



Full wwPDB EM Validation Report ⓘ

Dec 1, 2025 – 11:04 AM EST

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 Full wwPDB EM Validation 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:

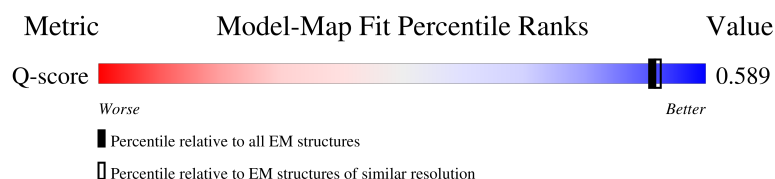
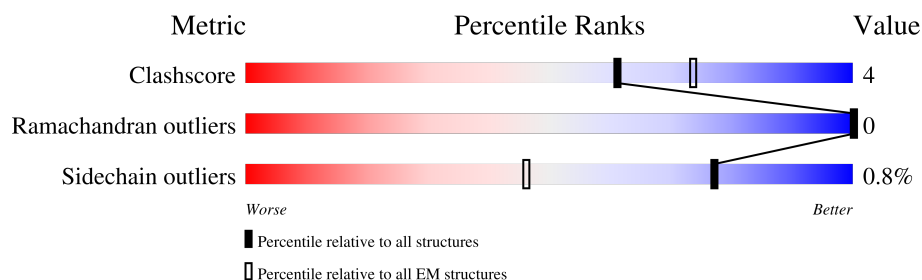
EMDB validation analysis : 0.0.1.dev129
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive 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) : 2.46

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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
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	<div> <div>10%</div> <div>86%</div> <div>13%</div> </div>
1	R	375	<div> <div>9%</div> <div>89%</div> <div>10%</div> </div>
1	S	375	<div> <div>9%</div> <div>87%</div> <div>12%</div> </div>
1	T	375	<div> <div>10%</div> <div>85%</div> <div>14%</div> </div>

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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).

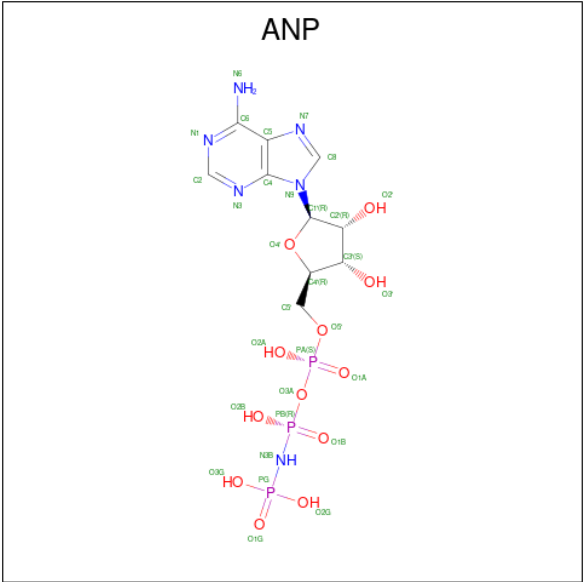
Mol	Chain	Residues	Atoms		AltConf
3	Q	1	Total 1	Mg 1	0
3	R	1	Total 1	Mg 1	0
3	S	1	Total 1	Mg 1	0
3	T	1	Total 1	Mg 1	0
3	U	1	Total 1	Mg 1	0
3	V	1	Total 1	Mg 1	0
3	W	1	Total 1	Mg 1	0
3	X	1	Total 1	Mg 1	0
3	Y	1	Total 1	Mg 1	0
3	Z	1	Total 1	Mg 1	0

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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	

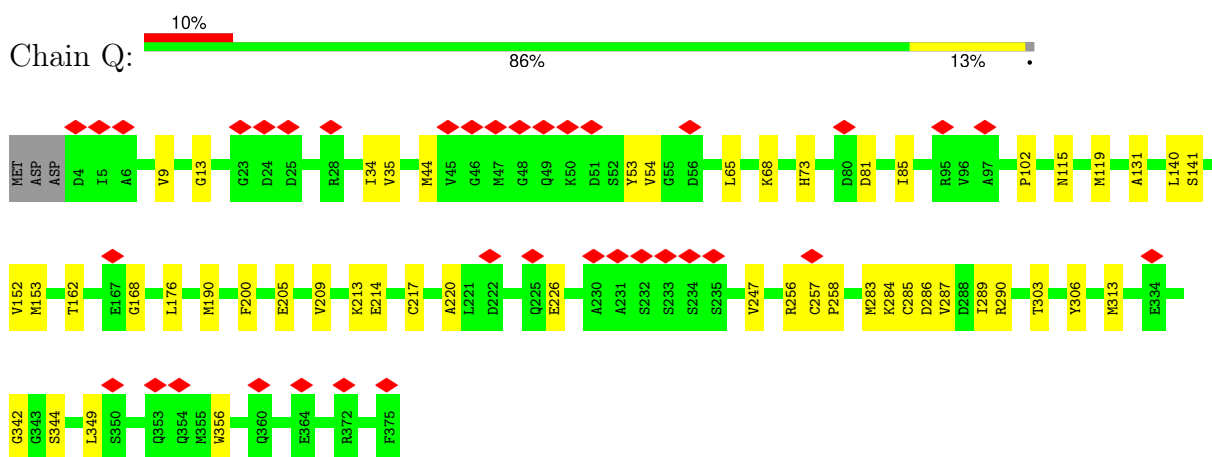
- Molecule 5 is water.

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	

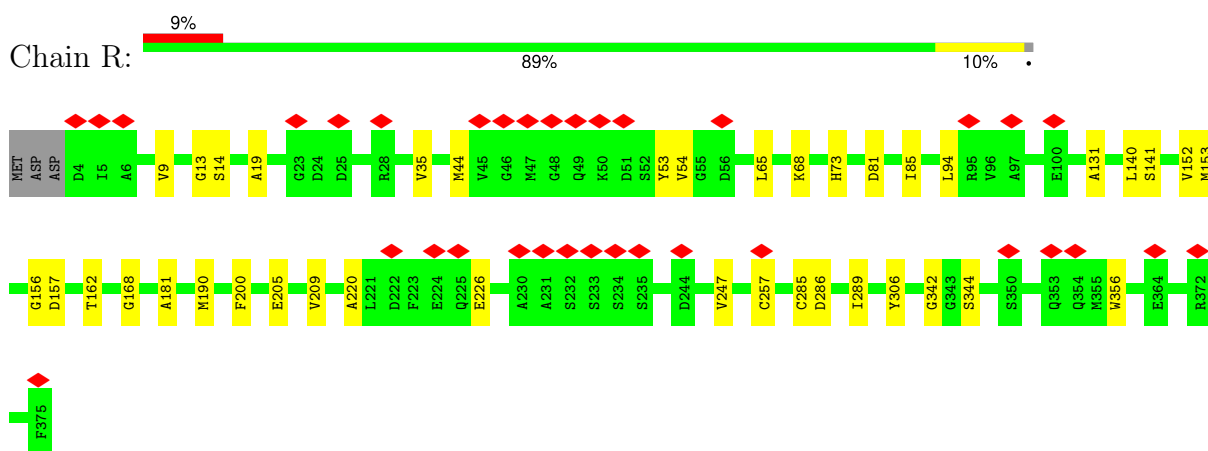
3 Residue-property plots

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.

