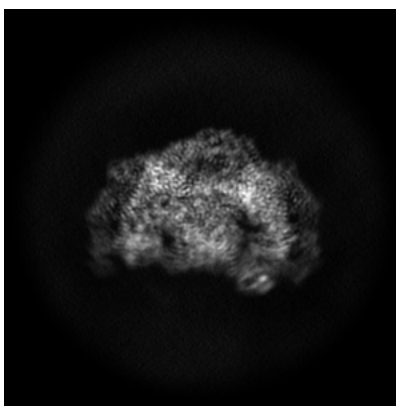
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

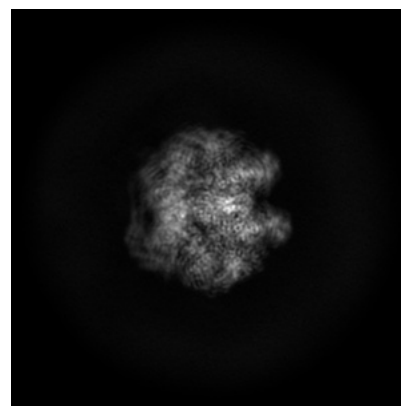
6.1.1 Primary map



X

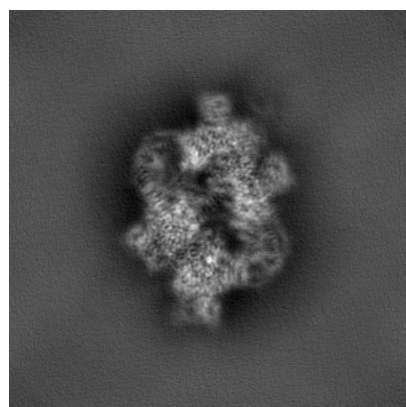


Y

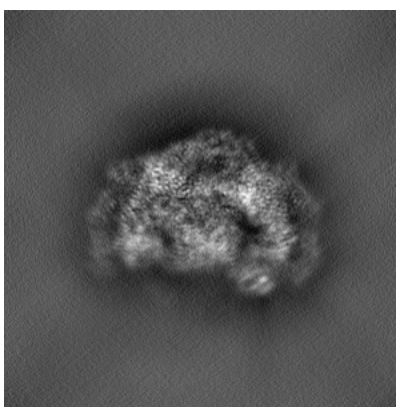


Z

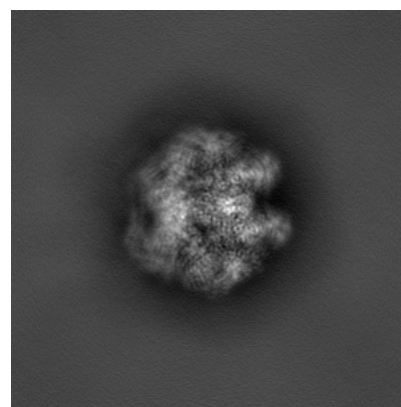
6.1.2 Raw map



X



Y

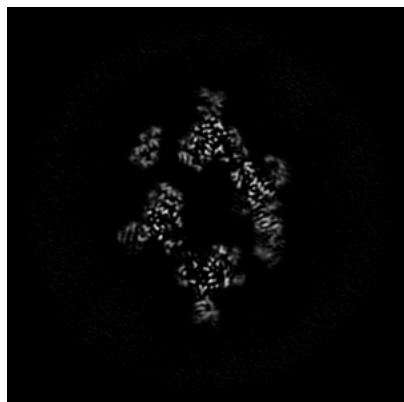


Z

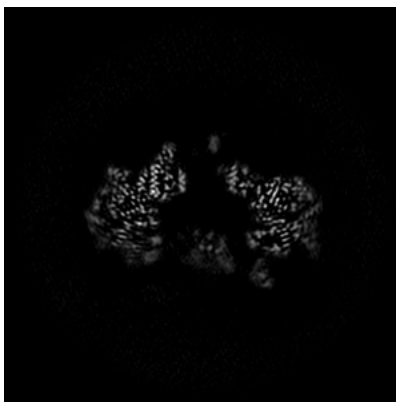
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

