



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 05:54 PM UTC

PDB ID : 9P1I / pdb_00009p1i
EMDB ID : EMD-71108
Title : Atomic structure of vibrio effector fragment VopV bound to Beta-cytoplasmic c/gamma1-cytoplasmic F-actin
Authors : Kreutzberger, M.A.; Kudryashova, E.; Egelman, E.H.; Kudryashov, D.S.
Deposited on : 2025-06-10
Resolution : 3.00 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:

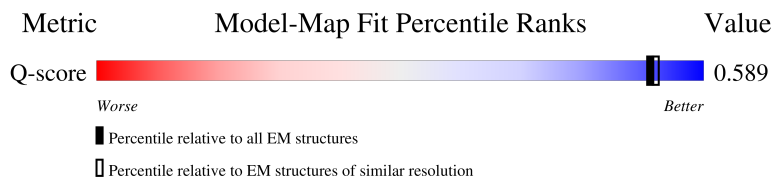
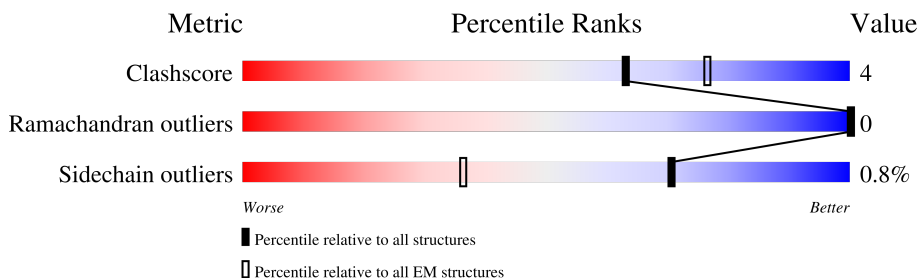
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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

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.



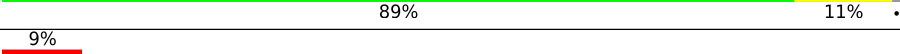
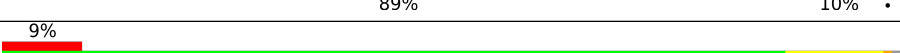
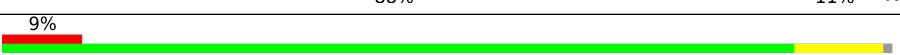
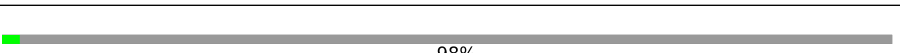
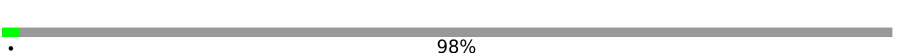
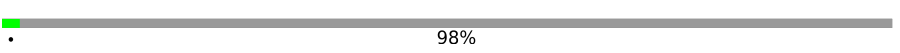
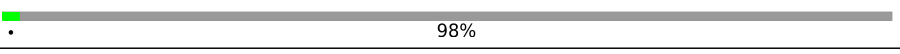
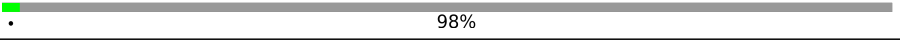
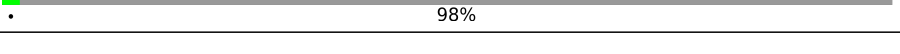
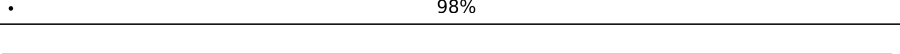
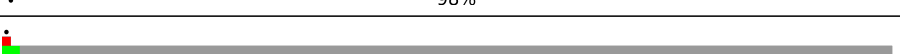
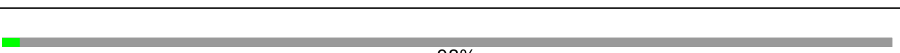
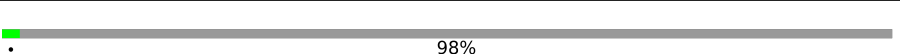
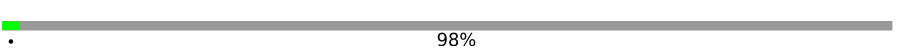
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	Q	375	10% 86% 13% .
1	R	375	9% 89% 10% .
1	S	375	9% 87% 12% .
1	T	375	10% 86% 14% .

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Mol	Chain	Length	Quality of chain
1	U	375	
1	V	375	
1	W	375	
1	X	375	
1	Y	375	
1	Z	375	
1	a	375	
1	b	375	
2	c	2402	
2	d	2402	
2	e	2402	
2	f	2402	
2	g	2402	
2	h	2402	
2	i	2402	
2	j	2402	
2	k	2402	
2	l	2402	
2	m	2402	
2	n	2402	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 39624 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 Actin, cytoplasmic 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Q	372	Total 2902	C 1838	N 488	O 554	S 22	0	0
1	R	372	Total 2902	C 1838	N 488	O 554	S 22	0	0
1	S	372	Total 2902	C 1838	N 488	O 554	S 22	0	0
1	T	372	Total 2902	C 1838	N 488	O 554	S 22	0	0
1	U	372	Total 2902	C 1838	N 488	O 554	S 22	0	0
1	V	372	Total 2902	C 1838	N 488	O 554	S 22	0	0
1	W	372	Total 2902	C 1838	N 488	O 554	S 22	0	0
1	X	372	Total 2902	C 1838	N 488	O 554	S 22	0	0
1	Y	372	Total 2902	C 1838	N 488	O 554	S 22	0	0
1	Z	372	Total 2902	C 1838	N 488	O 554	S 22	0	0
1	a	372	Total 2902	C 1838	N 488	O 554	S 22	0	0
1	b	372	Total 2902	C 1838	N 488	O 554	S 22	0	0

- Molecule 2 is a protein called VopV.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	c	47	Total 367	C 225	N 69	O 71	S 2	0	0
2	d	47	Total 367	C 225	N 69	O 71	S 2	0	0
2	e	47	Total 367	C 225	N 69	O 71	S 2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	f	47	Total 367	C 225	N 69	O 71	S 2	0	0
2	g	47	Total 367	C 225	N 69	O 71	S 2	0	0
2	h	47	Total 367	C 225	N 69	O 71	S 2	0	0
2	i	47	Total 367	C 225	N 69	O 71	S 2	0	0
2	j	47	Total 367	C 225	N 69	O 71	S 2	0	0
2	k	47	Total 367	C 225	N 69	O 71	S 2	0	0
2	l	47	Total 367	C 225	N 69	O 71	S 2	0	0
2	m	47	Total 367	C 225	N 69	O 71	S 2	0	0
2	n	47	Total 367	C 225	N 69	O 71	S 2	0	0

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

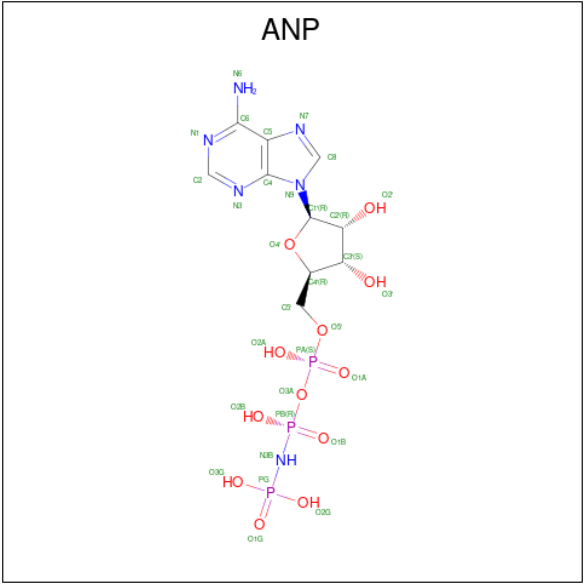
Mol	Chain	Residues	Atoms		AltConf
3	Q	1	Total 1	Mg 1	0
3	R	1	Total 1	Mg 1	0
3	S	1	Total 1	Mg 1	0
3	T	1	Total 1	Mg 1	0
3	U	1	Total 1	Mg 1	0
3	V	1	Total 1	Mg 1	0
3	W	1	Total 1	Mg 1	0
3	X	1	Total 1	Mg 1	0
3	Y	1	Total 1	Mg 1	0
3	Z	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
3	a	1	Total	Mg	0
			1	1	
3	b	1	Total	Mg	0
			1	1	

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



Mol	Chain	Residues	Atoms					AltConf
4	Q	1	Total	C	N	O	P	0
			31	10	6	12	3	
4	R	1	Total	C	N	O	P	0
			31	10	6	12	3	
4	S	1	Total	C	N	O	P	0
			31	10	6	12	3	
4	T	1	Total	C	N	O	P	0
			31	10	6	12	3	
4	U	1	Total	C	N	O	P	0
			31	10	6	12	3	
4	V	1	Total	C	N	O	P	0
			31	10	6	12	3	
4	W	1	Total	C	N	O	P	0
			31	10	6	12	3	
4	X	1	Total	C	N	O	P	0
			31	10	6	12	3	
4	Y	1	Total	C	N	O	P	0
			31	10	6	12	3	

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Mol	Chain	Residues	Atoms					AltConf
4	Z	1	Total	C	N	O	P	0
			31	10	6	12	3	
4	a	1	Total	C	N	O	P	0
			31	10	6	12	3	
4	b	1	Total	C	N	O	P	0
			31	10	6	12	3	

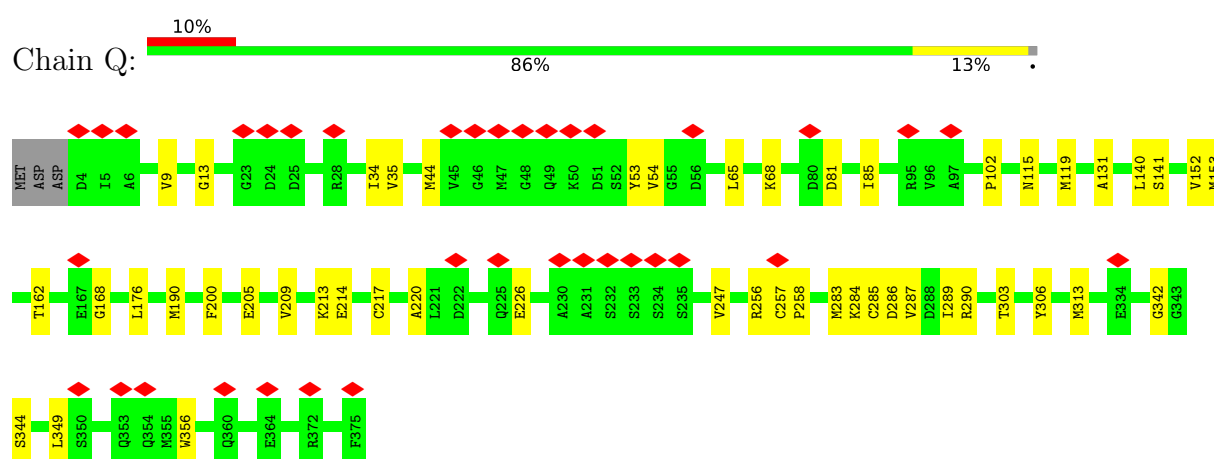
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		AltConf
5	Q	1	Total	O	0
			1	1	
5	R	1	Total	O	0
			1	1	
5	S	1	Total	O	0
			1	1	
5	T	1	Total	O	0
			1	1	
5	U	1	Total	O	0
			1	1	
5	V	1	Total	O	0
			1	1	
5	W	1	Total	O	0
			1	1	
5	X	1	Total	O	0
			1	1	
5	Y	1	Total	O	0
			1	1	
5	Z	1	Total	O	0
			1	1	
5	a	1	Total	O	0
			1	1	
5	b	1	Total	O	0
			1	1	

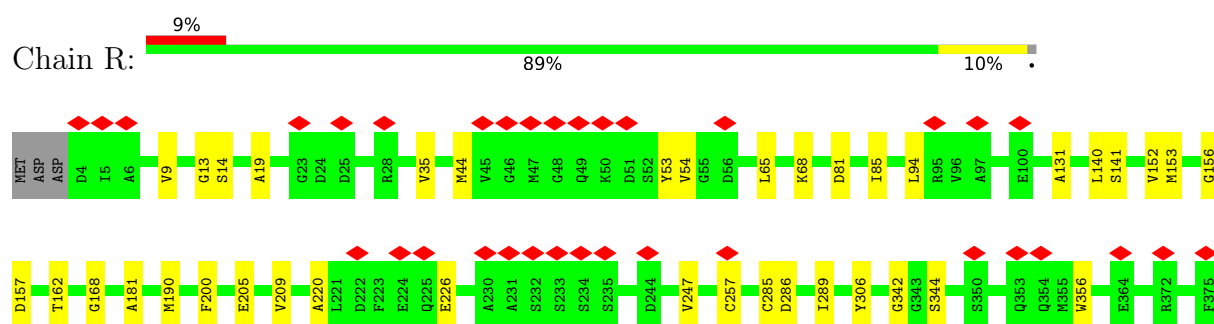
3 Residue-property plots

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.

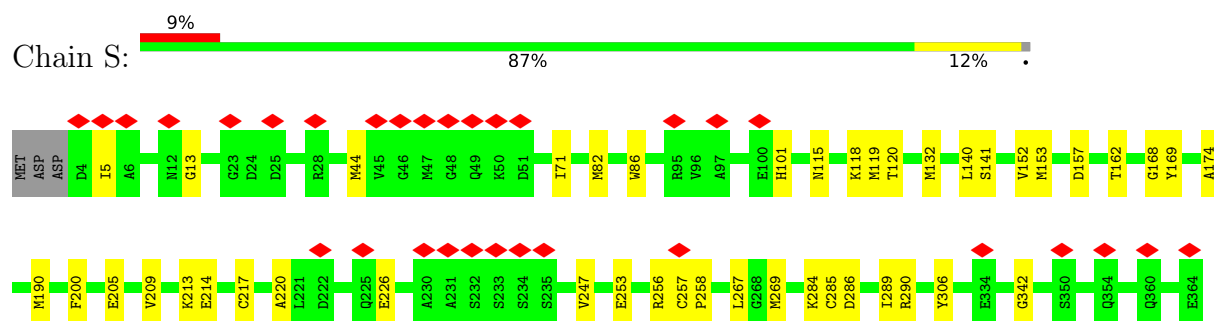
- Molecule 1: Actin, cytoplasmic 1



- Molecule 1: Actin, cytoplasmic 1

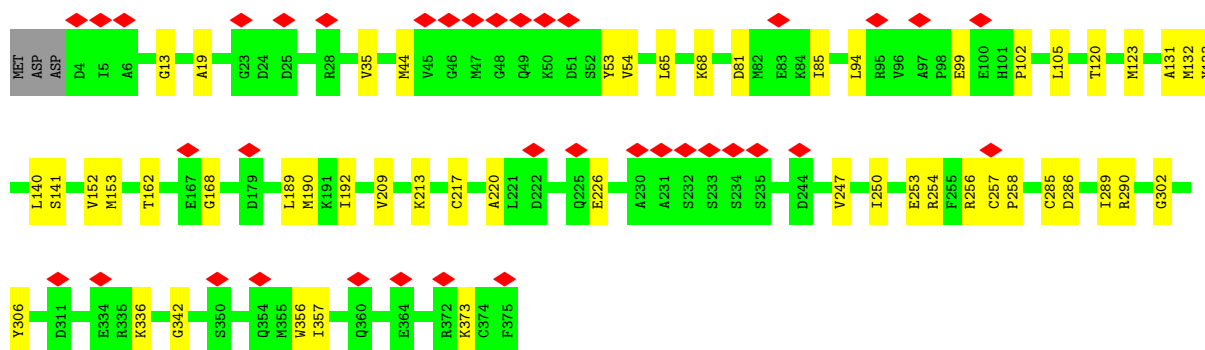
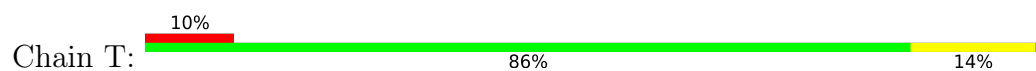