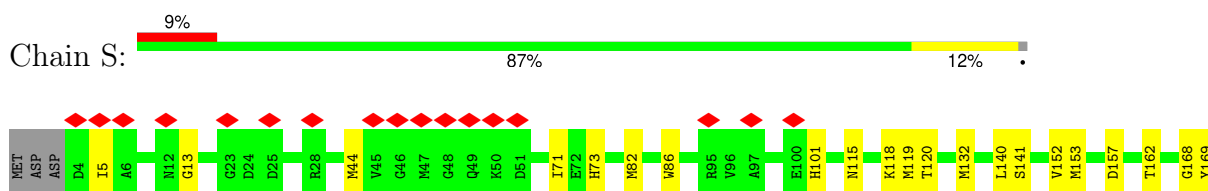
- Molecule 1: Actin, cytoplasmic 1

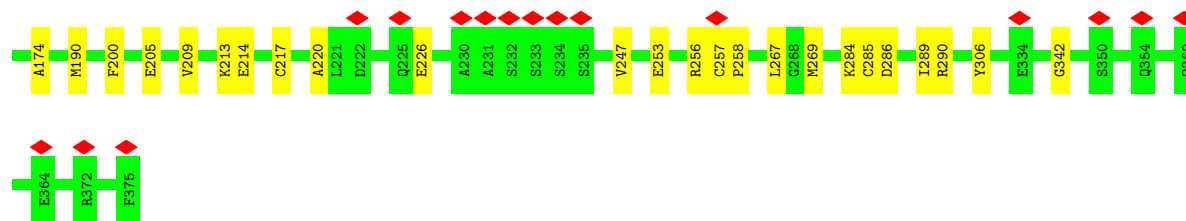


- Molecule 1: Actin, cytoplasmic 1

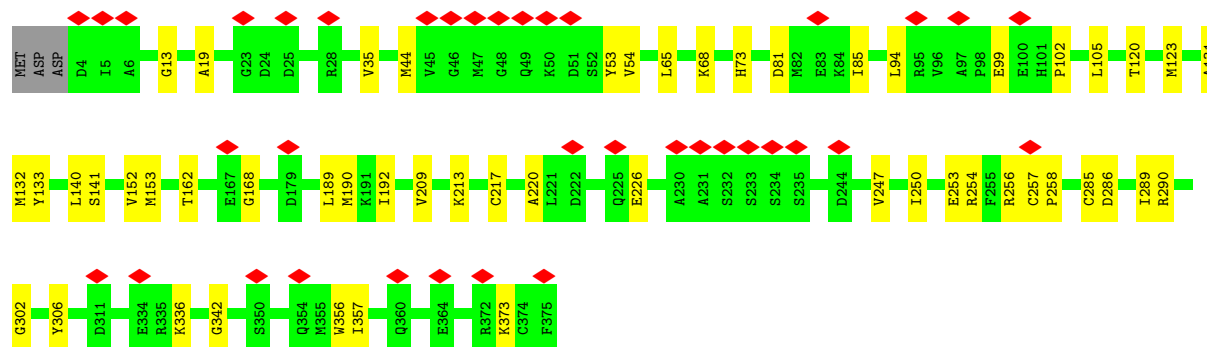
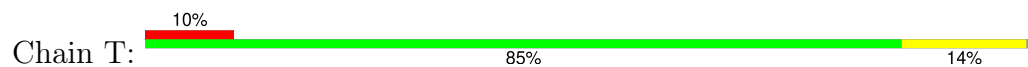


- Molecule 1: Actin, cytoplasmic 1

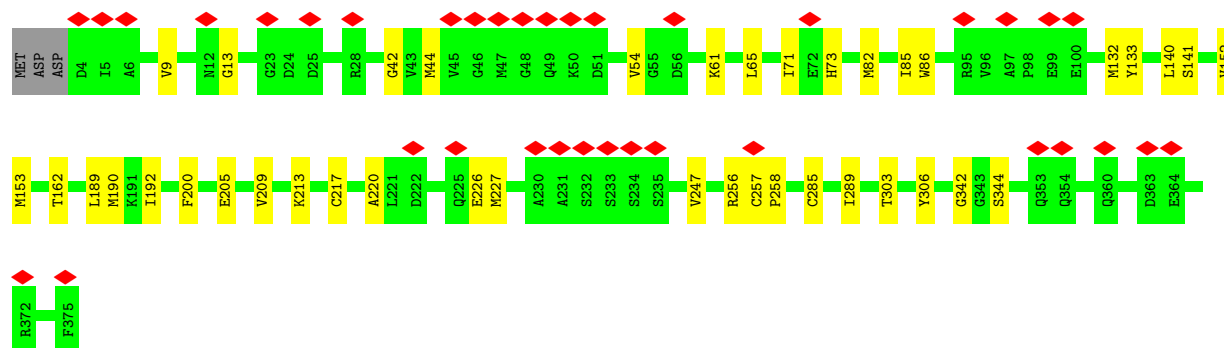
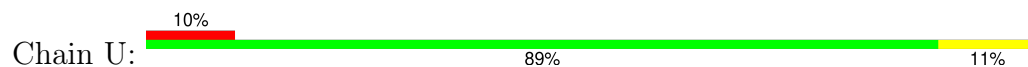




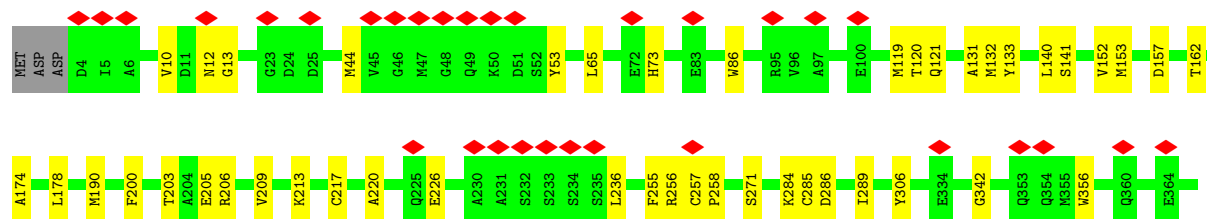
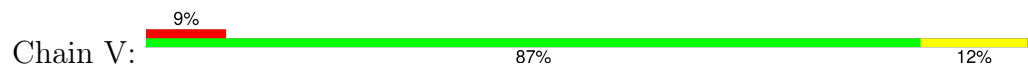
- Molecule 1: Actin, cytoplasmic 1



- Molecule 1: Actin, cytoplasmic 1

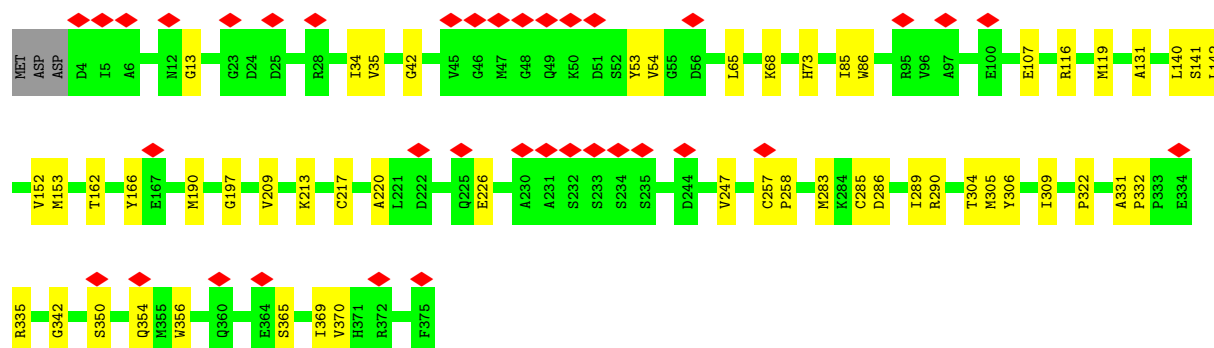
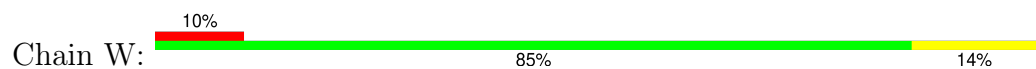