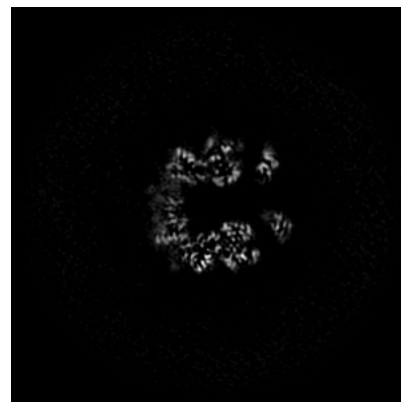
6.2.1 Primary map



X Index: 224

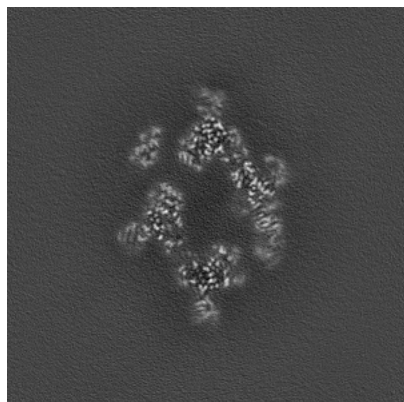


Y Index: 224

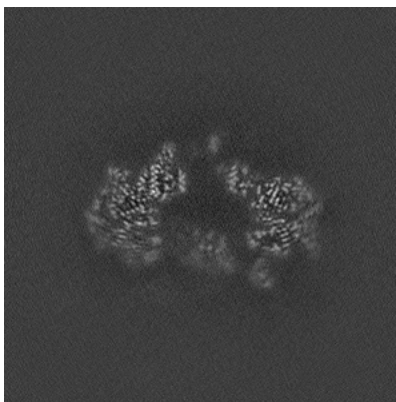


Z Index: 224

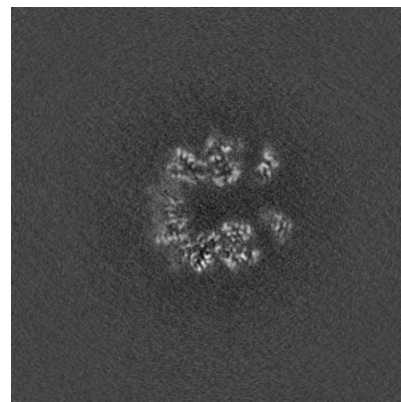
6.2.2 Raw map



X Index: 224



Y Index: 224

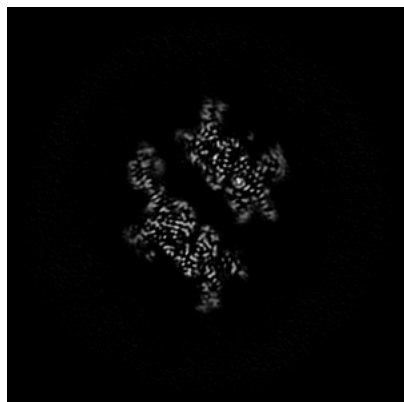


Z Index: 224

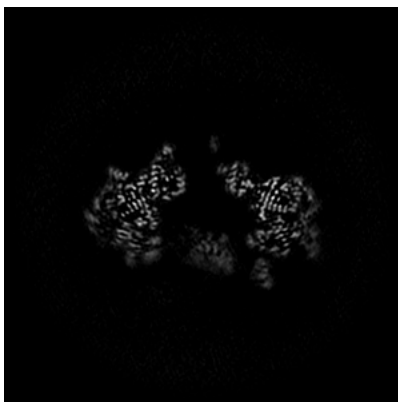
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