- Molecule 1: Actin, cytoplasmic 1

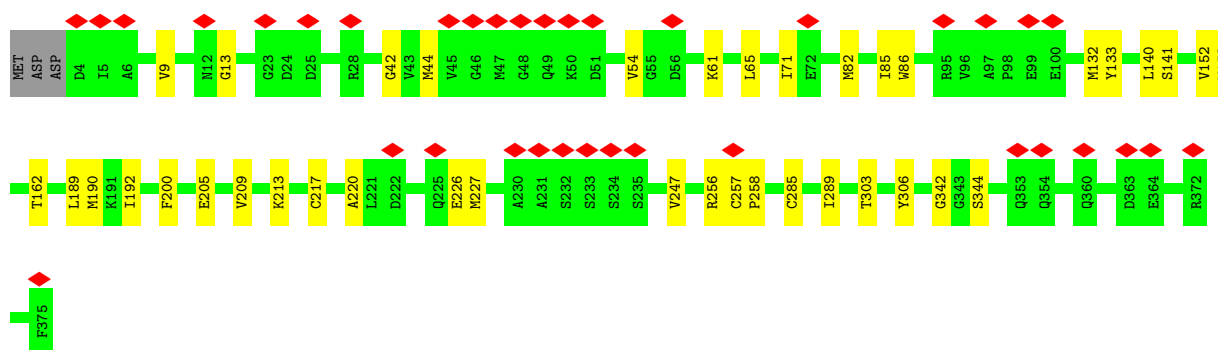
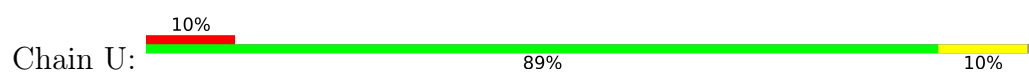




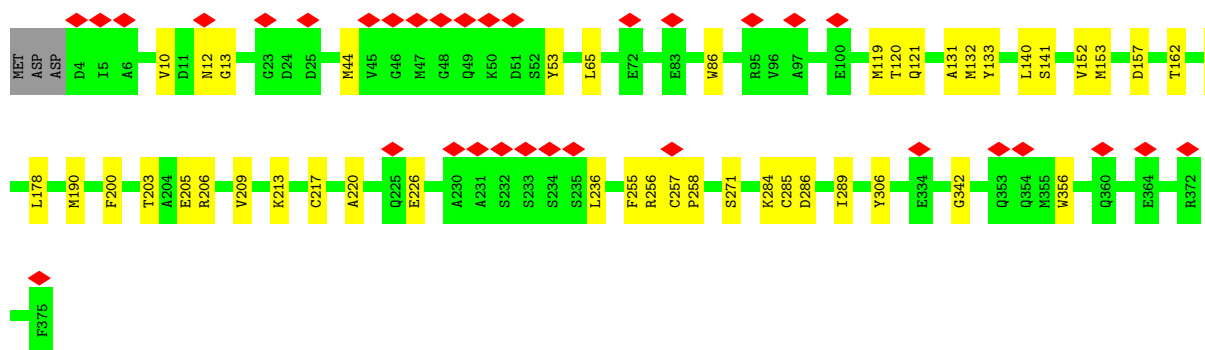
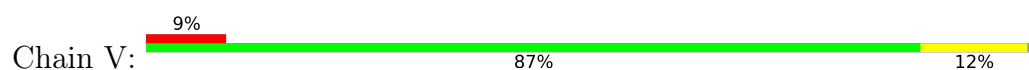
- Molecule 1: Actin, cytoplasmic 1



- Molecule 1: Actin, cytoplasmic 1

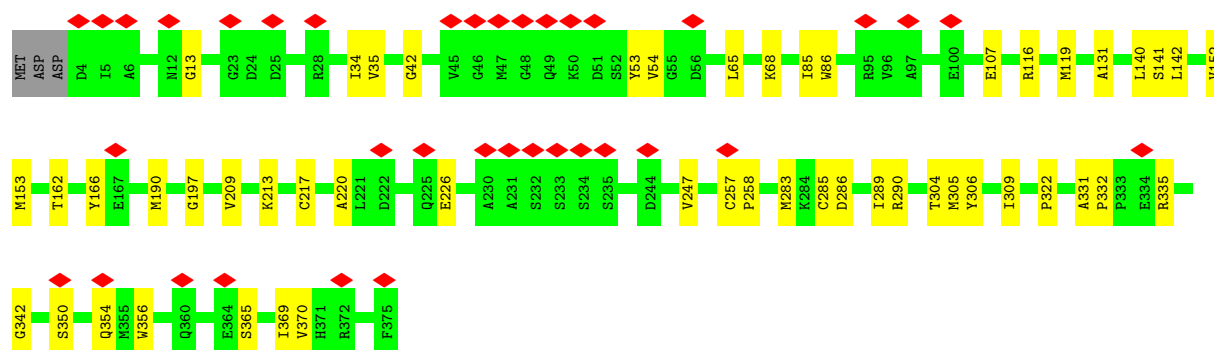


- Molecule 1: Actin, cytoplasmic 1



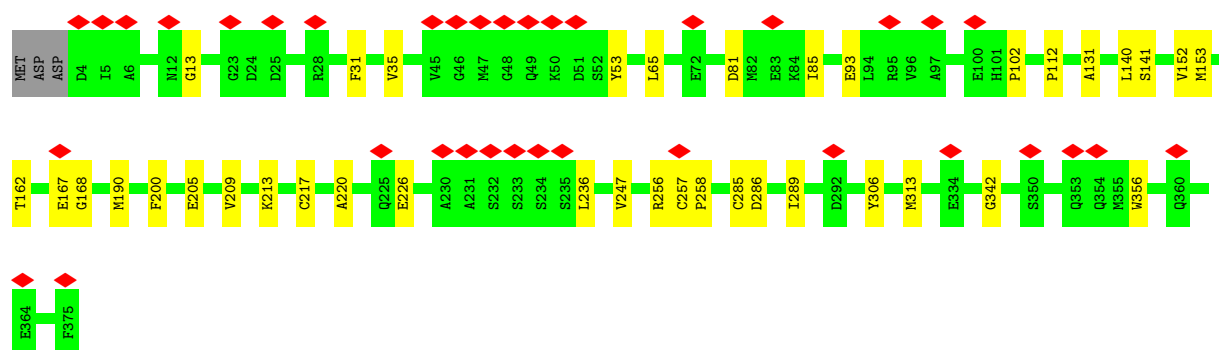
- Molecule 1: Actin, cytoplasmic 1

Chain W: 



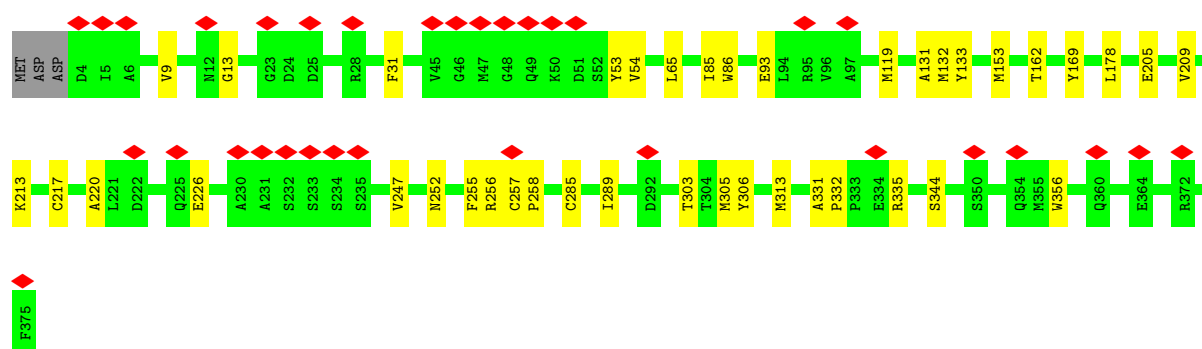
• Molecule 1: Actin, cytoplasmic 1

Chain X: 



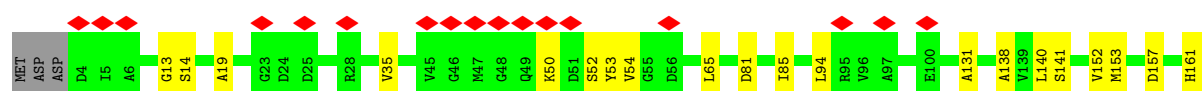
• Molecule 1: Actin, cytoplasmic 1

Chain Y: 



• Molecule 1: Actin, cytoplasmic 1

Chain Z: 













- Molecule 2: VopV

[illegible]



- Molecule 2: VopV

Chain h:

98%

MET	ILE	ASN	ASN	LEU	SER	ASN	ILE	GLN	ASN	THR	GLY	SER	ILE	SER	GLU	LEU	GLY	GLN	SER	PRO	ASN	LEU	THR	ILE	ASN	SER	ALA	ALA	PRO	PRO	PRO	SER	VAL	LEU	LEU	ARG	SER	GLU	LEU	ALA	ALA	ASN	SER	ASP	ASN	VAL	VAL	LEU	LEU	PRO	PRO	SER	ALA	THR	THR	GLN	GLN	ASP	CYS	PHE	GLU	GLN	GLY
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----







- Molecule 2: VopV

98%





Chain k: 

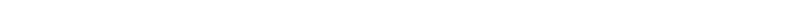
98%





ASP	LEU	ASN	THR	THR	ARG	LYS	GLU	TYR	GLU	THR	THR	LEU	VAL	SER	GLY	LEU	VAL	GLY	SER	ASN	SER	SER	SER	VAL	ILE	TRP	ALA	HIS	GLU	ARG	SER	MET	VAL	VAL	PRO	VAL	ALA	ASN	SER	SER	ASN	PHE	LYS	MET
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 2: VopV

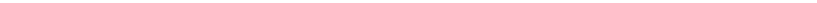
Chain 1:  98%

[illegible]





- Molecule 2: VopV

Chain n:  98%

[illegible]



TYR	GLU	VAL	SER	ASN	ASN	GLU	GLY
	THR	GLU	GLU	VAL	GLY	PRO	GLY
	THR	ASP	SER	GLU	GLY	ASN	THR
	LEU	GLY	SER	PRO	TYR	ALA	THR
	VAL	ILE	THR	VAL	PRO	ALA	GLN
	GLY	PHE	HIS	ALA	THR	ASP	ALA
	SER	LYS	HIS	ALA	THR	ASN	GLY
	GLY	GLU	SER	PRO	VAL	ASN	SER
	VAL	ALA	GLU	GLU	ASP	ALA	ASN
	SER	VAL	ILE	GLN	SER	VAL	VAL
ASN	VAL	LEU	LYS	ASN	ASN	GLY	GLU
	VAL	VAL	PHE	PRO	GLY	GLU	PRO
	THR	THR	HIS	SER	GLU	SER	ASN
	GLU	GLU	VAL	ALA	THR	VAL	VAL
	ASP	ASP	ASN	ASP	MET	PRO	ALA
	VAL	VAL	ALA	ALA	GLY	THR	THR
	LYS	LYS	GLU	PHE	TYR	HIS	PRO
	ASP	ASP	ILE	GLY	GLU	GLU	GLN
	THR	ILE	THR	GLY	ARG	GLY	ASN
	LEU	TRP	THR	PRO	ASP	SER	GLY
LYS	VAL	ALA	ASN	SER	VAL	VAL	SER
	ASN	ASN	ARG	ALA	THR	PRO	GLU
	PRO	ASP	PHE	PRO	PRO	GLU	GLU
	THR	GLY	THR	GLU	SER	GLN	THR
	GLN	GLU	SER	ILE	SER	SER	VAL
	LEU	LEU	THR	ASP	THR	GLY	ALA
	MET	ARG	LYS	ALA	ALA	GLY	GLN
	MET	PHE	VAL	GLY	ALA	PRO	GLY
	SER	ALA	ASN	VAL	SER	ALA	ASN
	GLY	LYS	GLY	SER	LYS	ARG	SER
GLY	HIS	LYS	GLY	LYS	TRP	PRO	GLY
	ALA	ILE	ILE	GLY	GLY	VAL	LEU
	THR	TRP	THR	GLY	SER	VAL	THR
	ASP	ASP	ASN	GLU	VAL	GLY	GLY
	THR	VAL	GLU	THR	GLY	THR	THR
	GLY	LYS	ILE	GLN	SER	ALA	ARG
	VAL	VAL	GLN	VAL	GLY	PRO	VAL
	SER	GLU	GLN	GLU	ALA	ARG	THR
	ASN	GLU	ALA	VAL	PRO	VAL	PRO
	THR	SER	SER	ASN	GLN	ILE	GLU
THR	THR	ARG	ASP	GLN	THR	GLY	LYS
	GLY	GLY	THR	THR	VAL	ILE	THR
	VAL	THR	VAL	THR	ALA	GLY	ALA
	ASN	ASN	ASN	ASN	VAL	GLY	ALA
	GLY	ASN	GLY	GLY	GLY	GLY	ALA
	THR	THR	THR	THR	THR	THR	THR
	ASN	THR	THR	THR	THR	THR	THR
	GLY	THR	THR	THR	THR	THR	THR
	VAL	THR	THR	THR	THR	THR	THR
	ASN	THR	THR	THR	THR	THR	THR
SER	THR	THR	THR	THR	THR	THR	THR
	GLY	THR	THR	THR	THR	THR	THR
	ASN	THR	THR	THR	THR	THR	THR
	GLY	THR	THR	THR	THR	THR	THR
	ASN	THR	THR	THR	THR	THR	THR
	GLY	THR	THR	THR	THR	THR	THR
	ASN	THR	THR	THR	THR	THR	THR
	GLY	THR	THR	THR	THR	THR	THR
	ASN	THR	THR	THR	THR	THR	THR
	GLY	THR	THR	THR	THR	THR	THR

4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-167°, rise=27.52 Å, axial sym=C1	Depositor
Number of segments used	140672	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 ($e^-/\text{Å}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.192	Depositor
Minimum map value	-0.697	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.045	Depositor
Recommended contour level	0.307	Depositor
Map size (Å)	265.6, 265.6, 424.96002	wwPDB
Map dimensions	320, 320, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83000004, 0.83000004, 0.83000004	Depositor