- Molecule 1: Actin, cytoplasmic 1

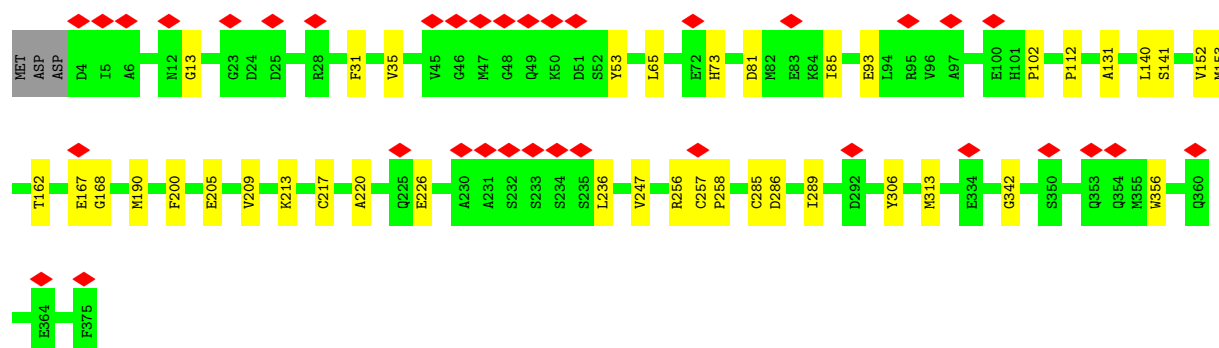
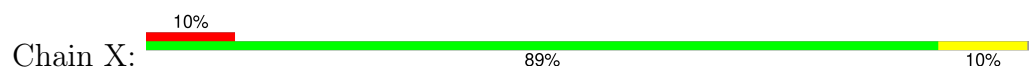




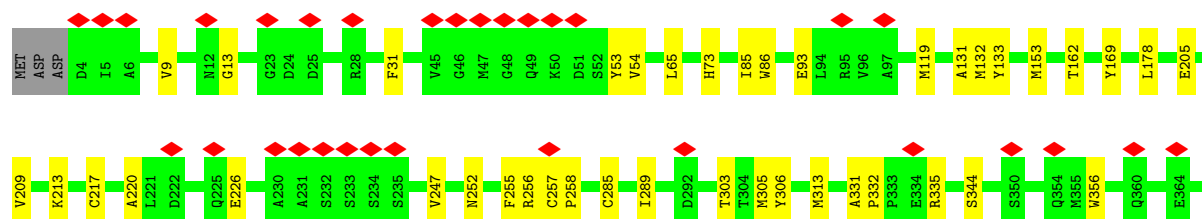
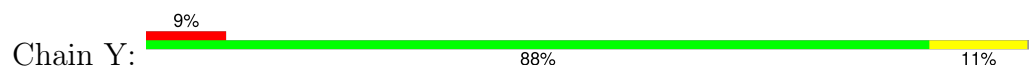
- Molecule 1: Actin, cytoplasmic 1




- Molecule 1: Actin, cytoplasmic 1

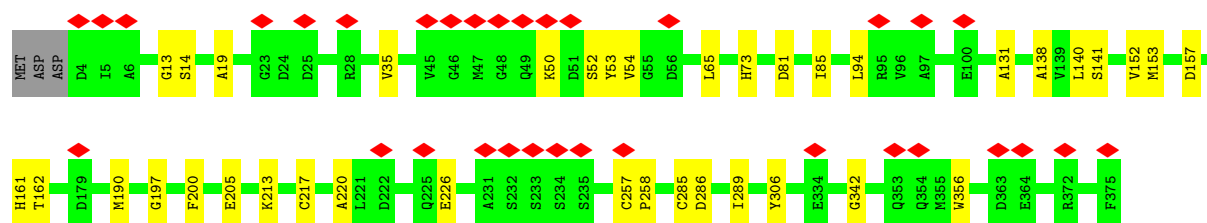


- Molecule 1: Actin, cytoplasmic 1




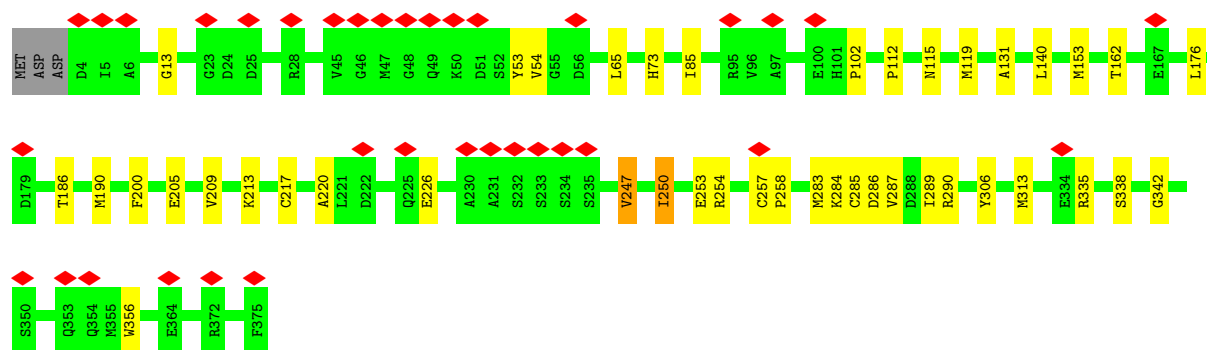
- Molecule 1: Actin, cytoplasmic 1

Chain Z: 




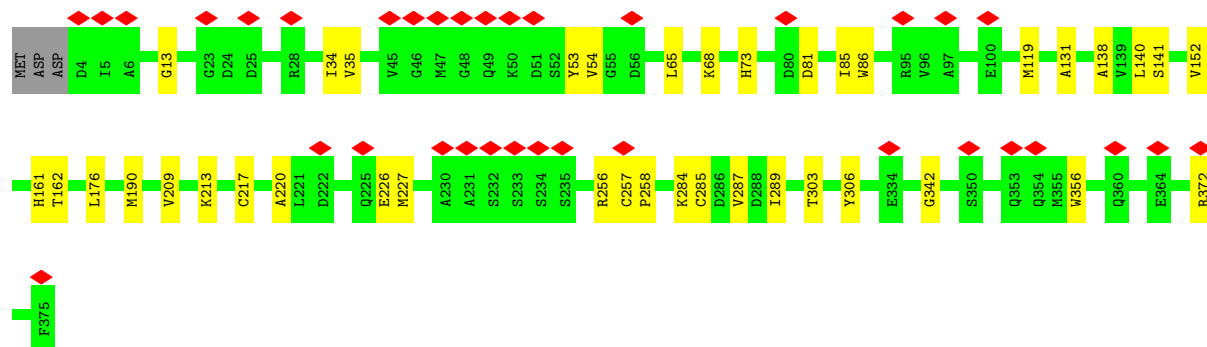
• Molecule 1: Actin, cytoplasmic 1

Chain a: 



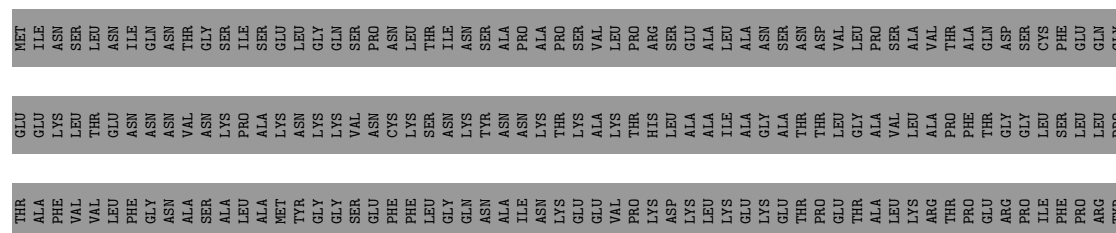
• Molecule 1: Actin, cytoplasmic 1

Chain b: 



• Molecule 2: VopV

Chain c: 















- Molecule 2: VopV

98%





- Molecule 2: VopV

Chain h: 98%

[illegible]



THR	THR	LEU	VAL	SER	GLY	LEU	VAL	GLY	SER	ASN	SER	SER	VAL	SER	ILE	TRP	ALA	HIS	SER	GLU	ARG	SER	MET	VAL	VAL	PRO	VAL	ALA	ASN	SER	SER	ASN	PHE	LYS	MET	MET
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- Molecule 2: VopV