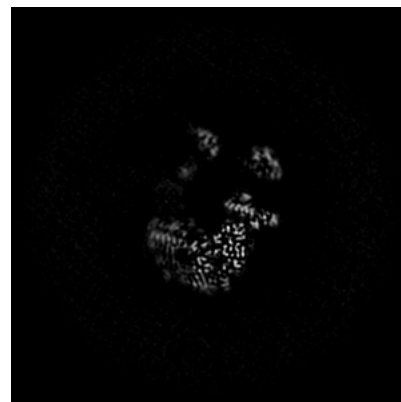
6.3.1 Primary map



X Index: 244

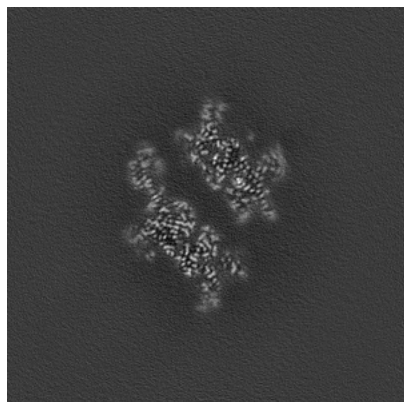


Y Index: 226

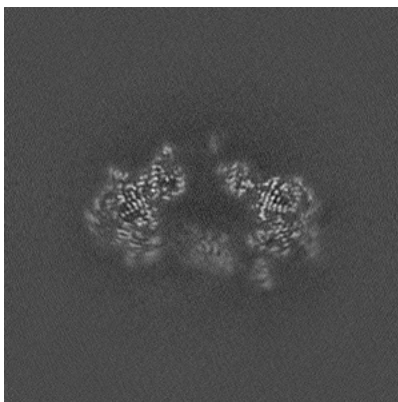


Z Index: 197

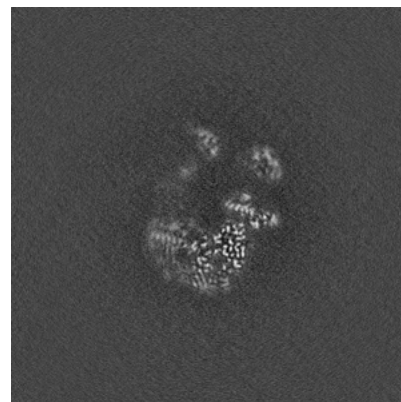
6.3.2 Raw map



X Index: 244



Y Index: 226

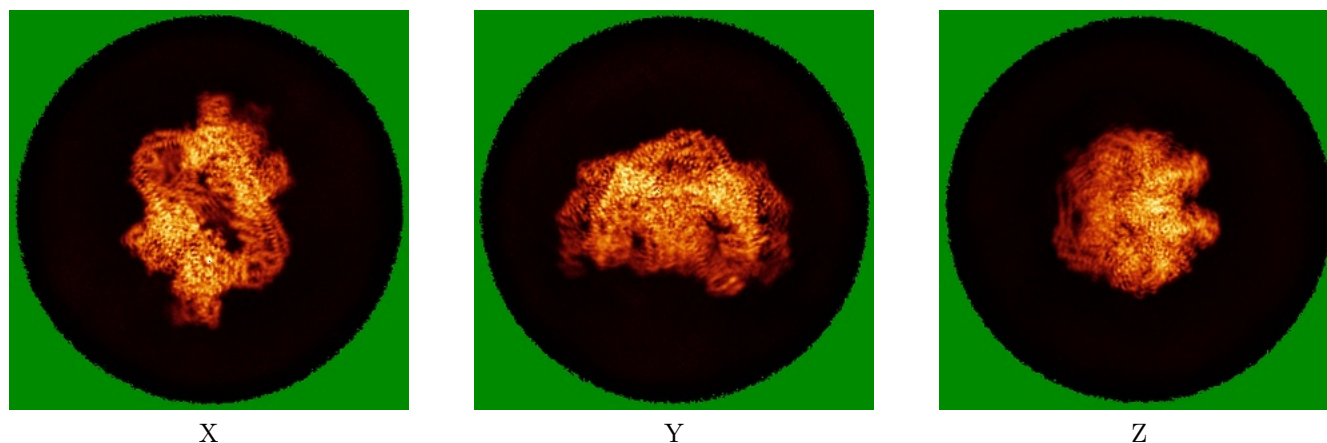


Z Index: 197

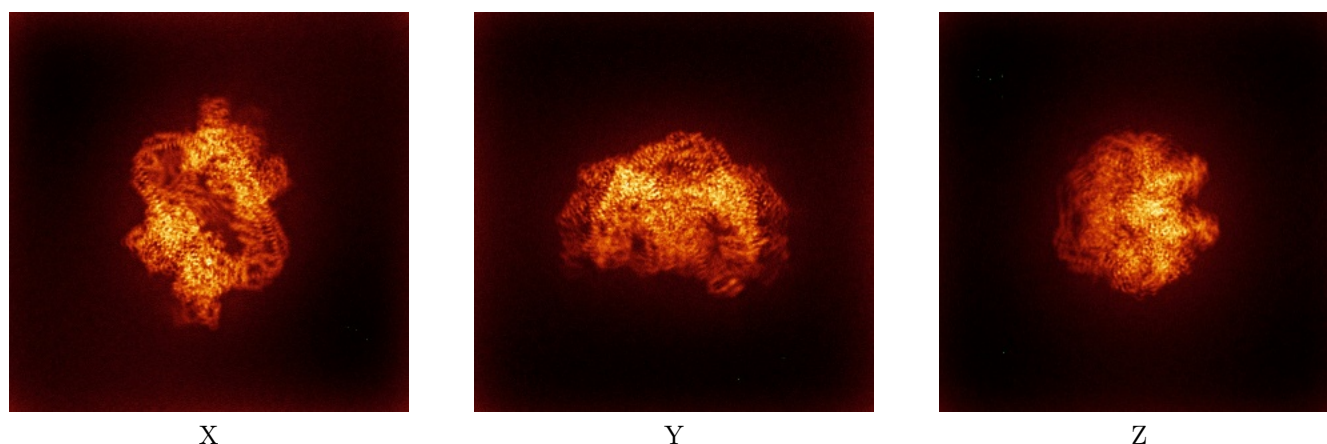
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