5 Model quality

5.1 Standard geometry

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

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	Q	0.13	0/2952	0.41	2/3995 (0.1%)
1	R	0.12	0/2952	0.38	0/3995
1	S	0.13	0/2952	0.41	2/3995 (0.1%)
1	T	0.12	0/2952	0.40	2/3995 (0.1%)
1	U	0.12	0/2952	0.39	2/3995 (0.1%)
1	V	0.14	0/2952	0.42	2/3995 (0.1%)
1	W	0.13	0/2952	0.40	0/3995
1	X	0.13	0/2952	0.40	2/3995 (0.1%)
1	Y	0.14	0/2952	0.42	2/3995 (0.1%)
1	Z	0.13	0/2952	0.41	0/3995
1	a	0.15	0/2952	0.43	0/3995
1	b	0.13	0/2952	0.41	2/3995 (0.1%)
2	c	0.18	0/374	0.55	0/505
2	d	0.16	0/374	0.54	0/505
2	e	0.17	0/374	0.52	0/505
2	f	0.16	0/374	0.51	0/505
2	g	0.16	0/374	0.52	0/505
2	h	0.17	0/374	0.52	0/505
2	i	0.16	0/374	0.52	0/505
2	j	0.16	0/374	0.50	0/505
2	k	0.17	0/374	0.55	0/505
2	l	0.52	0/374	0.87	0/505
2	m	0.16	0/374	0.52	0/505
2	n	0.16	0/374	0.53	0/505
All	All	0.14	0/39912	0.43	16/54000 (0.0%)

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
2	l	0	2

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	256	ARG	CA-C-N	5.99	127.20	119.78
1	Q	256	ARG	C-N-CA	5.99	127.20	119.78
1	b	256	ARG	CA-C-N	5.77	126.94	119.78
1	b	256	ARG	C-N-CA	5.77	126.94	119.78
1	S	256	ARG	CA-C-N	5.67	126.81	119.78

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	l	362	ARG	Sidechain
2	l	392	TYR	Sidechain

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	Q	2902	0	2870	30	0
1	R	2902	0	2870	22	0
1	S	2902	0	2870	31	0
1	T	2902	0	2870	29	0
1	U	2902	0	2870	21	0
1	V	2902	0	2870	29	0
1	W	2902	0	2870	32	0
1	X	2902	0	2870	23	0
1	Y	2902	0	2870	23	0
1	Z	2902	0	2870	26	0
1	a	2902	0	2870	29	0
1	b	2902	0	2870	20	0
2	c	367	0	362	5	0
2	d	367	0	362	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	e	367	0	362	4	0
2	f	367	0	362	4	0
2	g	367	0	362	6	0
2	h	367	0	362	3	0
2	i	367	0	362	4	0
2	j	367	0	362	4	0
2	k	367	0	362	7	0
2	l	367	0	362	3	0
2	m	367	0	362	4	0
2	n	367	0	362	2	0
3	Q	1	0	0	0	0
3	R	1	0	0	0	0
3	S	1	0	0	0	0
3	T	1	0	0	0	0
3	U	1	0	0	0	0
3	V	1	0	0	0	0
3	W	1	0	0	0	0
3	X	1	0	0	0	0
3	Y	1	0	0	0	0
3	Z	1	0	0	0	0
3	a	1	0	0	0	0
3	b	1	0	0	0	0
4	Q	31	0	13	3	0
4	R	31	0	13	2	0
4	S	31	0	13	4	0
4	T	31	0	13	2	0
4	U	31	0	13	2	0
4	V	31	0	13	3	0
4	W	31	0	13	2	0
4	X	31	0	13	2	0
4	Y	31	0	13	2	0
4	Z	31	0	13	2	0
4	a	31	0	13	2	0
4	b	31	0	13	2	0
5	Q	1	0	0	0	0
5	R	1	0	0	0	0
5	S	1	0	0	0	0
5	T	1	0	0	0	0
5	U	1	0	0	0	0
5	V	1	0	0	0	0
5	W	1	0	0	0	0
5	X	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	Y	1	0	0	0	0
5	Z	1	0	0	0	0
5	a	1	0	0	0	0
5	b	1	0	0	0	0
All	All	39624	0	38940	328	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 4.

The worst 5 of 328 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:V:121:GLN:HE22	2:h:356:GLU:HA	1.51	0.74
1:Y:257:CYS:HB3	1:Y:258:PRO:HD3	1.75	0.68
1:S:257:CYS:HB3	1:S:258:PRO:HD3	1.76	0.67
1:V:257:CYS:HB3	1:V:258:PRO:HD3	1.76	0.67
1:a:176:LEU:HD21	1:a:284:LYS:HZ1	1.62	0.64

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	Q	369/375 (98%)	363 (98%)	6 (2%)	0	100	100
1	R	369/375 (98%)	360 (98%)	9 (2%)	0	100	100
1	S	369/375 (98%)	360 (98%)	9 (2%)	0	100	100
1	T	369/375 (98%)	359 (97%)	10 (3%)	0	100	100
1	U	369/375 (98%)	357 (97%)	12 (3%)	0	100	100
1	V	369/375 (98%)	362 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	W	369/375 (98%)	360 (98%)	9 (2%)	0	100	100
1	X	369/375 (98%)	363 (98%)	6 (2%)	0	100	100
1	Y	369/375 (98%)	360 (98%)	9 (2%)	0	100	100
1	Z	369/375 (98%)	359 (97%)	10 (3%)	0	100	100
1	a	369/375 (98%)	359 (97%)	10 (3%)	0	100	100
1	b	369/375 (98%)	361 (98%)	8 (2%)	0	100	100
2	c	45/2402 (2%)	41 (91%)	4 (9%)	0	100	100
2	d	45/2402 (2%)	41 (91%)	4 (9%)	0	100	100
2	e	45/2402 (2%)	42 (93%)	3 (7%)	0	100	100
2	f	45/2402 (2%)	42 (93%)	3 (7%)	0	100	100
2	g	45/2402 (2%)	41 (91%)	4 (9%)	0	100	100
2	h	45/2402 (2%)	41 (91%)	4 (9%)	0	100	100
2	i	45/2402 (2%)	42 (93%)	3 (7%)	0	100	100
2	j	45/2402 (2%)	41 (91%)	4 (9%)	0	100	100
2	k	45/2402 (2%)	41 (91%)	4 (9%)	0	100	100
2	l	45/2402 (2%)	42 (93%)	3 (7%)	0	100	100
2	m	45/2402 (2%)	41 (91%)	4 (9%)	0	100	100
2	n	45/2402 (2%)	41 (91%)	4 (9%)	0	100	100
All	All	4968/33324 (15%)	4819 (97%)	149 (3%)	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	Q	314/317 (99%)	312 (99%)	2 (1%)	78	88
1	R	314/317 (99%)	312 (99%)	2 (1%)	78	88
1	S	314/317 (99%)	314 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	T	314/317 (99%)	313 (100%)	1 (0%)	86	91
1	U	314/317 (99%)	312 (99%)	2 (1%)	78	88
1	V	314/317 (99%)	314 (100%)	0	100	100
1	W	314/317 (99%)	311 (99%)	3 (1%)	68	84
1	X	314/317 (99%)	312 (99%)	2 (1%)	78	88
1	Y	314/317 (99%)	311 (99%)	3 (1%)	68	84
1	Z	314/317 (99%)	314 (100%)	0	100	100
1	a	314/317 (99%)	312 (99%)	2 (1%)	78	88
1	b	314/317 (99%)	311 (99%)	3 (1%)	68	84
2	c	40/1904 (2%)	39 (98%)	1 (2%)	42	72
2	d	40/1904 (2%)	38 (95%)	2 (5%)	22	56
2	e	40/1904 (2%)	38 (95%)	2 (5%)	22	56
2	f	40/1904 (2%)	38 (95%)	2 (5%)	22	56
2	g	40/1904 (2%)	40 (100%)	0	100	100
2	h	40/1904 (2%)	40 (100%)	0	100	100
2	i	40/1904 (2%)	38 (95%)	2 (5%)	22	56
2	j	40/1904 (2%)	39 (98%)	1 (2%)	42	72
2	k	40/1904 (2%)	39 (98%)	1 (2%)	42	72
2	l	40/1904 (2%)	40 (100%)	0	100	100
2	m	40/1904 (2%)	39 (98%)	1 (2%)	42	72
2	n	40/1904 (2%)	39 (98%)	1 (2%)	42	72
All	All	4248/26652 (16%)	4215 (99%)	33 (1%)	70	86

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	i	397	ARG
2	j	389	THR
2	n	384	ASP
1	Y	178	LEU
1	X	236	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	X	173	HIS
1	Y	263	GLN
1	b	173	HIS
1	Y	92	ASN
1	Z	92	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

12 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	HIC	X	73	1	10,11,12	0.47	0	9,14,16	0.53	0
1	HIC	V	73	1	10,11,12	0.47	0	9,14,16	0.51	0
1	HIC	Y	73	1	10,11,12	0.48	0	9,14,16	0.56	0
1	HIC	T	73	1	10,11,12	0.48	0	9,14,16	0.53	0
1	HIC	R	73	1	10,11,12	0.47	0	9,14,16	0.52	0
1	HIC	a	73	1	10,11,12	0.49	0	9,14,16	0.52	0
1	HIC	Z	73	1	10,11,12	0.48	0	9,14,16	0.57	0
1	HIC	Q	73	1	10,11,12	0.48	0	9,14,16	0.55	0
1	HIC	W	73	1	10,11,12	0.48	0	9,14,16	0.52	0
1	HIC	U	73	1	10,11,12	0.48	0	9,14,16	0.59	0
1	HIC	S	73	1	10,11,12	0.48	0	9,14,16	0.56	0
1	HIC	b	73	1	10,11,12	0.47	0	9,14,16	0.54	0

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
1	HIC	X	73	1	-	0/5/6/8	0/1/1/1
1	HIC	V	73	1	-	0/5/6/8	0/1/1/1
1	HIC	Y	73	1	-	0/5/6/8	0/1/1/1
1	HIC	T	73	1	-	0/5/6/8	0/1/1/1
1	HIC	R	73	1	-	0/5/6/8	0/1/1/1
1	HIC	a	73	1	-	0/5/6/8	0/1/1/1
1	HIC	Z	73	1	-	0/5/6/8	0/1/1/1
1	HIC	Q	73	1	-	0/5/6/8	0/1/1/1
1	HIC	W	73	1	-	0/5/6/8	0/1/1/1
1	HIC	U	73	1	-	0/5/6/8	0/1/1/1
1	HIC	S	73	1	-	0/5/6/8	0/1/1/1
1	HIC	b	73	1	-	0/5/6/8	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	$\# Z > 2$
4	ANP	U	802	3	33,33,33	2.27	5 (15%)	45,52,52	1.16	3 (6%)
4	ANP	V	802	3	33,33,33	2.28	5 (15%)	45,52,52	1.19	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ANP	S	802	3	33,33,33	2.29	5 (15%)	45,52,52	1.18	3 (6%)
4	ANP	Y	802	3	33,33,33	2.27	5 (15%)	45,52,52	1.17	3 (6%)
4	ANP	Q	802	3	33,33,33	2.26	5 (15%)	45,52,52	1.19	3 (6%)
4	ANP	X	802	3	33,33,33	2.29	5 (15%)	45,52,52	1.17	3 (6%)
4	ANP	T	802	3	33,33,33	2.28	5 (15%)	45,52,52	1.18	3 (6%)
4	ANP	b	802	3	33,33,33	2.30	5 (15%)	45,52,52	1.17	3 (6%)
4	ANP	R	802	3	33,33,33	2.28	5 (15%)	45,52,52	1.17	3 (6%)
4	ANP	W	802	3	33,33,33	2.28	5 (15%)	45,52,52	1.17	3 (6%)
4	ANP	a	802	3	33,33,33	2.27	5 (15%)	45,52,52	1.17	3 (6%)
4	ANP	Z	802	3	33,33,33	2.29	5 (15%)	45,52,52	1.16	3 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ANP	U	802	3	-	3/18/38/38	0/3/3/3
4	ANP	V	802	3	-	4/18/38/38	0/3/3/3
4	ANP	S	802	3	-	2/18/38/38	0/3/3/3
4	ANP	Y	802	3	-	2/18/38/38	0/3/3/3
4	ANP	Q	802	3	-	2/18/38/38	0/3/3/3
4	ANP	X	802	3	-	2/18/38/38	0/3/3/3
4	ANP	T	802	3	-	2/18/38/38	0/3/3/3
4	ANP	b	802	3	-	2/18/38/38	0/3/3/3
4	ANP	R	802	3	-	3/18/38/38	0/3/3/3
4	ANP	W	802	3	-	2/18/38/38	0/3/3/3
4	ANP	a	802	3	-	2/18/38/38	0/3/3/3
4	ANP	Z	802	3	-	3/18/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	b	802	ANP	PB-O3A	8.85	1.70	1.59
4	Z	802	ANP	PB-O3A	8.81	1.70	1.59
4	S	802	ANP	PB-O3A	8.81	1.70	1.59
4	X	802	ANP	PB-O3A	8.80	1.70	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	V	802	ANP	PB-O3A	8.78	1.70	1.59

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	V	802	ANP	O2B-PB-O1B	4.75	120.05	109.87
4	R	802	ANP	O2B-PB-O1B	4.72	119.99	109.87
4	U	802	ANP	O2B-PB-O1B	4.68	119.92	109.87
4	b	802	ANP	O2B-PB-O1B	4.68	119.91	109.87
4	Q	802	ANP	O2B-PB-O1B	4.68	119.90	109.87

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	Q	802	ANP	PB-N3B-PG-O1G
4	Q	802	ANP	PG-N3B-PB-O1B
4	R	802	ANP	PB-N3B-PG-O1G
4	S	802	ANP	PB-N3B-PG-O1G
4	S	802	ANP	PG-N3B-PB-O1B

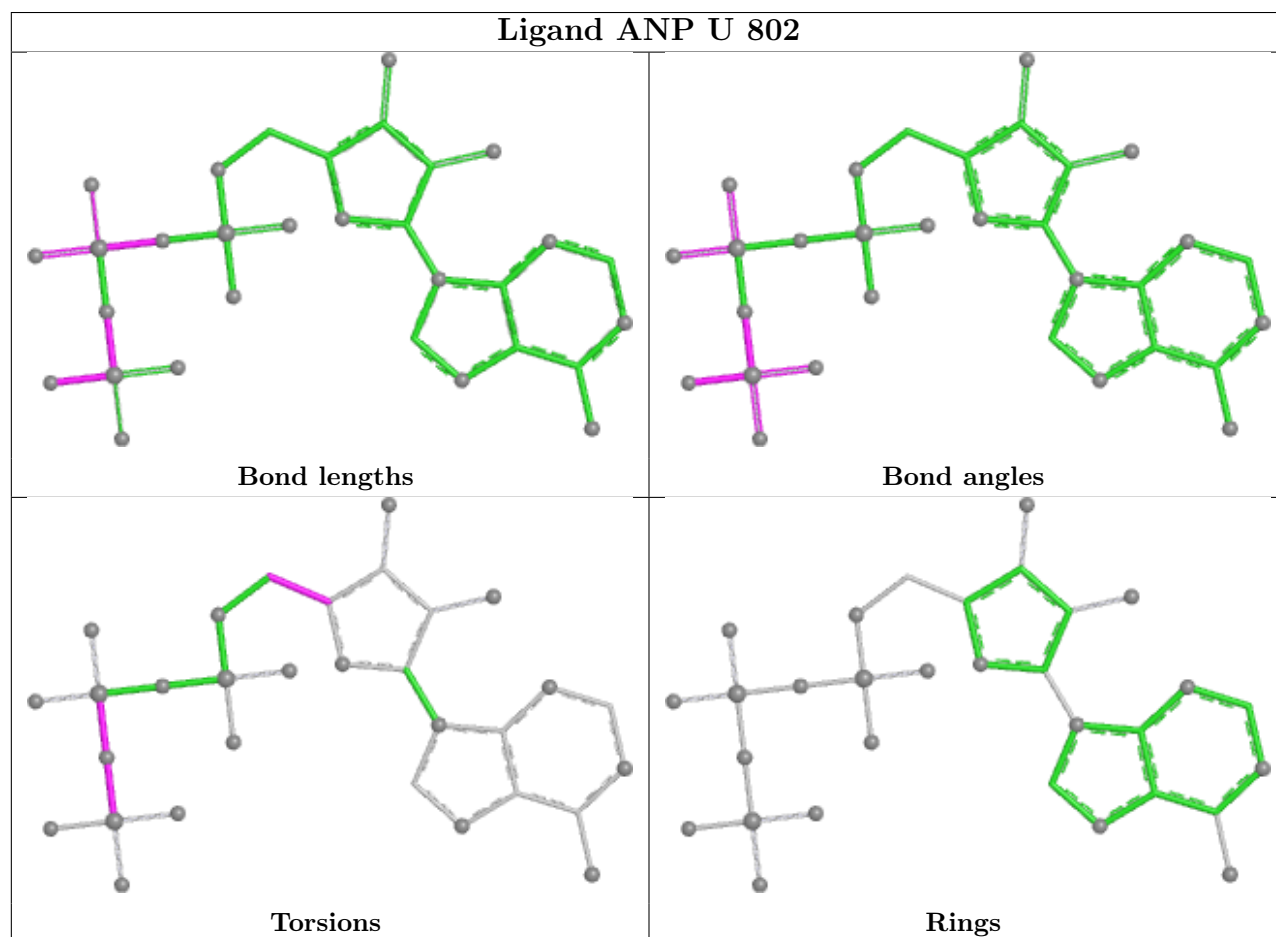
There are no ring outliers.