Chain i:  98%

SER	ALA	ALA	ALA	GLN	SER	ASP	VAL	SER	SER	SER	GLN	THR	THR	THR	LEU	PHE	ASP	ASP	GLU	ALA	ILE	GLN	ASN	MET	GLY	GLN	LEU	GLN	VAL	VAL	ASP	ASP	VAL	SER	SER	GLU	ILE	ILE	PRO	ASP	THR	THR	LEU	PHE	SER	SER	GLU	VAL	THR	THR	THR	THR	GLY	GLY	GLU	GLU	ASP	THR	THR	VAL	ASP	ASN	ASN	LEU	LEU	LEU	ILE	TYR
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ALA	LEU	GLU	SER	CYS	HIS	LEU	GLN	SER	GLY	GLN	ALA	LYS	LEU	VAL	LYS	VAL	THR	LEU	GLY	GLY	LEU	GLN	ALA	TYR	LEU	GLY	GLY	ILE	SER	ASP	THR	ALA	ASP	ALA	LEU	PRO	PRO	VAL	VAL	THR	THR	GLU	ASN	VAL	THR	SER	SER	PRO	VAL	K352	K353	K354	P355	K358	I359	T366
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D373
Y378
D384
S385
M386
G387
E388
M394
R395
D396
R397
V398
SER
SER
SER
SER
THR
PRO
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ARG
SER
ALA
THR
GLN
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ALA
ASP
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THR
LYS
GLY
VAL
GLU
PRO
ASN
VAL
SER

GLY	TYR	GLU	THR	GLY	ARG	ASP	ARG	VAL	VAL	SER	SER	SER	SER	THR	THR	PRO	PRO	PRO	PRO	LYS	GLY	SER	SER	VAL	VAL	ASN	ASN	GLU	GLU	GLY	ASN	GLY	ALA	ALA	ALA	ALA	ALA	ALA	GLN	GLN	THR	THR	PRO	PRO	PRO	GLY	GLY	LYS	SER	SER	GLY	VAL	VAL	GLU	GLU	PRO	PRO	ASN	ASN	VAL	VAL	THR	THR	ALA	ALA	THR	THR	PRO	PRO	GLY	GLY	LYS	LYS	PRO	PRO	SER	SER	ALA	ALA
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ASP	VAL	SER	SER	SER	GLY	GLU	PRO	THR	THR	SER	SER	ALA	ALA	GLN	GLY	ASN	ALA	GLY	GLY	GLY	ILE	ASP	SER	SER	GLY	VAL	VAL	ALA	ALA	THR	PRO	PRO	GLU	GLN	LYS	PRO	PRO
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SER	MET	GLY	ALA	SER	GLY	GLU	PRO	THR	SER	ALA	ALA	GLN	GLY	ASN	SER	ALA	SER	GLU	GLY	THR	ASP	SER	SER	GLY	VAL	GLY	THR	PRO	GLU	SER	THR	PRO	SER	VAL	ASP	ALA	ALA	THR	GLY	GLU	ASN	ASN	THR	THR	PRO	THR	HIS	GLU	SER	GLY	GLU
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SER	VAL	PRO	PRO	SER	VAL	GLU	SER	GLU	GLN	ALA	ALA	SER	SER	SER	GLY	PRO	PRO	GLU	VAL	VAL	LYS	THR	THR	PRO	ALA	ALA	ARG	VAL	ILE	THR	SER	SER	GLY	GLY	ASN	ASN	ASP	ILE	ASP	GLY	ASN	ASN	PRO	PRO	GLY	TYR	ARG	PRO	THR	THR	ARG	ARG	VAL	ASP	ASP	SER	ASN	GLY	GLY	GLU	THR	THR	MET	GLY	TYR	GLU	MET	MET	ARG	ASP
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[illegible][illegible]





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

- Molecule 2: VopV

Chain k: 98%

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

[illegible]



[illegible]

- Molecule 2: VopV

Chain 1: 98%

[illegible]





- Molecule 2: VopV





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 ($e^-/\text{\AA}^2$)	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: MG, HIC, ANP

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.

All (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
1	S	256	ARG	C-N-CA	5.67	126.81	119.78
1	V	256	ARG	CA-C-N	5.38	127.47	120.26
1	V	256	ARG	C-N-CA	5.38	127.47	120.26
1	X	256	ARG	CA-C-N	5.21	127.24	120.26
1	X	256	ARG	C-N-CA	5.21	127.24	120.26
1	U	256	ARG	CA-C-N	5.18	127.20	120.26
1	U	256	ARG	C-N-CA	5.18	127.20	120.26
1	T	256	ARG	CA-C-N	5.13	127.14	120.26
1	T	256	ARG	C-N-CA	5.13	127.14	120.26
1	Y	256	ARG	CA-C-N	5.12	127.12	120.26
1	Y	256	ARG	C-N-CA	5.12	127.12	120.26

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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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.