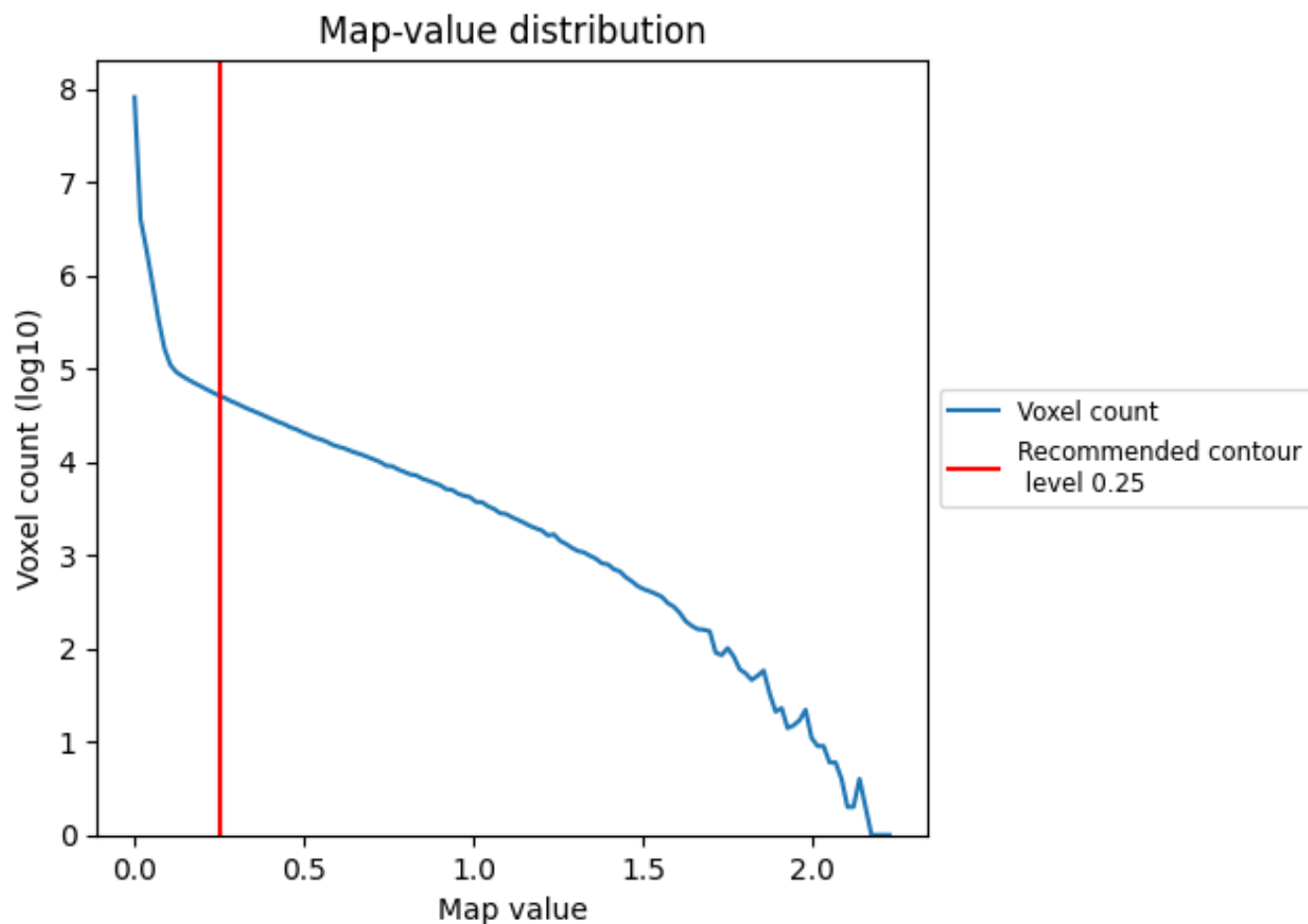
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