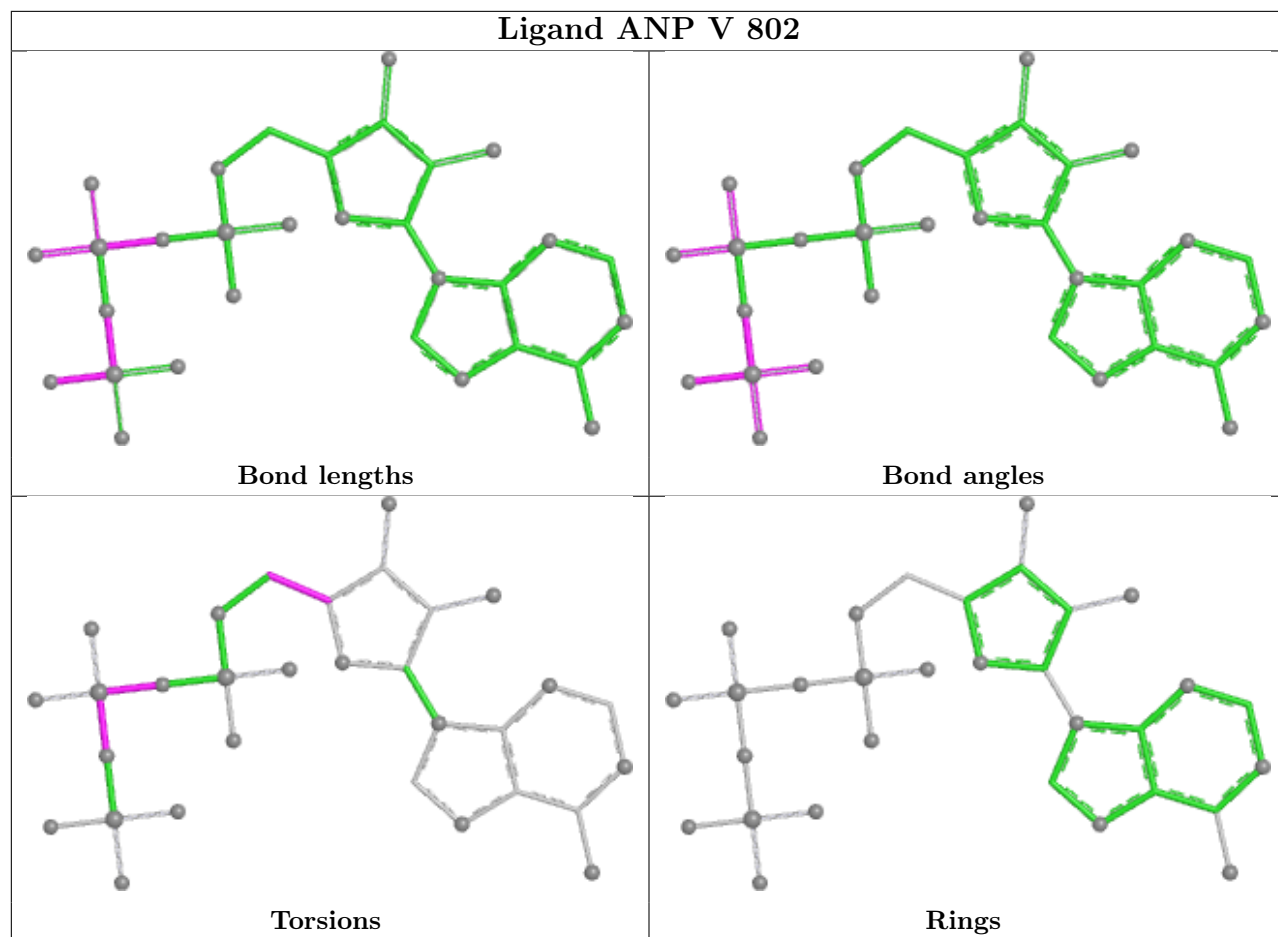
12 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	U	802	ANP	2	0
4	V	802	ANP	3	0
4	S	802	ANP	4	0
4	Y	802	ANP	2	0
4	Q	802	ANP	3	0
4	X	802	ANP	2	0
4	T	802	ANP	2	0
4	b	802	ANP	2	0
4	R	802	ANP	2	0
4	W	802	ANP	2	0
4	a	802	ANP	2	0
4	Z	802	ANP	2	0

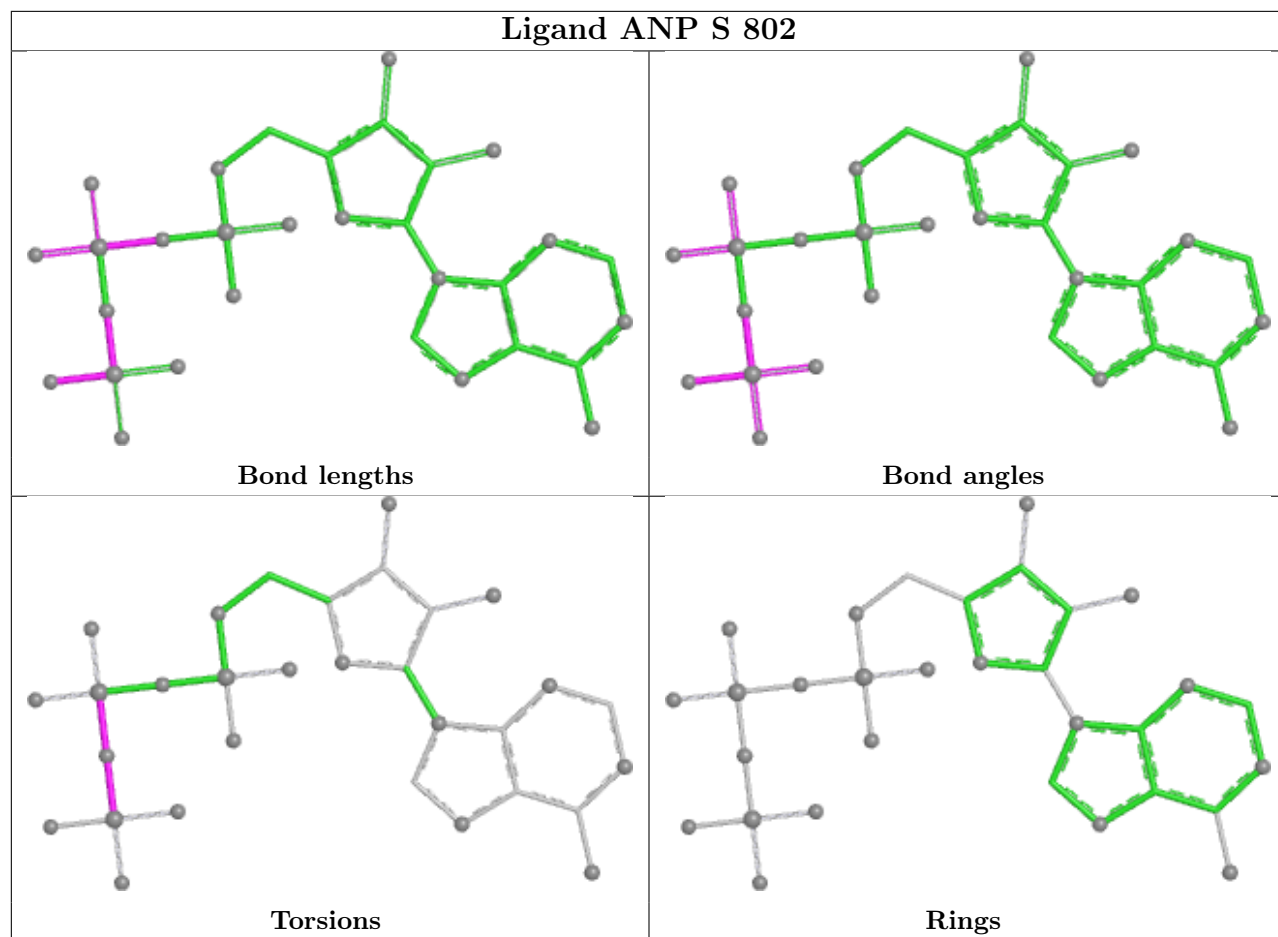
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

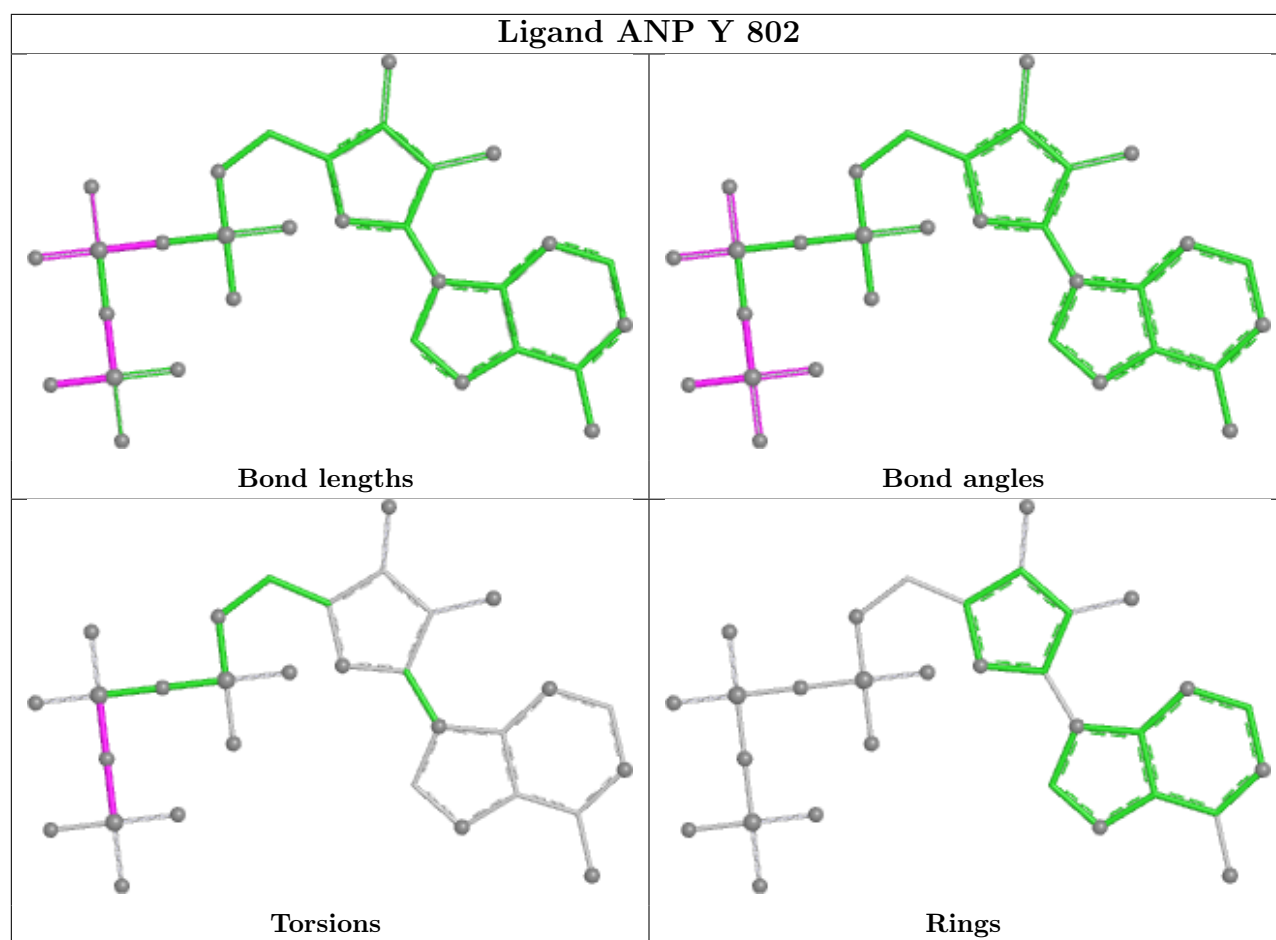
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted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