All (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
1:Q:44:MET:HE2	1:W:142:LEU:HD23	1.82	0.62
1:Q:257:CYS:HB3	1:Q:258:PRO:HD3	1.81	0.61
1:W:107:GLU:HG2	1:W:116:ARG:HH11	1.65	0.61
1:R:190:MET:HG2	1:R:209:VAL:HG21	1.82	0.61
1:b:257:CYS:HB3	1:b:258:PRO:HD3	1.83	0.60
1:V:174:ALA:HA	1:V:284:LYS:HE3	1.84	0.60
1:T:153:MET:HG2	1:T:162:THR:HG22	1.83	0.60
1:R:220:ALA:HB1	1:R:226:GLU:HG3	1.83	0.60
1:V:153:MET:HG2	1:V:162:THR:HG22	1.84	0.60
1:S:169:TYR:HA	1:U:42:GLY:HA2	1.82	0.60
1:S:168:GLY:HA2	1:U:44:MET:HG3	1.84	0.60
1:V:157:ASP:H	4:V:802:ANP:HNB1	1.49	0.59
1:V:86:TRP:HH2	1:V:119:MET:HG2	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:153:MET:HG2	1:S:162:THR:HG22	1.84	0.59
1:T:250:ILE:HG12	1:T:254:ARG:HG3	1.84	0.59
1:X:153:MET:HG2	1:X:162:THR:HG22	1.85	0.57
1:W:220:ALA:HB1	1:W:226:GLU:HG3	1.87	0.57
1:S:174:ALA:HA	1:S:284:LYS:HE3	1.87	0.56
1:Z:200:PHE:HB3	1:Z:205:GLU:HB3	1.87	0.56
1:Q:200:PHE:HB3	1:Q:205:GLU:HB3	1.87	0.56
1:a:153:MET:HG2	1:a:162:THR:HG22	1.87	0.56
2:k:378:TYR:HB3	2:k:394:MET:HB3	1.88	0.56
1:S:118:LYS:HD2	2:d:359:ILE:HD11	1.87	0.56
1:T:220:ALA:HB1	1:T:226:GLU:HG3	1.88	0.56
1:b:220:ALA:HB1	1:b:226:GLU:HG3	1.88	0.55
1:V:286:ASP:HA	2:e:366:THR:HG23	1.87	0.55
1:X:286:ASP:HA	2:i:366:THR:HG23	1.87	0.55
1:V:200:PHE:HB3	1:V:205:GLU:HB3	1.89	0.55
1:S:200:PHE:HB3	1:S:205:GLU:HB3	1.88	0.55
1:U:220:ALA:HB1	1:U:226:GLU:HG3	1.88	0.55
1:W:42:GLY:HA2	1:Y:169:TYR:HA	1.89	0.54
1:S:286:ASP:HA	2:h:366:THR:HG23	1.89	0.54
1:Q:168:GLY:HA2	1:S:44:MET:HG3	1.89	0.54
1:b:306:TYR:CE1	4:b:802:ANP:H2	2.43	0.54
1:Y:305:MET:HA	1:Y:335:ARG:HH11	1.73	0.54
1:Q:131:ALA:HB1	1:Q:356:TRP:HB3	1.90	0.54
1:U:190:MET:HG2	1:U:209:VAL:HG21	1.90	0.53
1:Q:285:CYS:HB3	1:Q:289:ILE:HD11	1.90	0.53
1:b:141:SER:HB2	1:b:152:VAL:HG11	1.91	0.53
1:T:357:ILE:HG12	1:T:373:LYS:HG2	1.90	0.53
2:h:378:TYR:HB3	2:h:394:MET:HB3	1.91	0.53
1:R:200:PHE:HB3	1:R:205:GLU:HB3	1.91	0.53
1:Y:86:TRP:HH2	1:Y:119:MET:HG2	1.73	0.53
1:a:186:THR:O	1:a:190:MET:HG3	2.08	0.53
1:T:247:VAL:HG21	2:c:388:GLU:HB2	1.91	0.52
1:a:285:CYS:HB3	1:a:289:ILE:HD11	1.91	0.52
1:R:306:TYR:CE1	4:R:802:ANP:H2	2.45	0.52
1:W:305:MET:HA	1:W:335:ARG:HH11	1.74	0.52
1:Z:138:ALA:HB2	1:Z:161:HIS:CD2	2.45	0.52
1:W:306:TYR:CE1	4:W:802:ANP:H2	2.45	0.52
1:R:153:MET:HG2	1:R:162:THR:HG22	1.91	0.52
1:X:13:GLY:HA3	4:X:802:ANP:PB	2.50	0.52
1:Q:141:SER:HB2	1:Q:152:VAL:HG11	1.91	0.52
1:S:306:TYR:CE1	4:S:802:ANP:H2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:131:ALA:HB1	1:Y:356:TRP:HB3	1.92	0.52
2:i:378:TYR:HB3	2:i:394:MET:HB3	1.91	0.52
2:f:378:TYR:HB3	2:f:394:MET:HB3	1.93	0.51
1:W:107:GLU:HG2	1:W:116:ARG:NH1	2.24	0.51
1:Y:285:CYS:HB3	1:Y:289:ILE:HD11	1.93	0.51
2:c:378:TYR:HB3	2:c:394:MET:HB3	1.93	0.51
2:l:378:TYR:HB3	2:l:394:MET:HB3	1.92	0.51
1:V:131:ALA:HB1	1:V:356:TRP:HB3	1.93	0.51
1:W:286:ASP:HA	2:f:366:THR:HG23	1.93	0.51
1:Y:153:MET:HG2	1:Y:162:THR:HG22	1.91	0.51
1:Y:213:LYS:HG3	1:Y:257:CYS:SG	2.51	0.51
1:b:287:VAL:H	2:m:366:THR:HG22	1.76	0.51
2:c:378:TYR:HB2	2:c:394:MET:HE3	1.92	0.51
1:R:14:SER:HB2	1:R:157:ASP:HB3	1.93	0.51
1:T:141:SER:HB2	1:T:152:VAL:HG11	1.93	0.51
1:W:86:TRP:HH2	1:W:119:MET:HG2	1.76	0.51
1:a:200:PHE:HB3	1:a:205:GLU:HB3	1.93	0.51
1:Q:287:VAL:H	2:g:366:THR:HG22	1.77	0.50
1:T:250:ILE:HG13	1:T:253:GLU:HB2	1.92	0.50
1:b:176:LEU:HD21	1:b:284:LYS:NZ	2.26	0.50
2:d:378:TYR:HB3	2:d:394:MET:HB3	1.93	0.50
1:a:102:PRO:HB3	1:a:131:ALA:HB3	1.94	0.50
1:Y:306:TYR:CE1	4:Y:802:ANP:H2	2.46	0.50
1:S:71:ILE:HD11	1:S:82:MET:HE1	1.94	0.50
1:T:131:ALA:HB1	1:T:356:TRP:HB3	1.93	0.50
1:W:131:ALA:HB1	1:W:356:TRP:HB3	1.94	0.50
1:W:331:ALA:HB1	1:W:335:ARG:NH2	2.27	0.50
1:Q:283:MET:HE2	1:Q:290:ARG:HD3	1.94	0.50
1:R:131:ALA:HB1	1:R:356:TRP:HB3	1.94	0.50
1:R:286:ASP:HA	2:c:366:THR:HG23	1.94	0.50
1:X:285:CYS:HB3	1:X:289:ILE:HD11	1.93	0.50
1:S:190:MET:HG2	1:S:209:VAL:HG11	1.94	0.49
1:Q:176:LEU:HD21	1:Q:284:LYS:NZ	2.27	0.49
1:Z:35:VAL:HG21	1:Z:81:ASP:HB3	1.93	0.49
2:e:378:TYR:HB3	2:e:394:MET:HB3	1.94	0.49
1:S:285:CYS:HB3	1:S:289:ILE:HD11	1.94	0.49
1:Z:213:LYS:HG3	1:Z:257:CYS:SG	2.53	0.49
1:R:285:CYS:HB3	1:R:289:ILE:HD11	1.94	0.49
1:W:141:SER:HB2	1:W:152:VAL:HG11	1.94	0.49
1:X:131:ALA:HB1	1:X:356:TRP:HB3	1.94	0.49
1:X:257:CYS:HB3	1:X:258:PRO:HD3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:306:TYR:CE1	4:Q:802:ANP:H2	2.47	0.49
1:U:200:PHE:HB3	1:U:205:GLU:HB3	1.93	0.49
1:R:13:GLY:HA3	4:R:802:ANP:PB	2.53	0.48
1:S:13:GLY:HA3	4:S:802:ANP:PB	2.53	0.48
1:W:13:GLY:HA3	4:W:802:ANP:PB	2.53	0.48
1:X:200:PHE:HB3	1:X:205:GLU:HB3	1.95	0.48
1:a:306:TYR:CE1	4:a:802:ANP:H2	2.48	0.48
1:X:140:LEU:O	1:X:342:GLY:HA3	2.14	0.48
1:Q:153:MET:HG2	1:Q:162:THR:HG22	1.96	0.48
1:Z:286:ASP:HA	2:k:366:THR:HG23	1.95	0.48
1:R:168:GLY:HA2	1:T:44:MET:HG3	1.96	0.48
1:T:257:CYS:HB3	1:T:258:PRO:HD3	1.94	0.48
1:X:247:VAL:HG22	2:k:389:THR:O	2.14	0.48
1:X:306:TYR:CE1	4:X:802:ANP:H2	2.48	0.48
1:Z:220:ALA:HB1	1:Z:226:GLU:HG3	1.95	0.48
1:U:306:TYR:CE1	4:U:802:ANP:H2	2.49	0.48
1:V:205:GLU:OE2	2:d:366:THR:HG23	2.13	0.48
1:X:220:ALA:HB1	1:X:226:GLU:HG3	1.96	0.48
1:Z:131:ALA:HB1	1:Z:356:TRP:HB3	1.96	0.48
1:R:9:VAL:HG21	1:R:344:SER:HA	1.95	0.48
1:W:257:CYS:HB3	1:W:258:PRO:HD3	1.96	0.48
1:Z:205:GLU:OE2	2:m:366:THR:HG23	2.14	0.48
1:S:115:ASN:ND2	1:S:119:MET:HE3	2.29	0.48
1:Y:205:GLU:OE2	2:l:366:THR:HG23	2.14	0.48
1:Z:13:GLY:HA3	4:Z:802:ANP:PB	2.54	0.48
1:S:141:SER:HB2	1:S:152:VAL:HG11	1.95	0.48
1:W:153:MET:HG2	1:W:162:THR:HG22	1.96	0.48
1:Y:332:PRO:O	1:Y:335:ARG:HG3	2.13	0.48
1:U:82:MET:HE3	1:U:86:TRP:CZ2	2.49	0.48
1:a:115:ASN:ND2	1:a:119:MET:HE3	2.29	0.48
1:b:54:VAL:HG13	1:b:85:ILE:HD13	1.95	0.48
1:Q:102:PRO:HB3	1:Q:131:ALA:HB3	1.96	0.47
1:S:205:GLU:OE2	2:g:366:THR:HG23	2.14	0.47
1:U:13:GLY:HA3	4:U:802:ANP:PB	2.54	0.47
1:R:19:ALA:HB1	1:R:94:LEU:HD11	1.96	0.47
1:T:102:PRO:HB3	1:T:131:ALA:HB3	1.96	0.47
1:Z:306:TYR:CE1	4:Z:802:ANP:H2	2.50	0.47
1:Q:13:GLY:HA3	4:Q:802:ANP:PB	2.54	0.47
1:T:35:VAL:O	1:T:68:LYS:HG2	2.14	0.47
1:X:102:PRO:HB3	1:X:131:ALA:HB3	1.96	0.47
1:a:54:VAL:HG13	1:a:85:ILE:HD13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:190:MET:HG2	1:X:209:VAL:HG21	1.96	0.47
1:b:86:TRP:HH2	1:b:119:MET:HG2	1.80	0.47
2:j:378:TYR:HB3	2:j:394:MET:HB3	1.95	0.47
1:V:141:SER:HB2	1:V:152:VAL:HG11	1.97	0.47
1:Z:205:GLU:OE2	2:m:365:THR:HB	2.15	0.47
2:j:397:ARG:HA	2:j:397:ARG:NE	2.30	0.47
2:k:359:ILE:H	2:k:359:ILE:HG13	1.46	0.47
1:Q:220:ALA:HB1	1:Q:226:GLU:HG3	1.97	0.46
1:T:285:CYS:HB3	1:T:289:ILE:HD11	1.97	0.46
1:Z:285:CYS:HB3	1:Z:289:ILE:HD11	1.97	0.46
1:a:220:ALA:HB1	1:a:226:GLU:HG3	1.96	0.46
1:Q:35:VAL:O	1:Q:68:LYS:HG2	2.15	0.46
1:S:214:GLU:HG2	4:S:802:ANP:C5	2.45	0.46
1:Z:141:SER:HB2	1:Z:152:VAL:HG11	1.97	0.46
2:g:378:TYR:HB3	2:g:394:MET:HB3	1.98	0.46
1:W:190:MET:HG2	1:W:209:VAL:HG21	1.97	0.46
1:b:285:CYS:HB3	1:b:289:ILE:HD11	1.96	0.46
1:S:205:GLU:OE2	2:g:365:THR:HB	2.16	0.46
1:U:140:LEU:O	1:U:342:GLY:HA3	2.15	0.46
1:Y:331:ALA:HB1	1:Y:335:ARG:NH2	2.30	0.46
1:T:105:LEU:HD21	1:T:123:MET:HE3	1.98	0.46
1:W:285:CYS:HB3	1:W:289:ILE:HD11	1.96	0.46
1:a:313:MET:HE3	1:a:313:MET:HB3	1.85	0.46