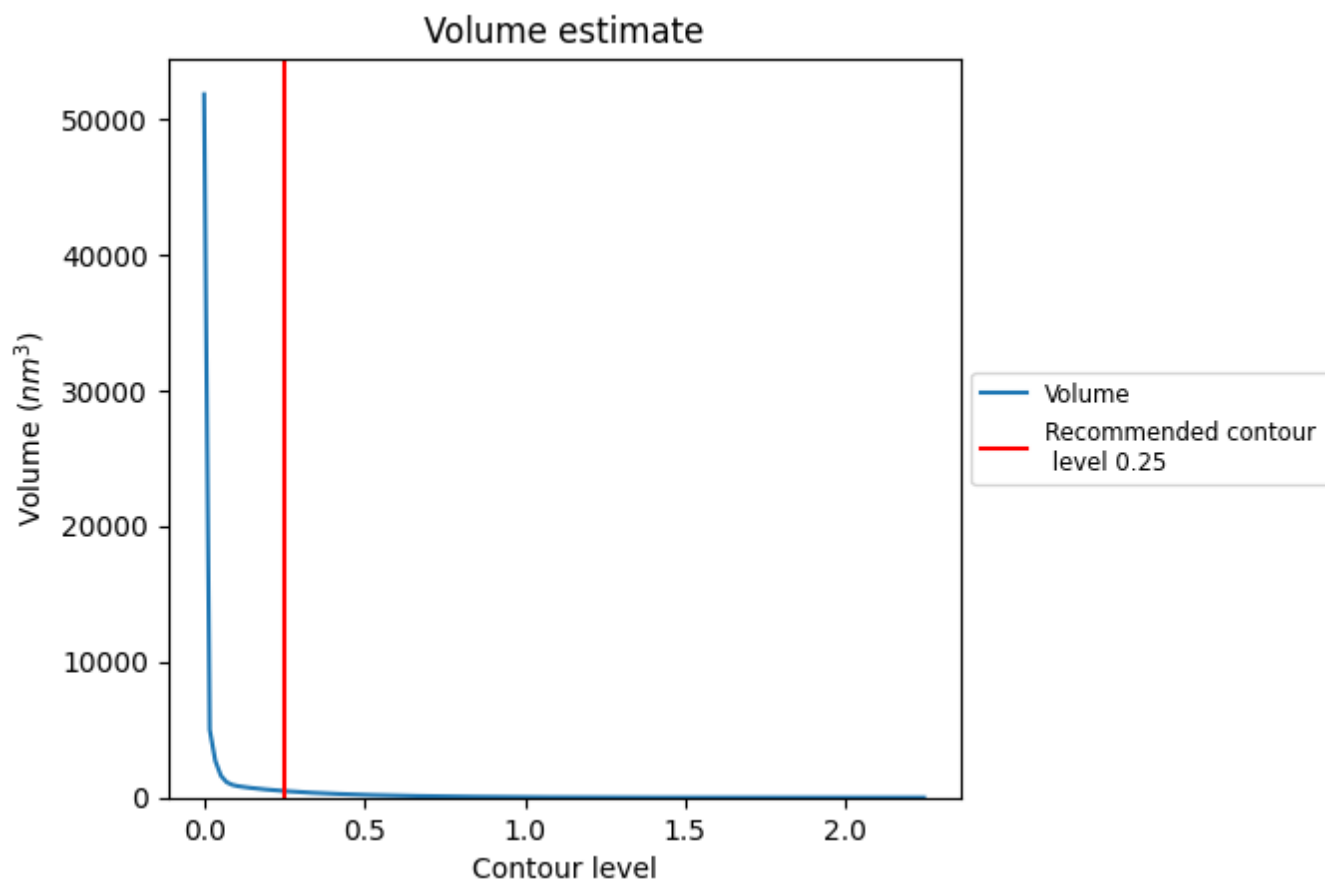
This section contains the results of statistical analysis of the map.

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.