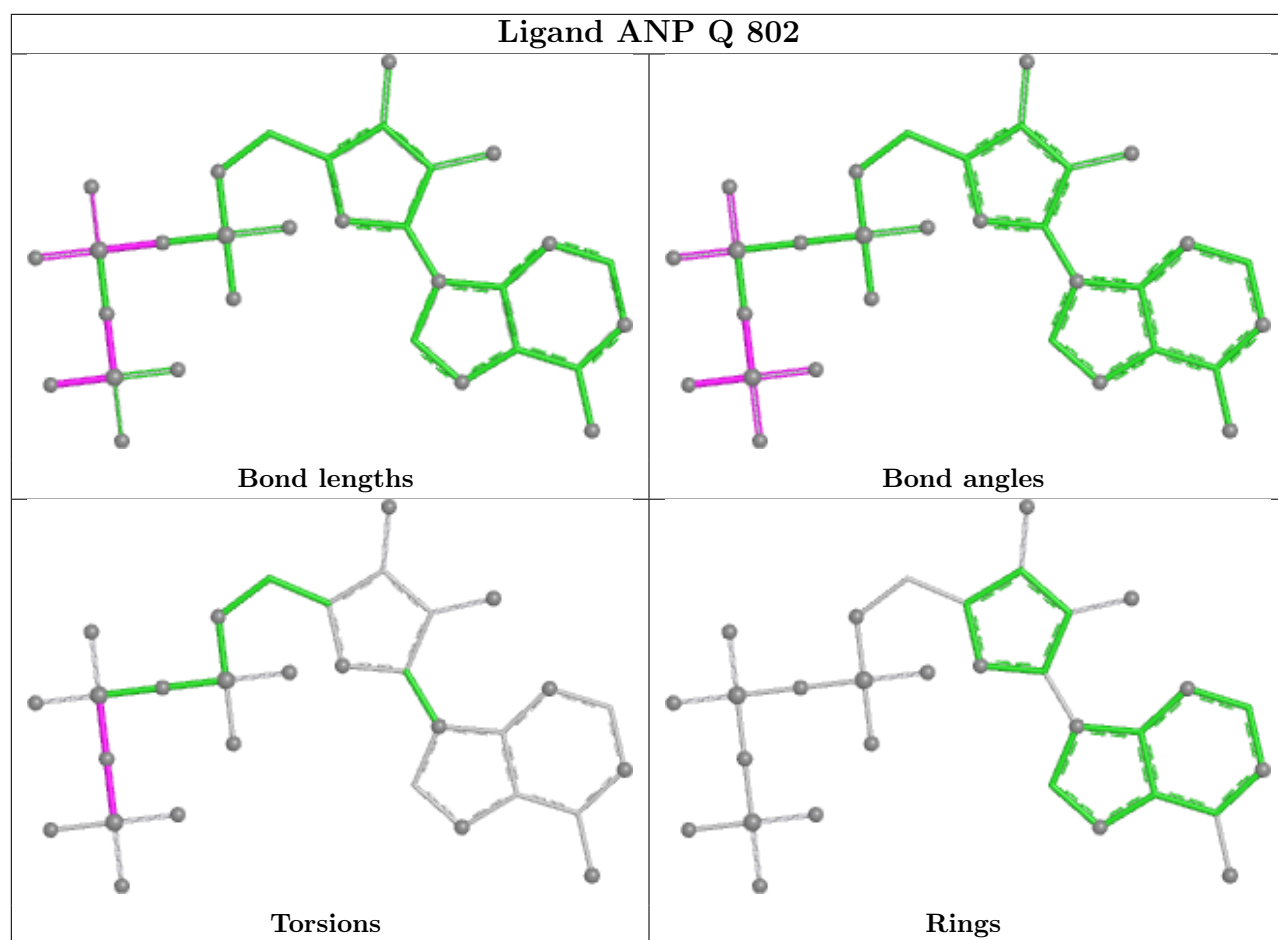


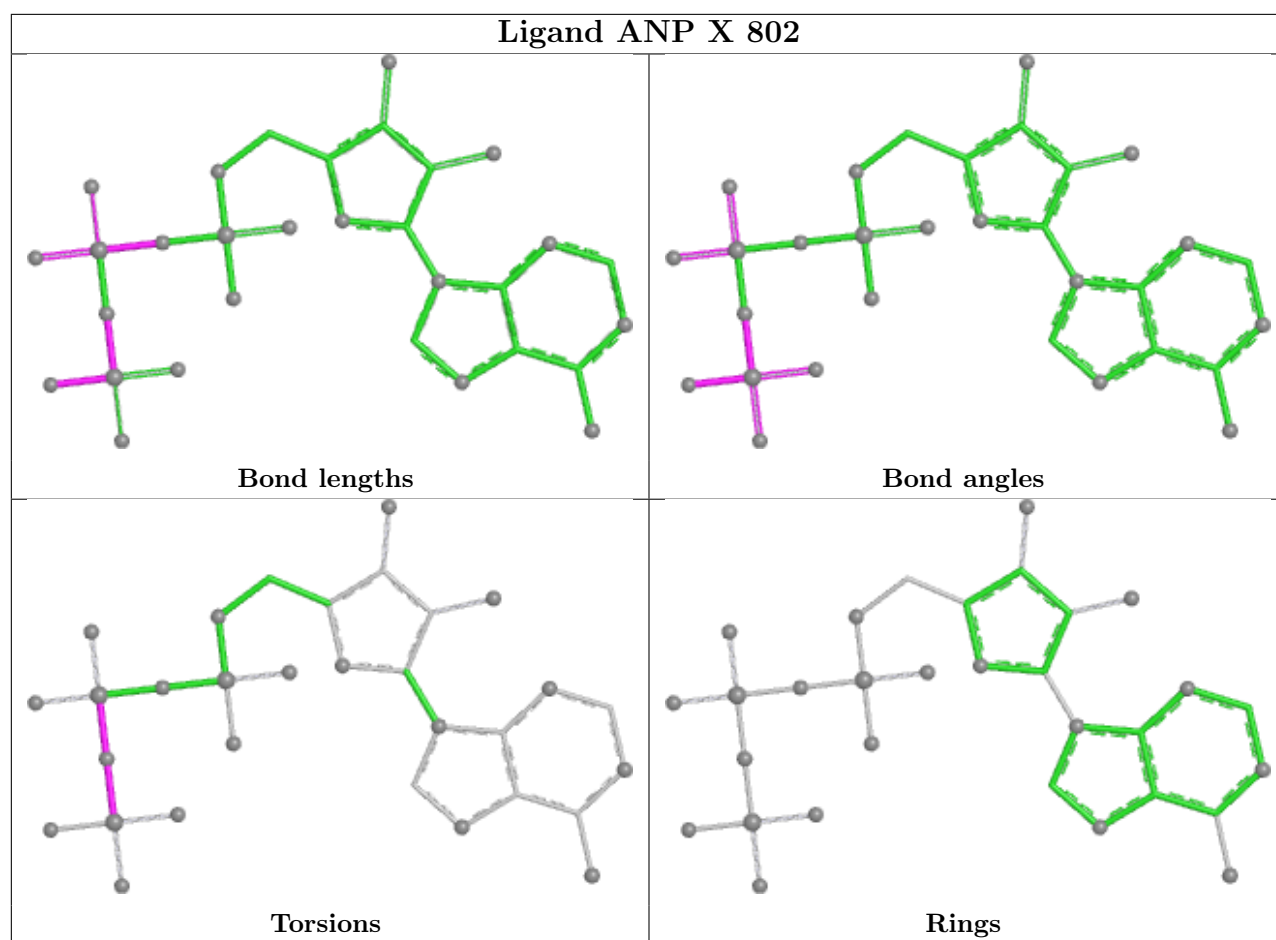


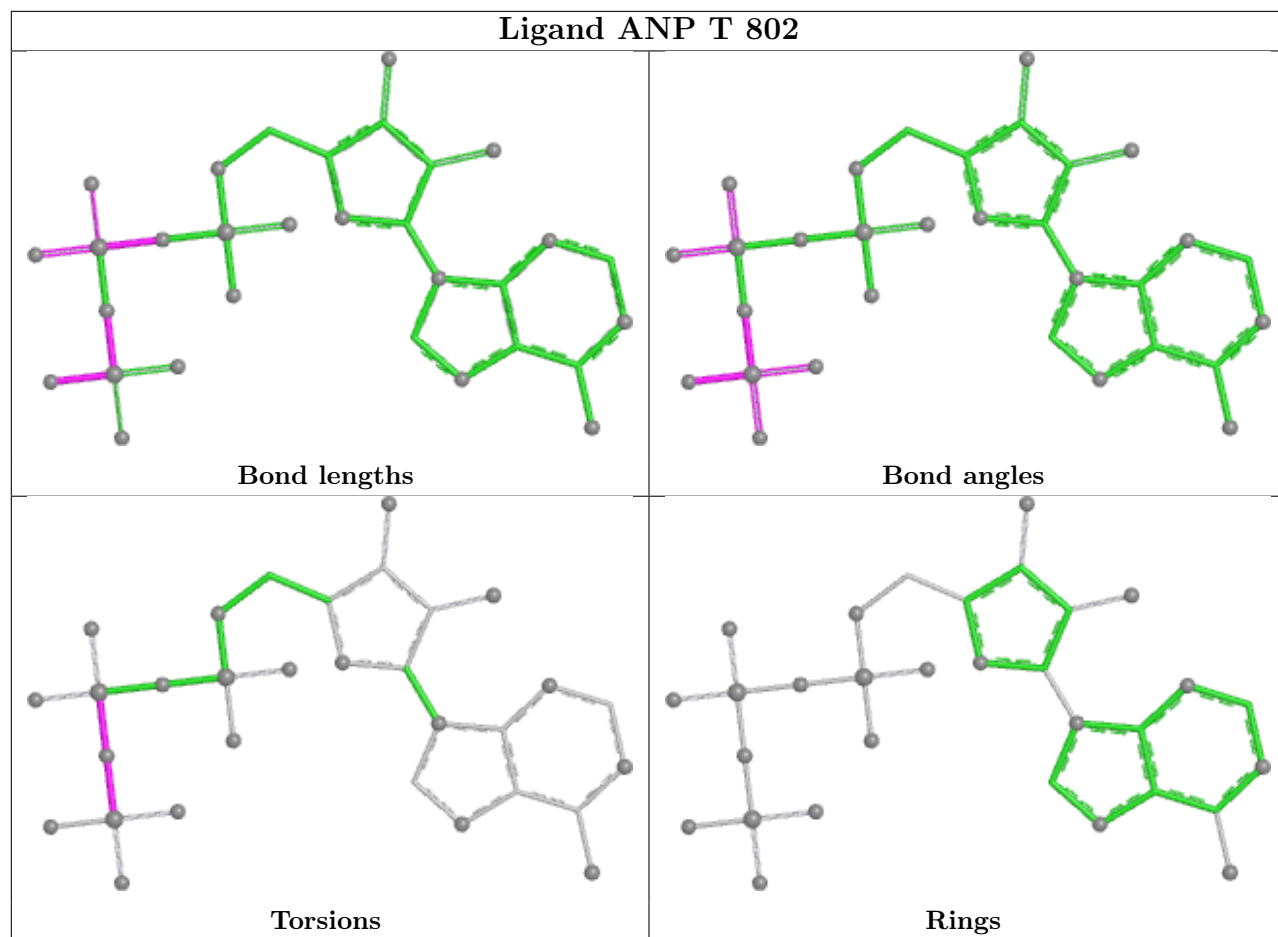
Ligand ANP S 802



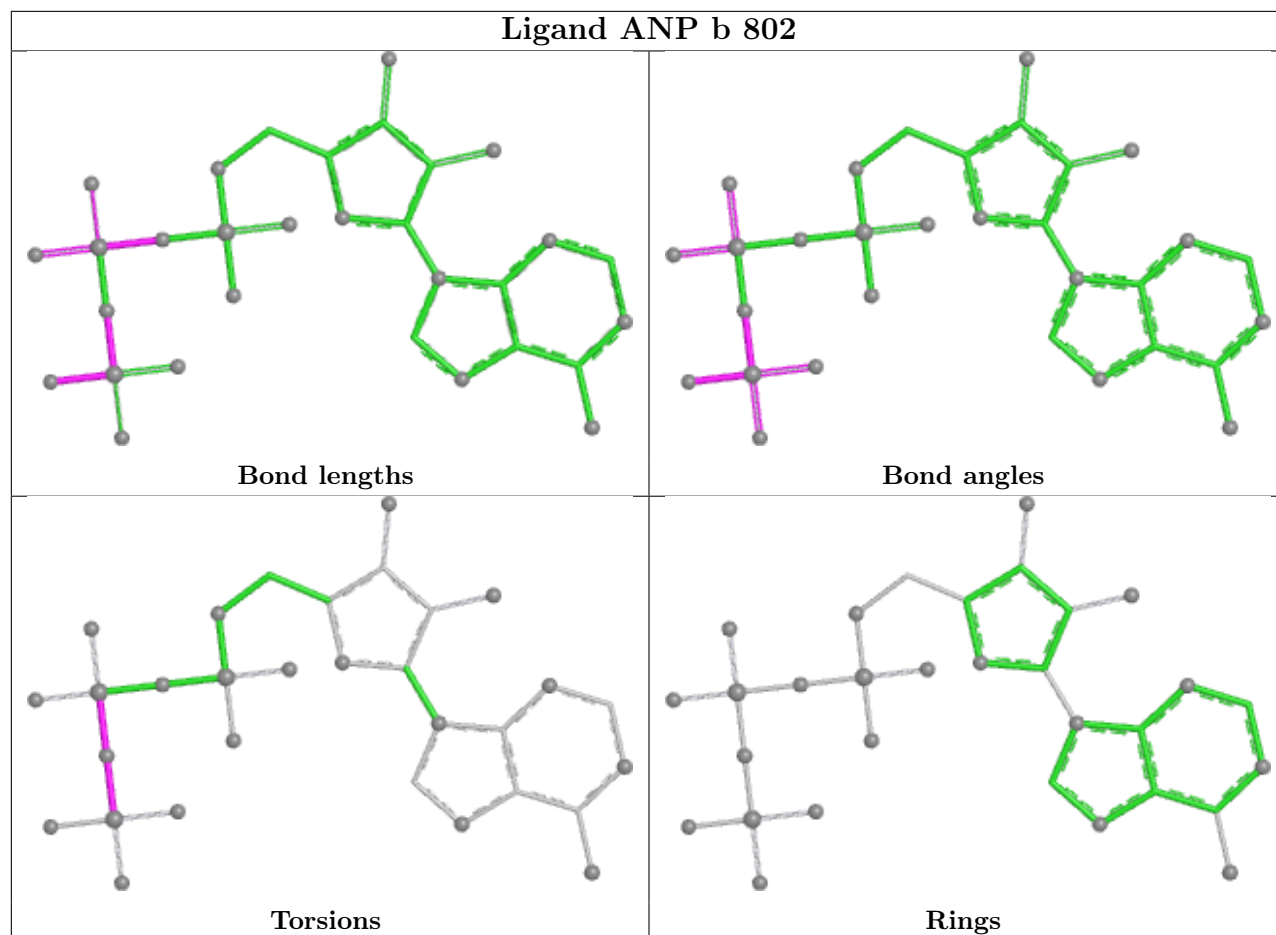


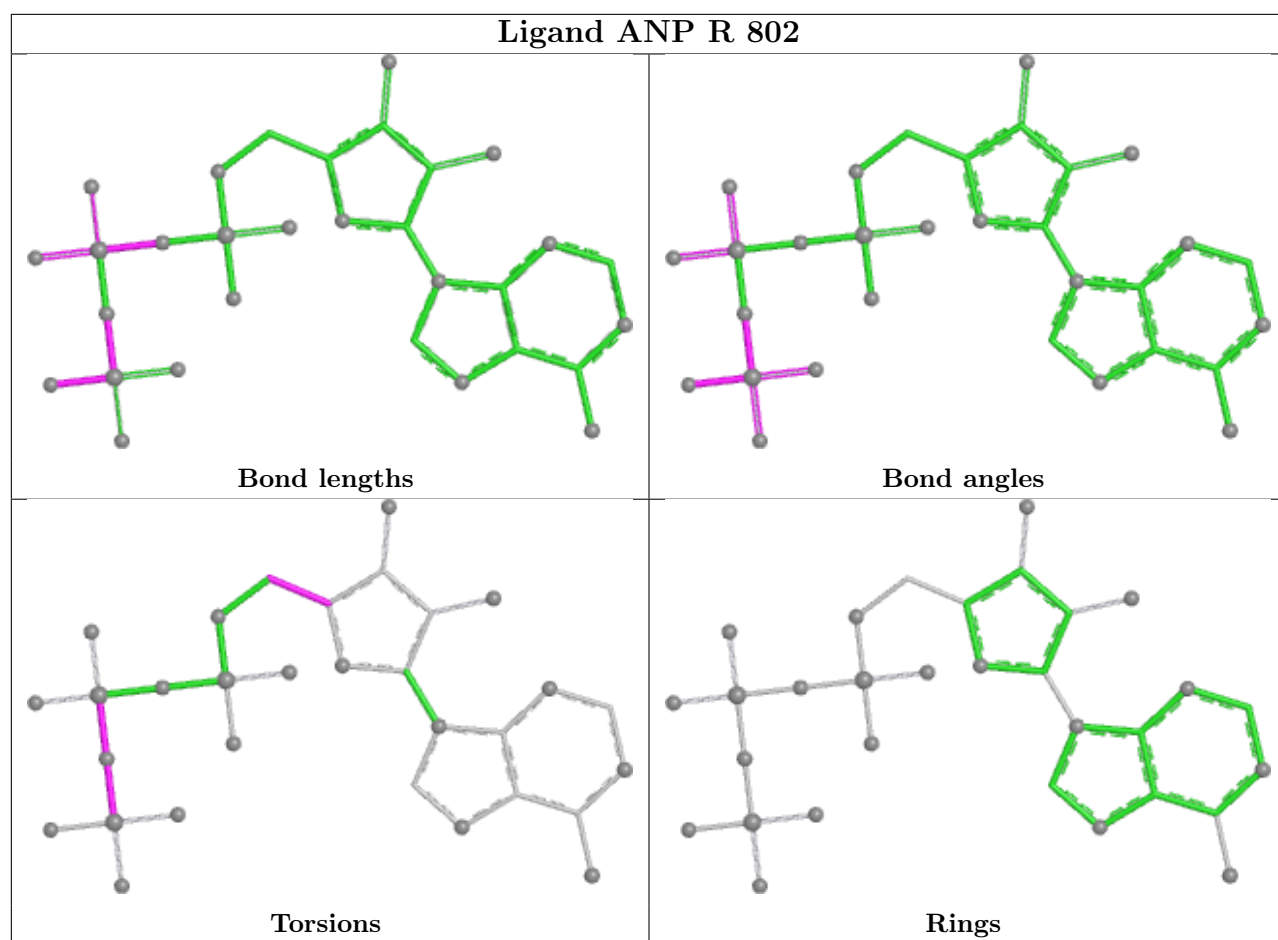


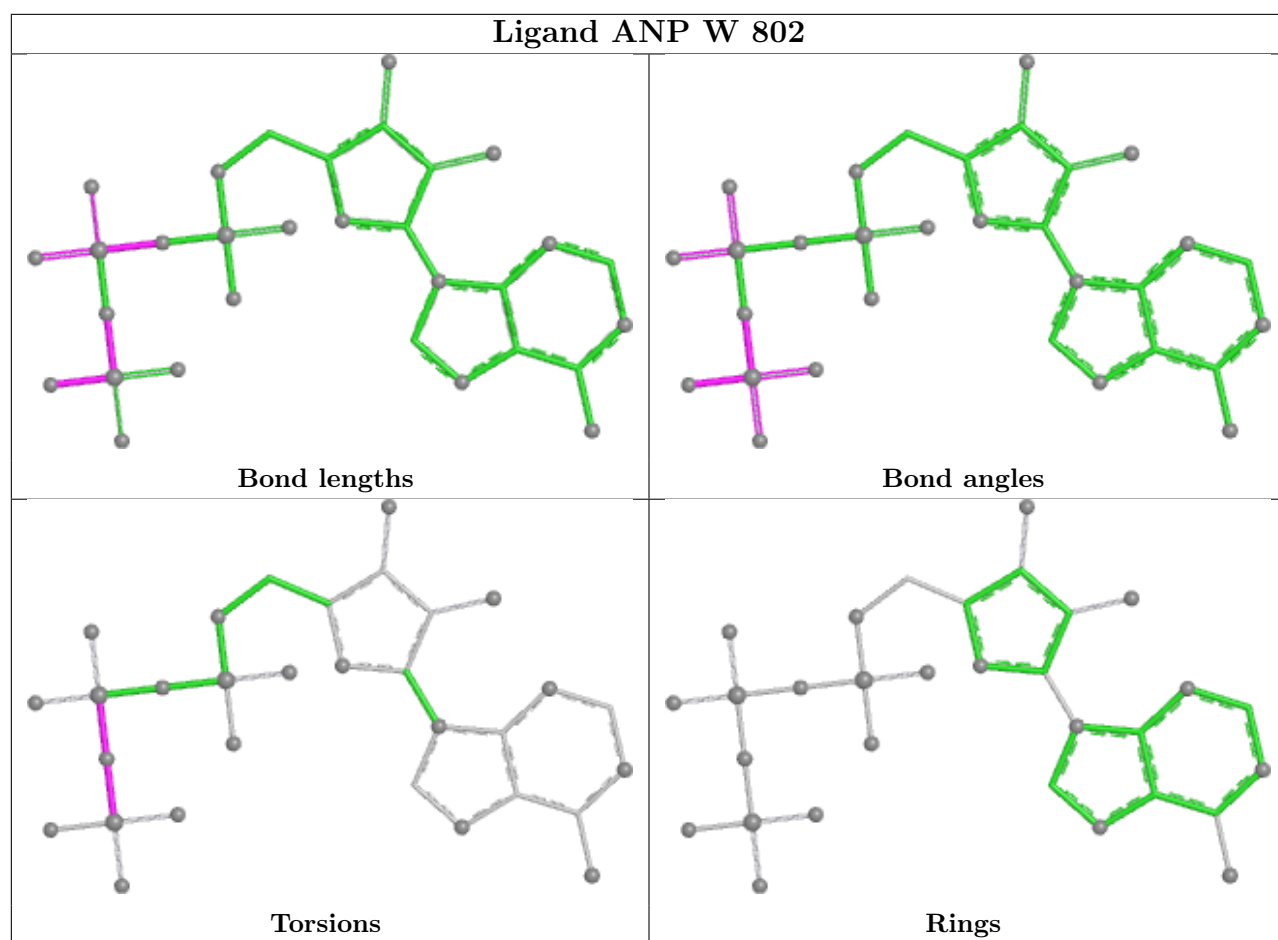




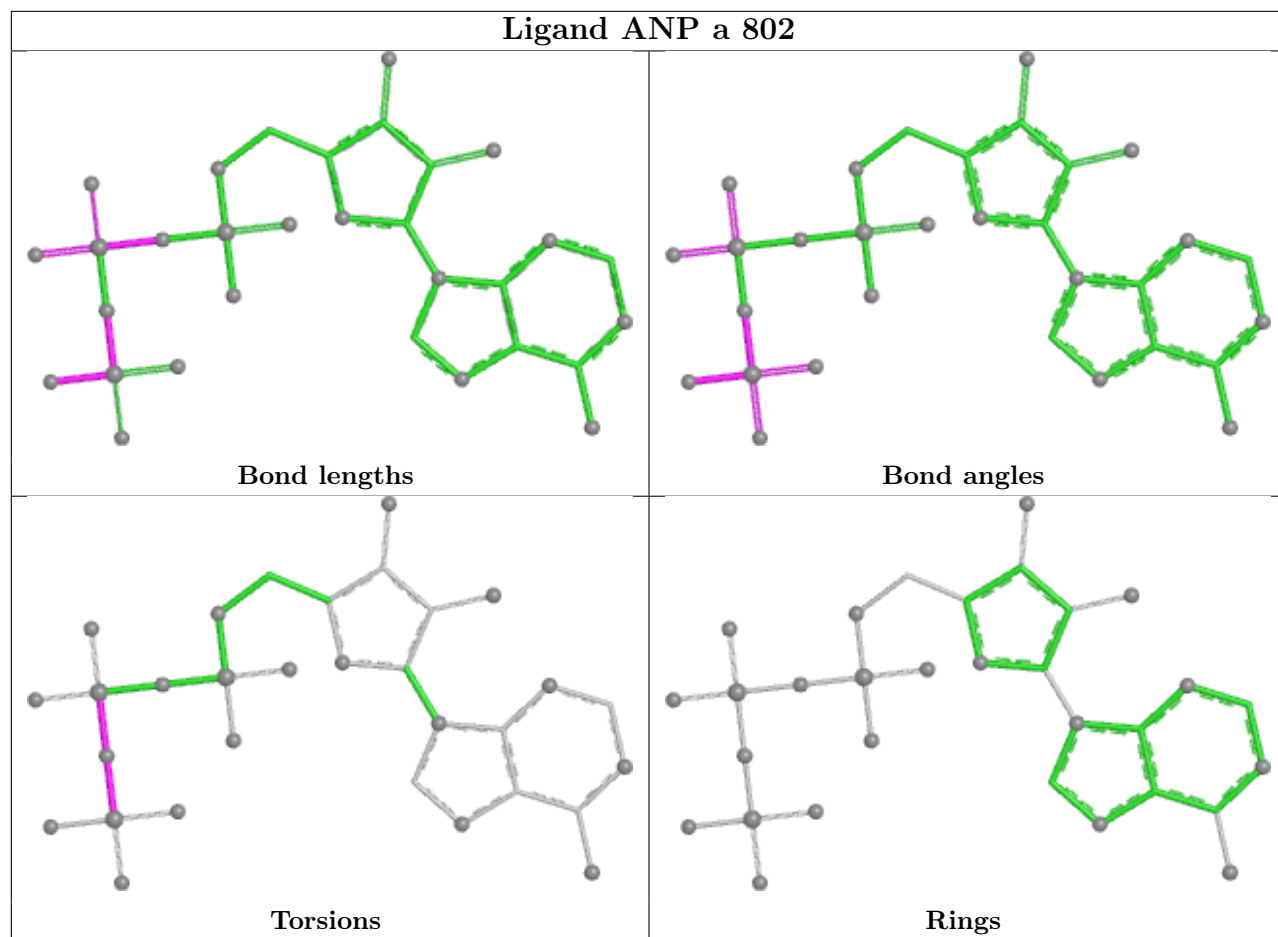
Ligand ANP b 802