1:Y:9:VAL:HG21	1:Y:344:SER:HA	1.98	0.46
1:Z:257:CYS:HB3	1:Z:258:PRO:HD3	1.97	0.46
1:Y:54:VAL:HG13	1:Y:85:ILE:HD13	1.97	0.46
1:S:220:ALA:HB1	1:S:226:GLU:HG3	1.97	0.45
1:a:247:VAL:HG22	2:n:389:THR:O	2.16	0.45
1:S:82:MET:HE3	1:S:86:TRP:CZ2	2.50	0.45
1:S:247:VAL:HG22	2:g:389:THR:O	2.16	0.45
1:T:302:GLY:HA2	1:T:336:LYS:HG2	1.97	0.45
1:W:213:LYS:HG3	1:W:257:CYS:SG	2.57	0.45
1:a:213:LYS:HA	1:a:217:CYS:SG	2.56	0.45
2:k:397:ARG:HA	2:k:397:ARG:NE	2.31	0.45
1:b:13:GLY:HA3	4:b:802:ANP:PB	2.56	0.45
2:n:378:TYR:HB2	2:n:394:MET:HE3	1.98	0.45
1:Q:213:LYS:HA	1:Q:217:CYS:SG	2.56	0.45
1:W:116:ARG:HG2	1:W:370:VAL:HG11	1.98	0.45
1:V:190:MET:HG2	1:V:209:VAL:HG21	1.97	0.45
1:W:35:VAL:O	1:W:68:LYS:HG2	2.16	0.45
1:S:267:LEU:HB2	1:S:269:MET:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:13:GLY:HA3	4:a:802:ANP:PB	2.57	0.45
1:a:131:ALA:HB1	1:a:356:TRP:HB3	1.99	0.45
2:e:378:TYR:HB2	2:e:394:MET:HE3	1.98	0.45
2:c:359:ILE:H	2:c:359:ILE:HG13	1.48	0.45
1:Q:287:VAL:HG23	2:g:366:THR:HG22	2.00	0.44
1:R:53:TYR:CD2	1:R:65:LEU:HD21	2.52	0.44
1:R:54:VAL:HG13	1:R:85:ILE:HD13	1.98	0.44
1:U:71:ILE:HD11	1:U:82:MET:HE1	1.98	0.44
1:Y:252:ASN:HA	1:Y:255:PHE:CE2	2.53	0.44
1:R:44:MET:HG3	1:X:168:GLY:HA2	1.99	0.44
1:W:322:PRO:HB3	2:f:389:THR:HG21	1.99	0.44
1:Y:313:MET:HB3	1:Y:313:MET:HE3	1.84	0.44
1:Z:19:ALA:HB1	1:Z:94:LEU:HD11	1.99	0.44
1:R:44:MET:HE3	1:R:44:MET:HB3	1.94	0.44
1:R:35:VAL:HG21	1:R:81:ASP:HB3	2.00	0.44
1:b:131:ALA:HB1	1:b:356:TRP:HB3	1.99	0.44
1:Y:220:ALA:HB1	1:Y:226:GLU:HG3	1.99	0.44
1:T:190:MET:HG3	1:T:209:VAL:HG11	1.99	0.44
1:U:54:VAL:HG13	1:U:85:ILE:HD13	1.99	0.44
1:V:213:LYS:HA	1:V:217:CYS:SG	2.58	0.44
1:Z:54:VAL:HG13	1:Z:85:ILE:HD13	1.98	0.44
1:a:286:ASP:O	1:a:290:ARG:HG3	2.18	0.44
1:V:306:TYR:CE1	4:V:802:ANP:H2	2.53	0.44
1:W:140:LEU:O	1:W:342:GLY:HA3	2.18	0.44
1:X:35:VAL:HG21	1:X:81:ASP:HB3	1.98	0.44
1:Z:140:LEU:O	1:Z:342:GLY:HA3	2.18	0.44
1:R:140:LEU:O	1:R:342:GLY:HA3	2.18	0.44
1:U:132:MET:HG2	1:U:133:TYR:N	2.33	0.44
1:U:257:CYS:HB3	1:U:258:PRO:HD3	1.99	0.44
1:T:54:VAL:HG13	1:T:85:ILE:HD13	2.00	0.44
1:W:332:PRO:O	1:W:335:ARG:HG3	2.18	0.44
1:Y:213:LYS:HA	1:Y:217:CYS:SG	2.58	0.44
1:b:190:MET:HG2	1:b:209:VAL:HG21	2.00	0.44
2:j:378:TYR:HB2	2:j:394:MET:HE3	2.00	0.44
1:R:141:SER:OG	1:R:152:VAL:HG11	2.18	0.43
1:T:120:THR:HA	1:T:132:MET:SD	2.58	0.43
1:U:189:LEU:HA	1:U:192:ILE:HG12	1.99	0.43
1:a:250:ILE:HG12	1:a:254:ARG:HG3	2.00	0.43
2:i:378:TYR:HB2	2:i:394:MET:HE3	2.00	0.43
2:k:362:ARG:HG2	2:k:392:TYR:O	2.18	0.43
1:T:53:TYR:CD2	1:T:65:LEU:HD21	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:176:LEU:HD21	1:a:284:LYS:NZ	2.29	0.43
1:b:140:LEU:O	1:b:342:GLY:HA3	2.18	0.43
1:V:13:GLY:HA3	4:V:802:ANP:PB	2.58	0.43
1:V:285:CYS:HB3	1:V:289:ILE:HD11	2.00	0.43
1:X:53:TYR:CD2	1:X:65:LEU:HD21	2.53	0.43
1:a:257:CYS:HB3	1:a:258:PRO:HD3	2.00	0.43
1:S:213:LYS:HA	1:S:217:CYS:SG	2.58	0.43
1:V:213:LYS:HG3	1:V:257:CYS:SG	2.59	0.43
1:a:140:LEU:O	1:a:342:GLY:HA3	2.19	0.43
1:Z:14:SER:HB2	1:Z:157:ASP:HB3	2.01	0.43
1:Q:349:LEU:HD23	1:Q:349:LEU:HA	1.91	0.43
1:U:141:SER:HB3	1:U:152:VAL:HG11	2.00	0.43
1:V:190:MET:HG2	1:V:209:VAL:HG11	2.01	0.43
1:Y:13:GLY:HA3	4:Y:802:ANP:PB	2.58	0.43
1:Z:138:ALA:HB2	1:Z:161:HIS:HD2	1.82	0.43
1:Q:286:ASP:O	1:Q:290:ARG:HG3	2.19	0.43
1:a:115:ASN:HD21	1:a:119:MET:HE3	1.84	0.43
1:Q:35:VAL:HG21	1:Q:81:ASP:HB3	2.01	0.43
1:T:213:LYS:HA	1:T:217:CYS:SG	2.58	0.43
1:b:213:LYS:HA	1:b:217:CYS:SG	2.59	0.43
1:T:286:ASP:O	1:T:290:ARG:HG3	2.18	0.43
1:U:285:CYS:HB3	1:U:289:ILE:HD11	2.01	0.43
2:e:359:ILE:H	2:e:359:ILE:HG13	1.48	0.43
1:T:140:LEU:O	1:T:342:GLY:HA3	2.18	0.43
1:Z:190:MET:HE3	1:Z:200:PHE:O	2.19	0.43
1:V:203:THR:HG22	1:V:206:ARG:HH22	1.84	0.42
1:W:213:LYS:HA	1:W:217:CYS:SG	2.59	0.42
1:Z:153:MET:HG2	1:Z:162:THR:HG22	2.01	0.42
1:b:35:VAL:HG21	1:b:81:ASP:HB3	2.00	0.42
1:Q:53:TYR:CD1	1:Q:65:LEU:HD21	2.54	0.42
1:Q:54:VAL:HG13	1:Q:85:ILE:HD13	2.00	0.42
1:T:35:VAL:HG21	1:T:81:ASP:HB3	2.01	0.42
1:V:140:LEU:O	1:V:342:GLY:HA3	2.19	0.42
1:W:197:GLY:HA2	1:X:112:PRO:HG3	2.02	0.42
1:Z:81:ASP:O	1:Z:85:ILE:HG12	2.19	0.42
2:m:378:TYR:HB3	2:m:394:MET:HB3	2.00	0.42
1:Q:115:ASN:ND2	1:Q:119:MET:HE3	2.34	0.42
1:Q:190:MET:HG3	1:Q:209:VAL:HG11	2.02	0.42
1:Q:247:VAL:HG22	2:f:389:THR:O	2.18	0.42
1:U:9:VAL:HG21	1:U:344:SER:HA	2.01	0.42
1:W:53:TYR:CD2	1:W:65:LEU:HD21	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:53:TYR:CD2	1:Y:65:LEU:HD21	2.55	0.42
1:a:283:MET:HE2	1:a:290:ARG:HD3	2.02	0.42
1:U:213:LYS:HA	1:U:217:CYS:SG	2.60	0.42
1:a:250:ILE:HG13	1:a:253:GLU:HB2	2.01	0.42
1:S:5:ILE:HB	1:S:101:HIS:CE1	2.55	0.42
1:T:168:GLY:HA2	1:V:44:MET:HG3	2.01	0.42
1:Y:205:GLU:O	1:Y:209:VAL:HG23	2.20	0.42
1:T:19:ALA:HB1	1:T:94:LEU:HD11	2.01	0.42
1:U:61:LYS:O	1:U:65:LEU:HG	2.20	0.42
1:X:141:SER:OG	1:X:152:VAL:HG11	2.19	0.42
1:b:35:VAL:O	1:b:68:LYS:HG2	2.20	0.42
1:V:120:THR:HA	1:V:132:MET:SD	2.60	0.42
1:V:220:ALA:HB1	1:V:226:GLU:HG3	2.01	0.42
1:X:313:MET:HE3	1:X:313:MET:HB3	1.96	0.42
1:Y:31:PHE:CE1	1:Y:93:GLU:HG3	2.55	0.42
1:W:166:TYR:CD1	1:W:289:ILE:HB	2.55	0.42
1:W:304:THR:HA	1:W:309:ILE:HD13	2.02	0.42
1:X:213:LYS:HG3	1:X:257:CYS:SG	2.60	0.42
1:b:138:ALA:HB2	1:b:161:HIS:CD2	2.54	0.42
1:a:205:GLU:O	1:a:209:VAL:HG23	2.20	0.41
1:b:153:MET:HG2	1:b:162:THR:HG22	2.01	0.41
1:X:81:ASP:O	1:X:85:ILE:HG12	2.20	0.41
1:b:53:TYR:CD1	1:b:65:LEU:HD21	2.55	0.41
1:T:189:LEU:HA	1:T:192:ILE:HG12	2.02	0.41
1:V:53:TYR:CD1	1:V:65:LEU:HD21	2.56	0.41
1:W:247:VAL:HG21	2:j:388:GLU:HB3	2.02	0.41
1:X:31:PHE:CE1	1:X:93:GLU:HG3	2.55	0.41
1:Z:53:TYR:CD1	1:Z:65:LEU:HD21	2.55	0.41
1:S:140:LEU:O	1:S:342:GLY:HA3	2.20	0.41
1:Q:313:MET:HE3	1:Q:313:MET:HB3	1.97	0.41
1:V:10:VAL:HG12	1:V:12:ASN:HB2	2.03	0.41
1:V:178:LEU:HD11	1:V:271:SER:HB2	2.03	0.41
1:T:13:GLY:HA3	4:T:802:ANP:PB	2.60	0.41
1:Z:197:GLY:HA2	1:a:112:PRO:HG3	2.03	0.41
1:a:53:TYR:CD2	1:a:65:LEU:HD21	2.55	0.41
1:Q:140:LEU:O	1:Q:342:GLY:HA3	2.20	0.41
1:W:365:SER:HB2	1:W:369:ILE:HB	2.02	0.41
1:R:156:GLY:O	1:R:181:ALA:HB1	2.21	0.41
1:V:132:MET:HG2	1:V:133:TYR:N	2.36	0.41
1:Z:213:LYS:HA	1:Z:217:CYS:SG	2.61	0.41
1:Q:9:VAL:HG21	1:Q:344:SER:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:120:THR:HA	1:S:132:MET:HE3	2.03	0.41
1:a:213:LYS:HG3	1:a:257:CYS:SG	2.61	0.41
1:S:115:ASN:HD21	1:S:119:MET:HE3	1.86	0.41
1:S:157:ASP:H	4:S:802:ANP:HNB1	1.69	0.41
1:T:132:MET:HG2	1:T:133:TYR:N	2.36	0.41
1:T:306:TYR:CE1	4:T:802:ANP:H2	2.56	0.41
1:W:283:MET:HE2	1:W:290:ARG:HD3	2.02	0.41
1:X:213:LYS:HA	1:X:217:CYS:SG	2.61	0.41
1:a:335:ARG:HA	1:a:338:SER:OG	2.21	0.41
1:Q:214:GLU:HG2	4:Q:802:ANP:C5	2.51	0.40
1:U:153:MET:HG2	1:U:162:THR:HG22	2.01	0.40
1:U:227:MET:HE3	1:U:227:MET:HB3	1.82	0.40
1:V:205:GLU:O	1:V:209:VAL:HG23	2.21	0.40
1:W:54:VAL:HG13	1:W:85:ILE:HD13	2.03	0.40
1:a:287:VAL:H	2:l:366:THR:HG22	1.87	0.40
1:R:247:VAL:HG21	2:i:388:GLU:HB3	2.03	0.40
1:Y:132:MET:HG2	1:Y:133:TYR:N	2.36	0.40
1:Z:50:LYS:HE2	1:Z:52:SER:O	2.20	0.40
1:b:227:MET:HE3	1:b:227:MET:HB3	1.91	0.40
2:k:362:ARG:HG2	2:k:362:ARG:H	1.70	0.40
1:S:253:GLU:O	1:S:257:CYS:HB2	2.21	0.40
1:V:236:LEU:HD23	1:V:255:PHE:HE2	1.85	0.40
1:S:286:ASP:O	1:S:290:ARG:HG3	2.22	0.40