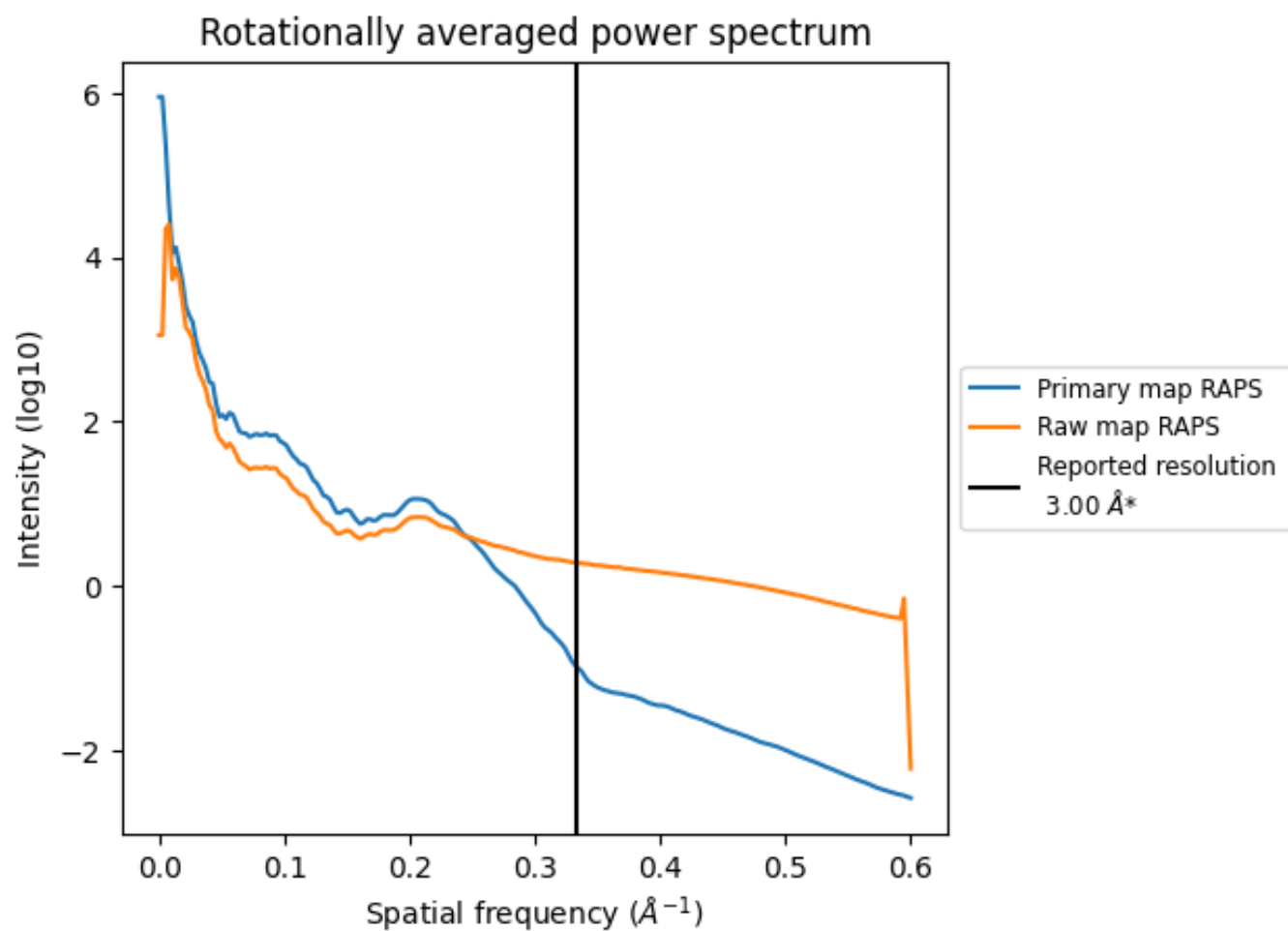
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 482 nm³; this corresponds to an approximate mass of 436 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 ⓘ