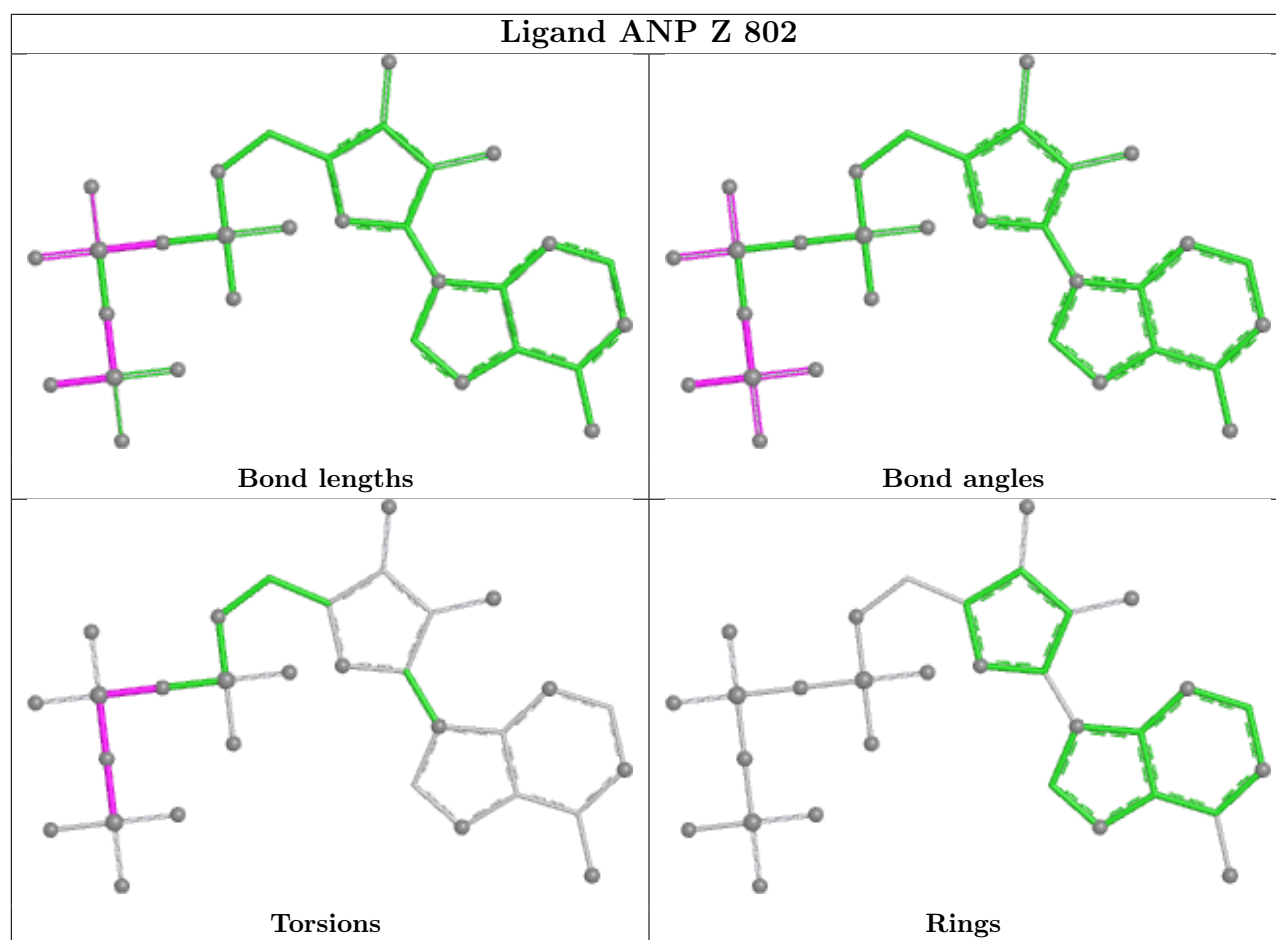






Ligand ANP a 802





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.

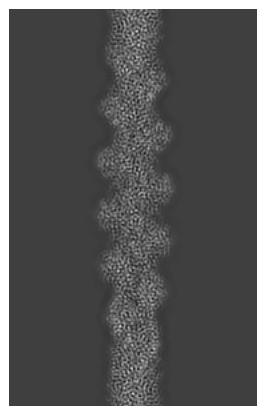
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71108. These allow visual inspection of the internal detail of the map and identification of artifacts.