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	Q	369/375 (98%)	363 (98%)	6 (2%)	0	100	100
1	R	369/375 (98%)	360 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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%)	84	93
1	R	314/317 (99%)	312 (99%)	2 (1%)	84	93
1	S	314/317 (99%)	314 (100%)	0	100	100
1	T	314/317 (99%)	313 (100%)	1 (0%)	91	96
1	U	314/317 (99%)	312 (99%)	2 (1%)	84	93
1	V	314/317 (99%)	314 (100%)	0	100	100
1	W	314/317 (99%)	311 (99%)	3 (1%)	73	88
1	X	314/317 (99%)	312 (99%)	2 (1%)	84	93
1	Y	314/317 (99%)	311 (99%)	3 (1%)	73	88
1	Z	314/317 (99%)	314 (100%)	0	100	100
1	a	314/317 (99%)	312 (99%)	2 (1%)	84	93
1	b	314/317 (99%)	311 (99%)	3 (1%)	73	88
2	c	40/1904 (2%)	39 (98%)	1 (2%)	42	73
2	d	40/1904 (2%)	38 (95%)	2 (5%)	20	53
2	e	40/1904 (2%)	38 (95%)	2 (5%)	20	53
2	f	40/1904 (2%)	38 (95%)	2 (5%)	20	53
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%)	20	53
2	j	40/1904 (2%)	39 (98%)	1 (2%)	42	73
2	k	40/1904 (2%)	39 (98%)	1 (2%)	42	73
2	l	40/1904 (2%)	40 (100%)	0	100	100
2	m	40/1904 (2%)	39 (98%)	1 (2%)	42	73
2	n	40/1904 (2%)	39 (98%)	1 (2%)	42	73
All	All	4248/26652 (16%)	4215 (99%)	33 (1%)	77	90