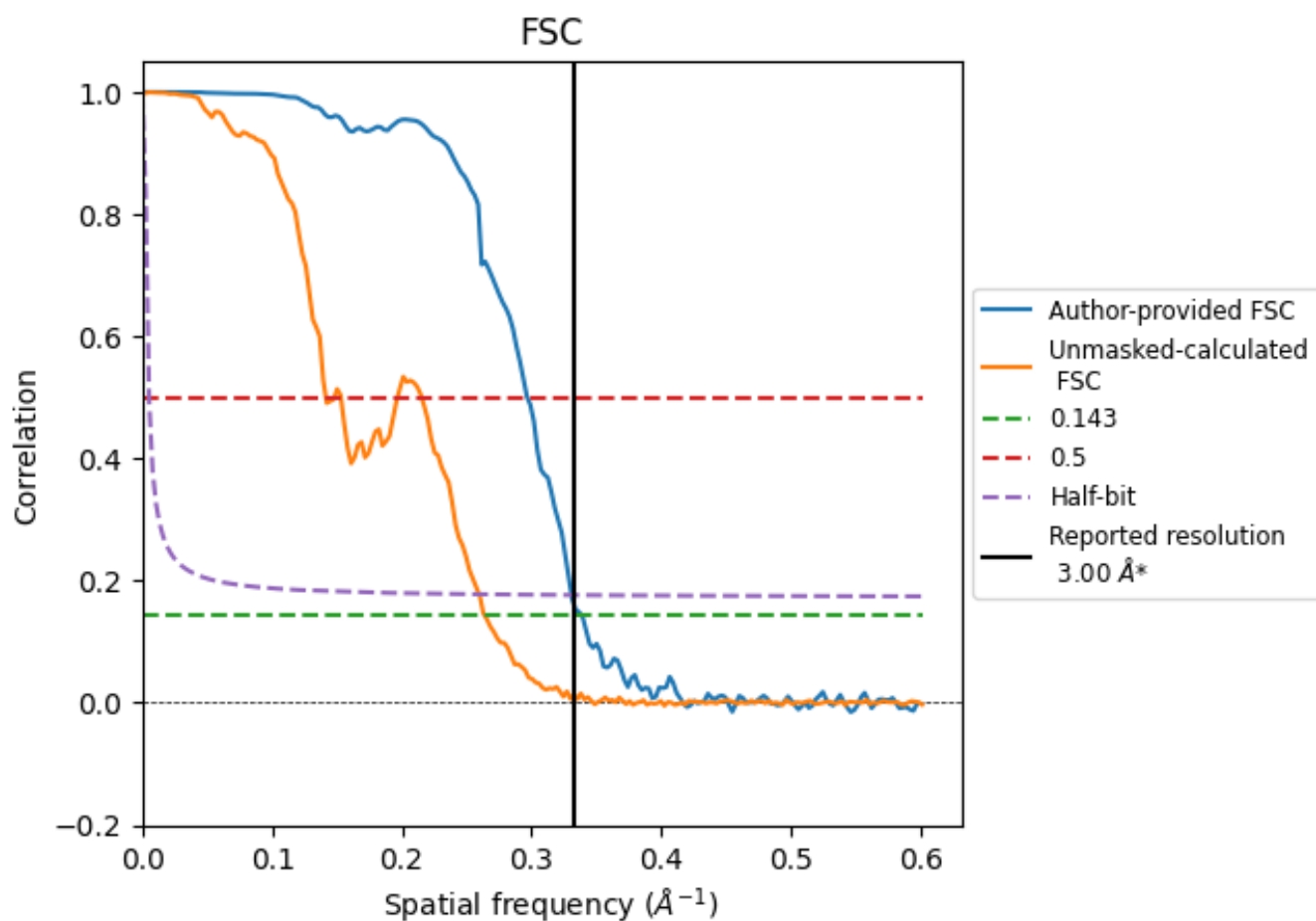


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

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 0.333 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.95	3.37	3.02
Unmasked-calculated*	3.79	7.07	3.85

*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 3.79 differs from the reported value 3.0 by more than 10 %

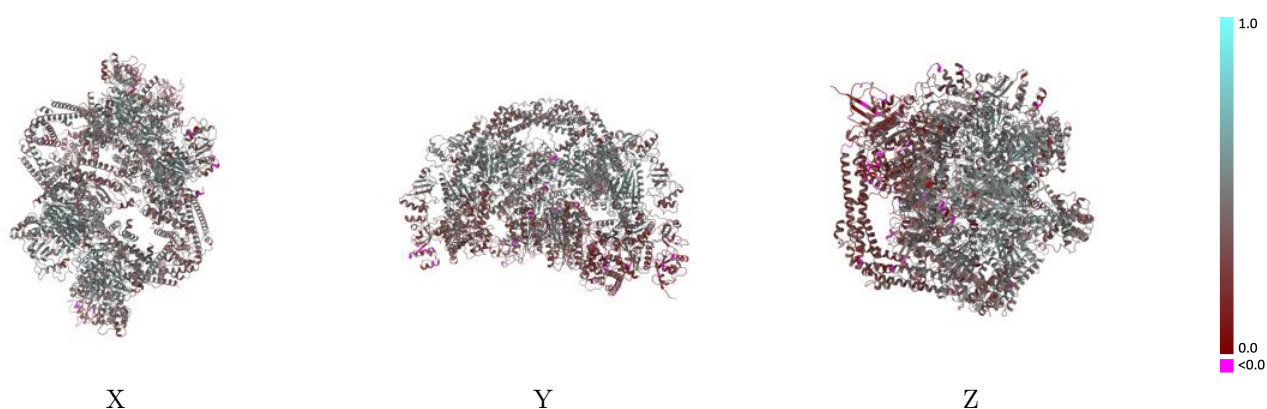
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-17641 and PDB model 8PEY. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)

This section was not generated.