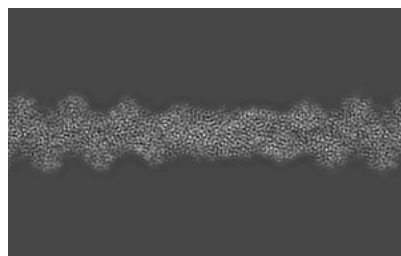
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

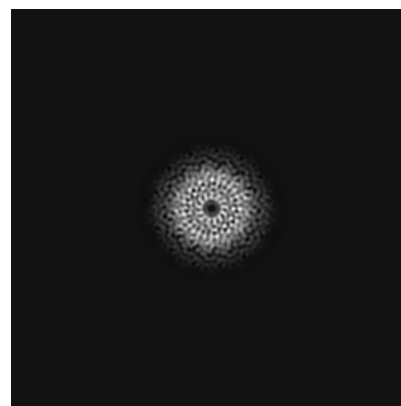
6.1.1 Primary map



X

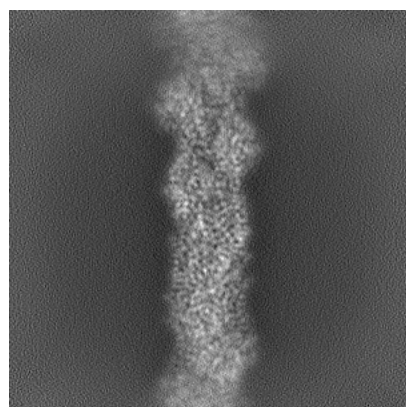


Y

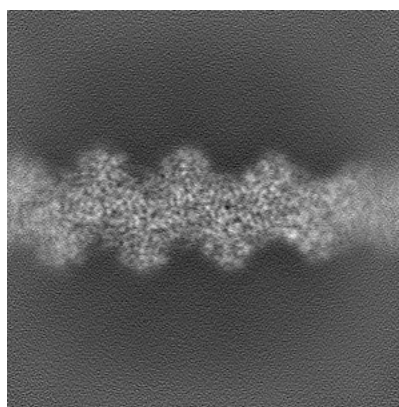


Z

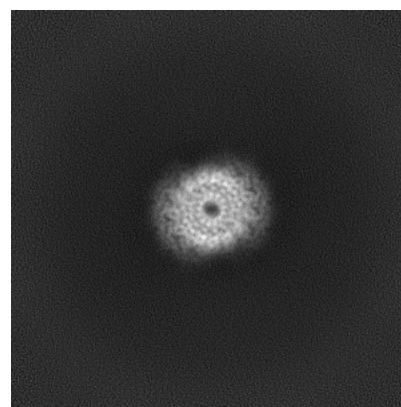
6.1.2 Raw map



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: 160

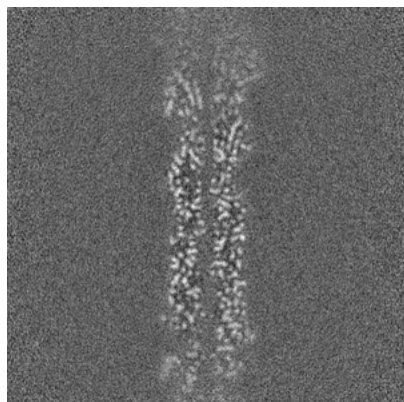


Y Index: 160

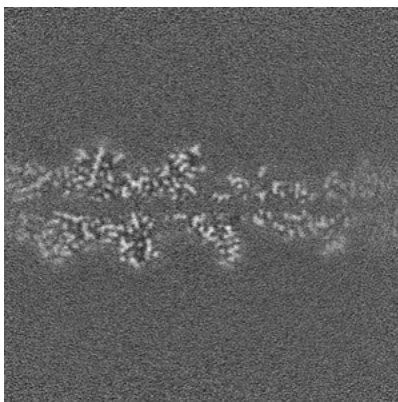


Z Index: 256

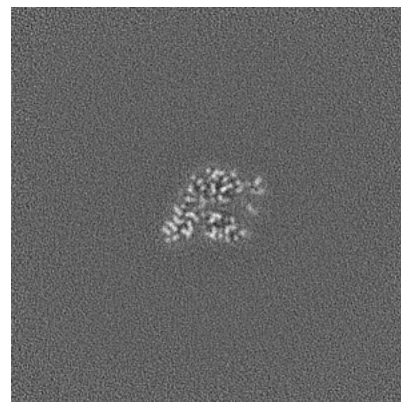
6.2.2 Raw map



X Index: 160



Y Index: 160

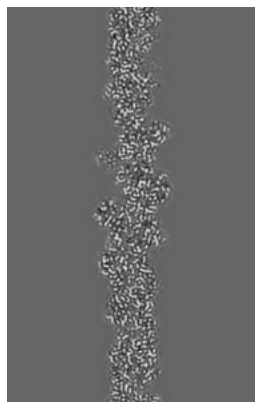


Z Index: 160

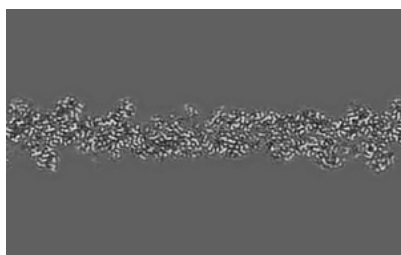
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

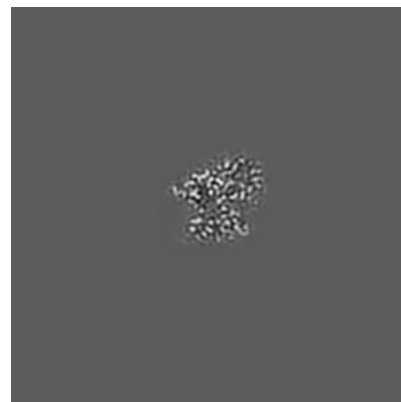
6.3.1 Primary map



X Index: 152

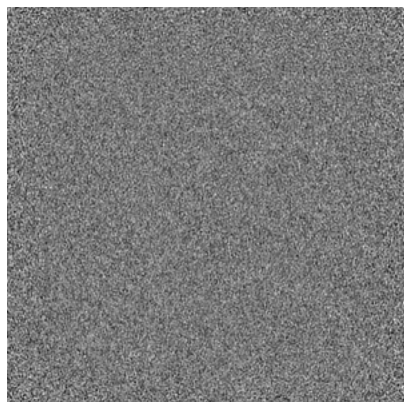


Y Index: 170

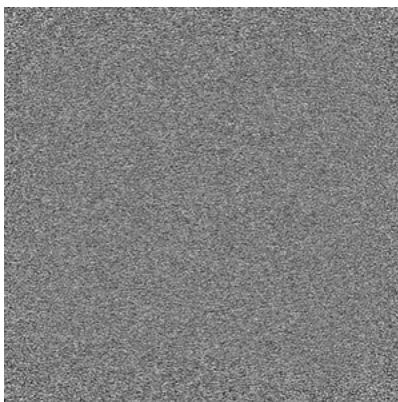


Z Index: 143

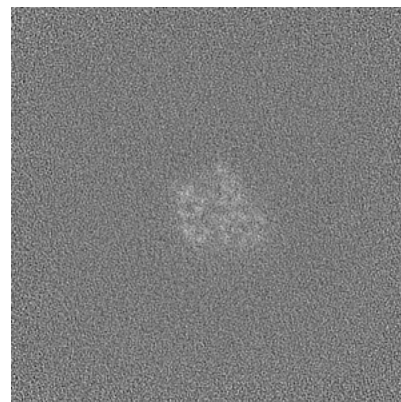
6.3.2 Raw map



X Index: 0



Y Index: 0

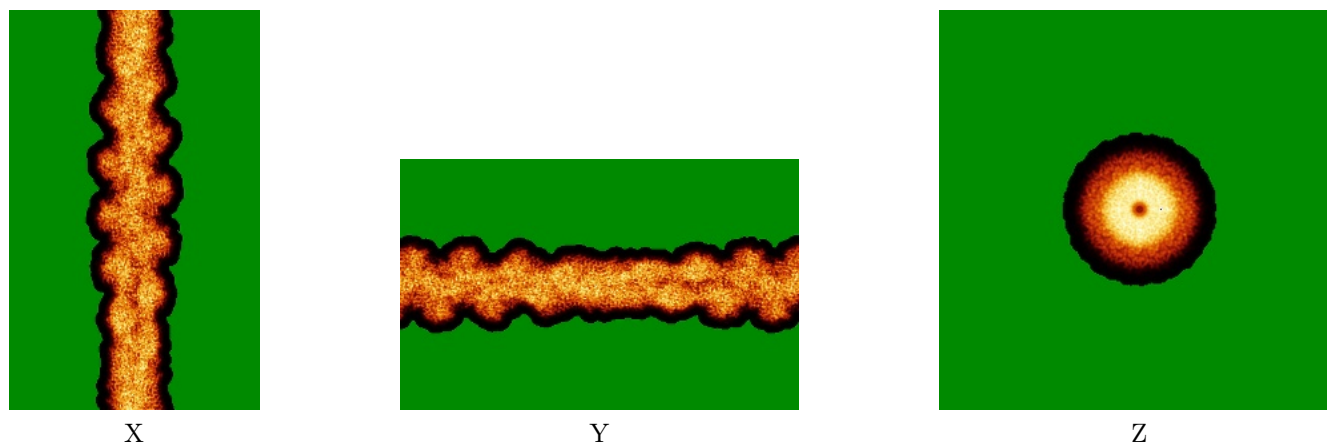


Z Index: 0

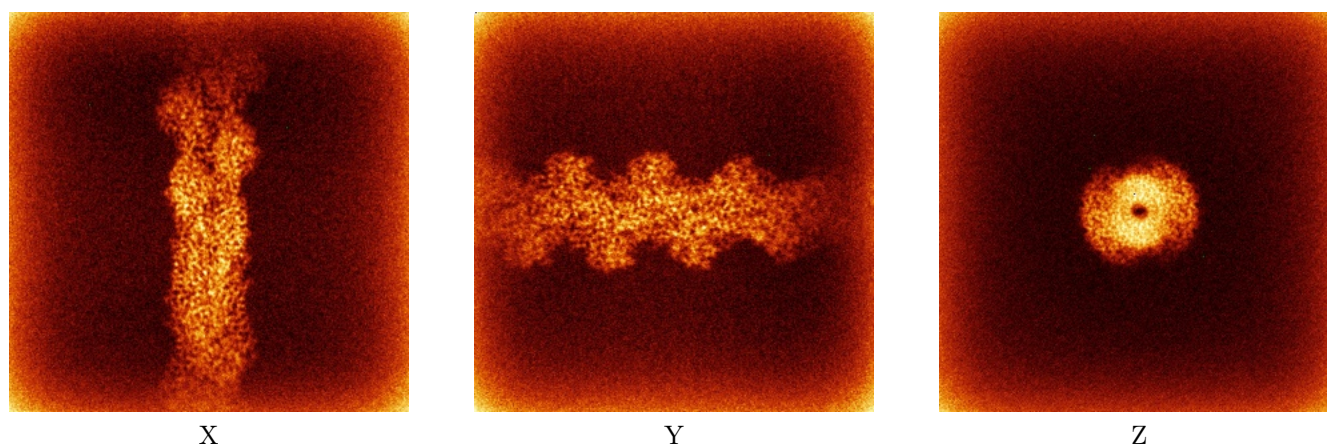
The images above show the largest variance slices of the map in three orthogonal directions.

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.

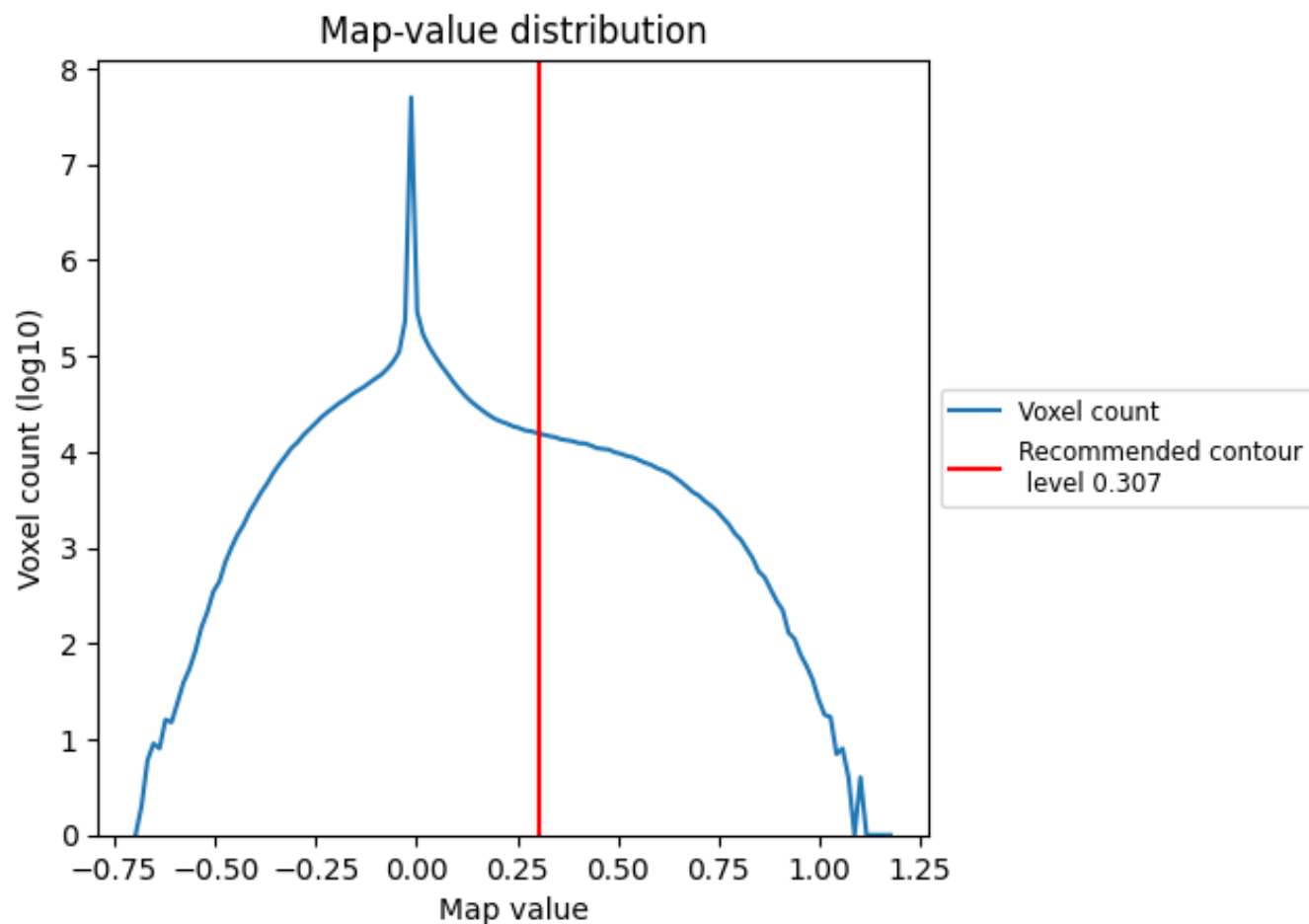
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

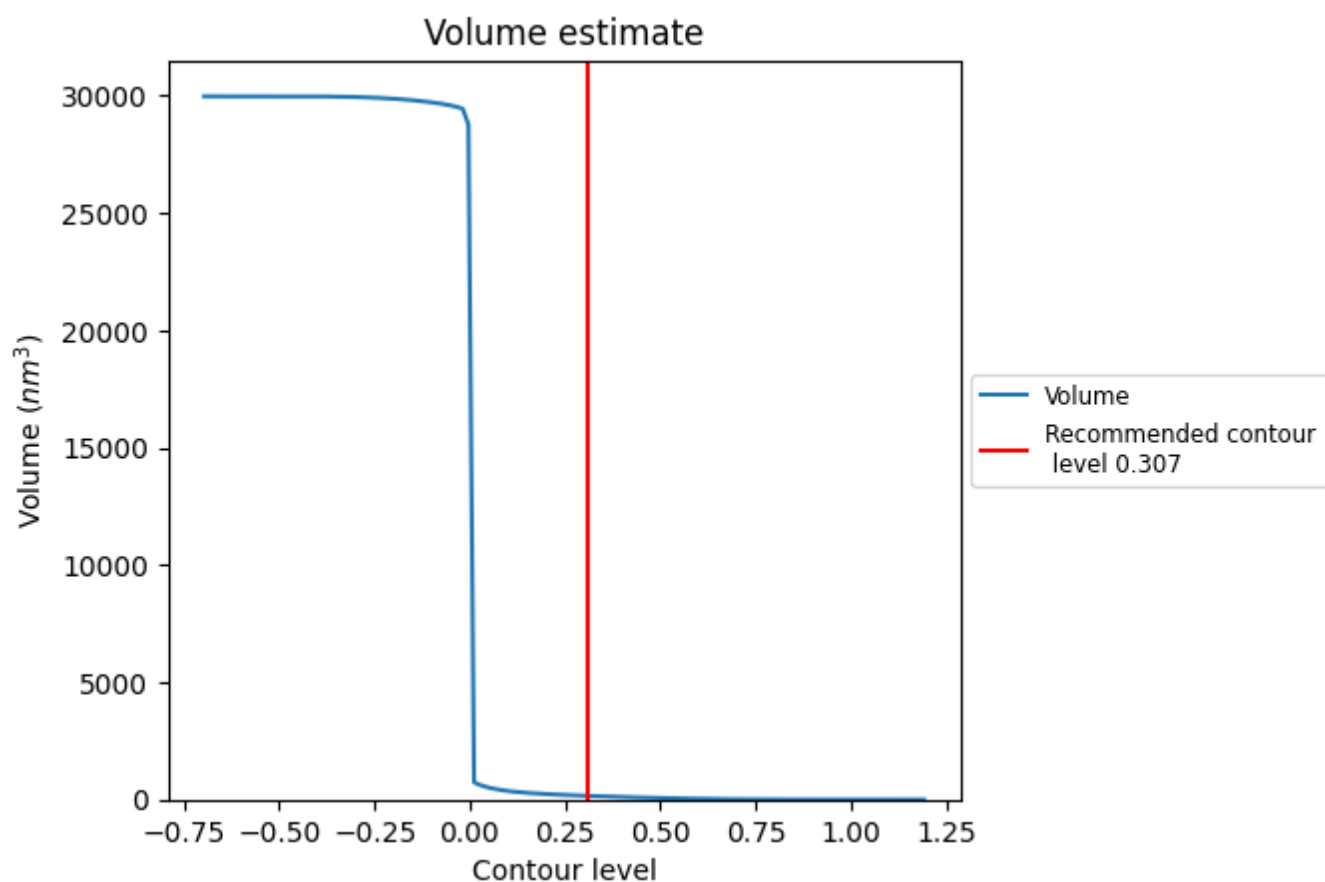
This section contains the results of statistical analysis of the map.