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

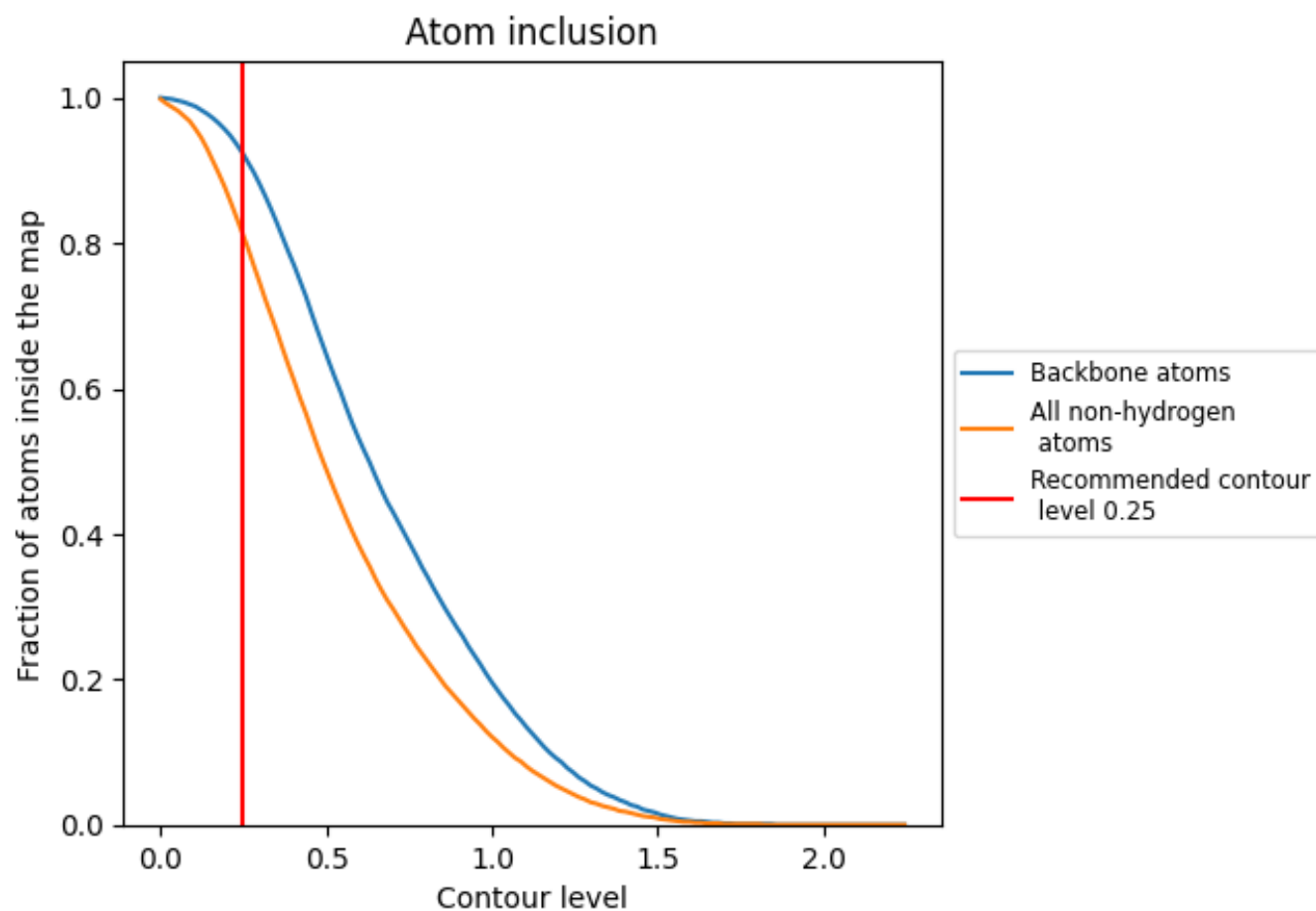


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 81% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8100	 0.4070
A	 0.6300	 0.3010
B	 0.7740	 0.3790
C	 0.8730	 0.4650
D	 0.8880	 0.4880
E	 0.8680	 0.4690
F	 0.7360	 0.3800
G	 0.5020	 0.2600
I	 0.6500	 0.3170
J	 0.8860	 0.4680
K	 0.9150	 0.5030
L	 0.9220	 0.5060
M	 0.8710	 0.4530
N	 0.6850	 0.3190
a	 0.6620	 0.2690
b	 0.7630	 0.3390
c	 0.8830	 0.3960
d	 0.9090	 0.4280
e	 0.9000	 0.4320
f	 0.9050	 0.4300
g	 0.9040	 0.4280
h	 0.9010	 0.4250
i	 0.8760	 0.3800
j	 0.8480	 0.3480