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 160 nm³; this corresponds to an approximate mass of 144 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.

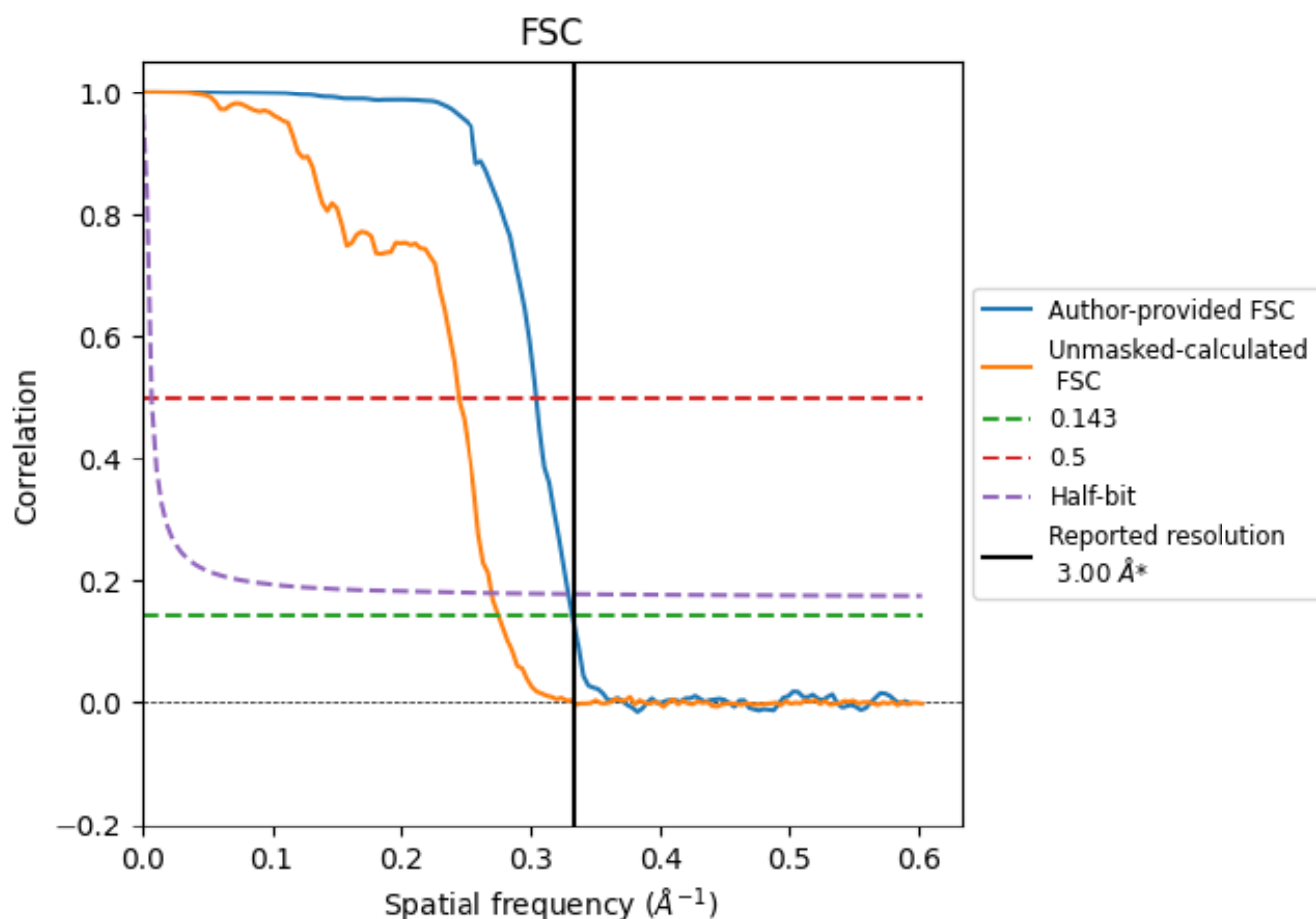
7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

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 Å⁻¹

8.2 Resolution estimates [i](#)

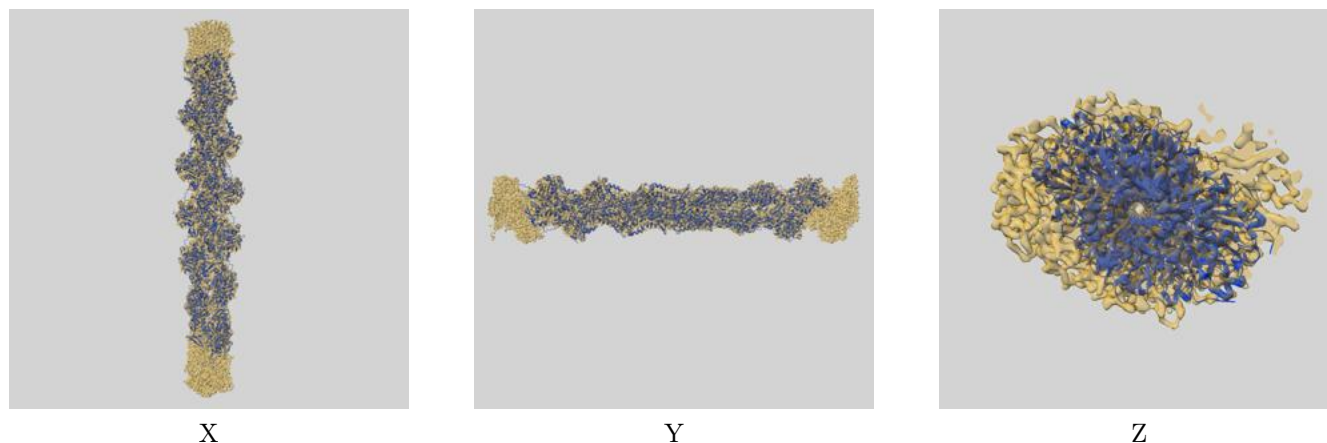
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.01	3.29	3.04
Unmasked-calculated*	3.63	4.09	3.70

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

9 Map-model fit [i](#)

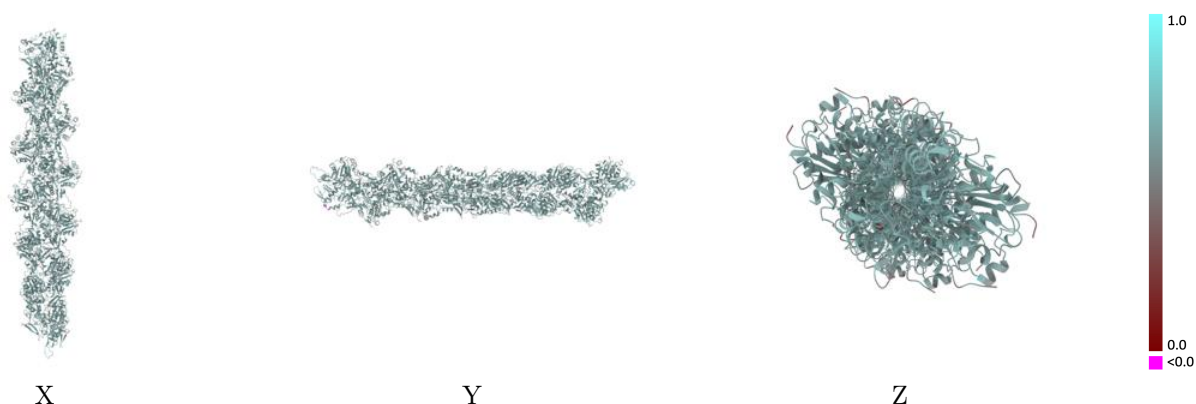
This section contains information regarding the fit between EMDB map EMD-71108 and PDB model 9P1I. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



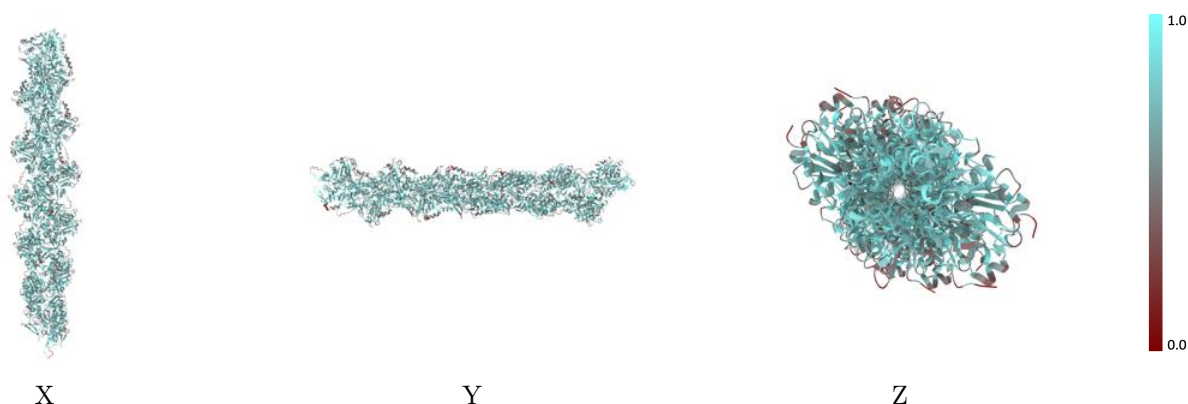
The images above show the 3D surface view of the map at the recommended contour level 0.307 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



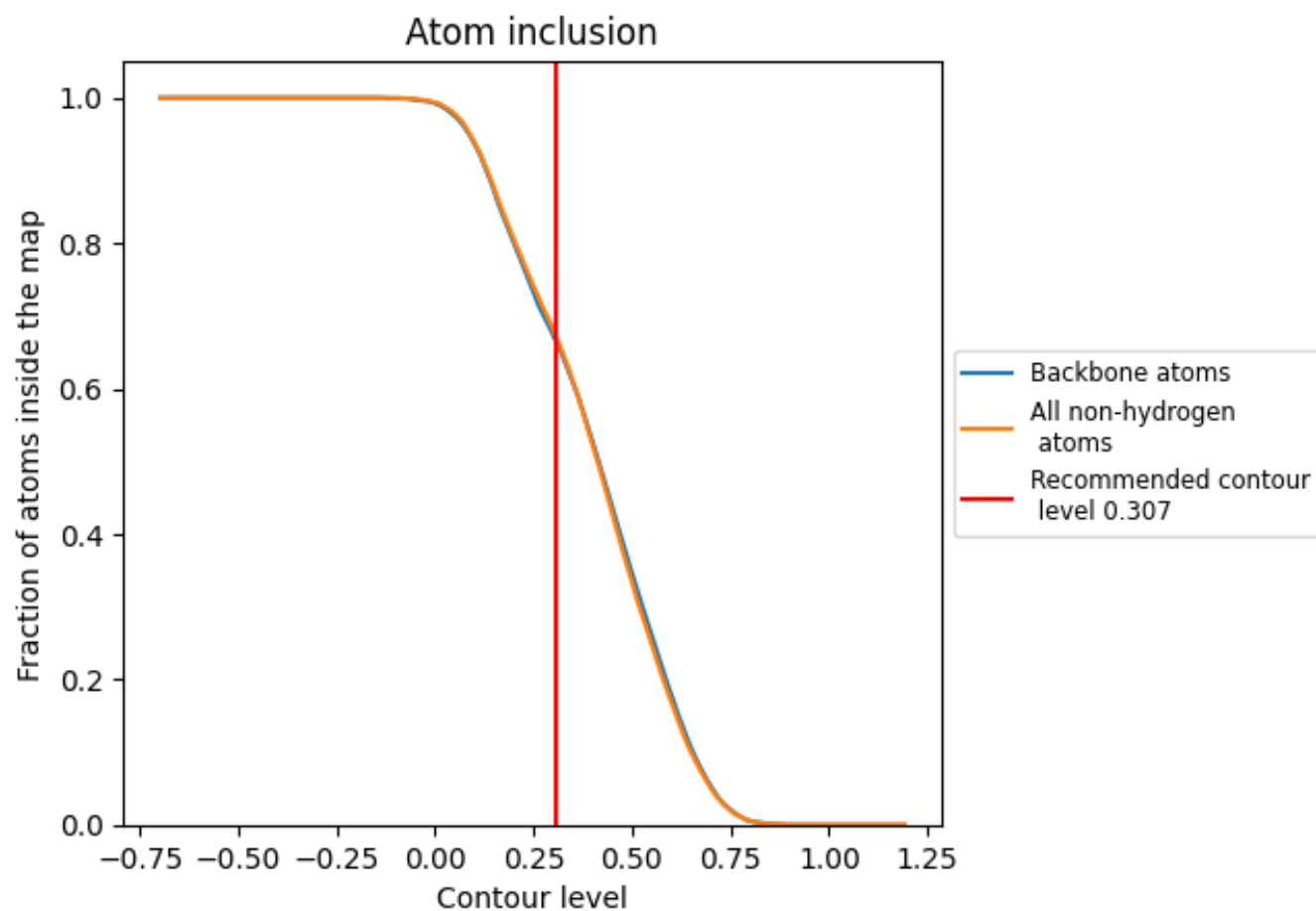
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.307).

9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 67% 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 (0.307) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6710	0.5890
Q	0.6940	0.5930
R	0.6900	0.5940
S	0.6920	0.5920
T	0.6930	0.5940
U	0.6930	0.5940
V	0.6940	0.5950
W	0.6890	0.5930
X	0.6960	0.5920
Y	0.6910	0.5930
Z	0.6910	0.5940
a	0.6920	0.5940
b	0.6900	0.5920
c	0.5850	0.5570
d	0.5650	0.5550
e	0.5680	0.5600
f	0.5560	0.5550
g	0.5880	0.5610
h	0.5620	0.5570
i	0.5650	0.5530
j	0.5790	0.5600
k	0.5590	0.5590
l	0.5880	0.5600
m	0.5790	0.5480
n	0.5850	0.5550

1.0

0.0

<0.0