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Q	34	ILE
1	Q	303	THR
1	R	68	LYS
1	R	257	CYS
1	T	99	GLU
1	U	247	VAL

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Mol	Chain	Res	Type
1	U	303	THR
1	W	34	ILE
1	W	350	SER
1	W	354	GLN
1	X	167	GLU
1	X	236	LEU
1	Y	178	LEU
1	Y	247	VAL
1	Y	303	THR
1	a	247	VAL
1	a	250	ILE
1	b	34	ILE
1	b	303	THR
1	b	372	ARG
2	c	359	ILE
2	d	389	THR
2	d	397	ARG
2	e	359	ILE
2	e	397	ARG
2	f	384	ASP
2	f	397	ARG
2	i	359	ILE
2	i	397	ARG
2	j	389	THR
2	k	359	ILE
2	m	359	ILE
2	n	384	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	Q	92	ASN
1	Q	173	HIS
1	Q	225	GLN
1	Q	263	GLN
1	S	101	HIS
1	S	353	GLN
1	T	88	HIS
1	U	88	HIS
1	U	92	ASN
1	V	121	GLN
1	V	137	GLN

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Mol	Chain	Res	Type
1	V	263	GLN
1	V	353	GLN
1	W	41	GLN
1	X	173	HIS
1	X	225	GLN
1	Y	92	ASN
1	Y	263	GLN
1	Z	92	ASN
1	Z	263	GLN
1	a	59	GLN
1	a	137	GLN
1	a	173	HIS
1	a	353	GLN
1	b	173	HIS

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	Q	73	1	8,11,12	1.07	1 (12%)	5,14,16	0.75	0
1	HIC	X	73	1	8,11,12	1.07	1 (12%)	5,14,16	0.80	0
1	HIC	W	73	1	8,11,12	1.08	1 (12%)	5,14,16	0.77	0
1	HIC	S	73	1	8,11,12	1.07	1 (12%)	5,14,16	0.79	0
1	HIC	Y	73	1	8,11,12	1.07	1 (12%)	5,14,16	0.79	0
1	HIC	T	73	1	8,11,12	1.08	1 (12%)	5,14,16	0.78	0
1	HIC	R	73	1	8,11,12	1.08	1 (12%)	5,14,16	0.80	0
1	HIC	b	73	1	8,11,12	1.07	1 (12%)	5,14,16	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	HIC	a	73	1	8,11,12	1.07	1 (12%)	5,14,16	0.78	0
1	HIC	V	73	1	8,11,12	1.06	1 (12%)	5,14,16	0.80	0
1	HIC	U	73	1	8,11,12	1.09	1 (12%)	5,14,16	0.79	0
1	HIC	Z	73	1	8,11,12	1.08	1 (12%)	5,14,16	0.75	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	Q	73	1	-	0/5/6/8	0/1/1/1
1	HIC	X	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	S	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	b	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	V	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	Z	73	1	-	0/5/6/8	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	U	73	HIC	CE1-ND1	-2.30	1.31	1.34
1	R	73	HIC	CE1-ND1	-2.30	1.31	1.34
1	S	73	HIC	CE1-ND1	-2.27	1.31	1.34
1	Z	73	HIC	CE1-ND1	-2.27	1.31	1.34
1	X	73	HIC	CE1-ND1	-2.26	1.31	1.34
1	T	73	HIC	CE1-ND1	-2.26	1.31	1.34
1	W	73	HIC	CE1-ND1	-2.25	1.31	1.34
1	Q	73	HIC	CE1-ND1	-2.25	1.31	1.34
1	b	73	HIC	CE1-ND1	-2.24	1.31	1.34
1	a	73	HIC	CE1-ND1	-2.23	1.31	1.34
1	Y	73	HIC	CE1-ND1	-2.21	1.31	1.34
1	V	73	HIC	CE1-ND1	-2.20	1.31	1.34

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	R	802	3	29,33,33	2.49	6 (20%)	31,52,52	1.45	3 (9%)
4	ANP	Y	802	3	29,33,33	2.48	6 (20%)	31,52,52	1.46	3 (9%)
4	ANP	T	802	3	29,33,33	2.48	6 (20%)	31,52,52	1.47	3 (9%)
4	ANP	b	802	3	29,33,33	2.50	6 (20%)	31,52,52	1.45	3 (9%)
4	ANP	U	802	3	29,33,33	2.48	6 (20%)	31,52,52	1.45	3 (9%)
4	ANP	X	802	3	29,33,33	2.49	6 (20%)	31,52,52	1.45	3 (9%)
4	ANP	a	802	3	29,33,33	2.47	6 (20%)	31,52,52	1.46	3 (9%)
4	ANP	S	802	3	29,33,33	2.49	6 (20%)	31,52,52	1.46	3 (9%)
4	ANP	V	802	3	29,33,33	2.48	6 (20%)	31,52,52	1.47	3 (9%)
4	ANP	W	802	3	29,33,33	2.49	6 (20%)	31,52,52	1.46	3 (9%)
4	ANP	Z	802	3	29,33,33	2.50	6 (20%)	31,52,52	1.45	3 (9%)
4	ANP	Q	802	3	29,33,33	2.47	6 (20%)	31,52,52	1.48	3 (9%)

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	R	802	3	-	3/14/38/38	0/3/3/3
4	ANP	Y	802	3	-	2/14/38/38	0/3/3/3
4	ANP	T	802	3	-	2/14/38/38	0/3/3/3
4	ANP	b	802	3	-	2/14/38/38	0/3/3/3
4	ANP	U	802	3	-	3/14/38/38	0/3/3/3
4	ANP	X	802	3	-	2/14/38/38	0/3/3/3
4	ANP	a	802	3	-	2/14/38/38	0/3/3/3
4	ANP	S	802	3	-	2/14/38/38	0/3/3/3
4	ANP	V	802	3	-	4/14/38/38	0/3/3/3
4	ANP	W	802	3	-	2/14/38/38	0/3/3/3
4	ANP	Z	802	3	-	3/14/38/38	0/3/3/3
4	ANP	Q	802	3	-	2/14/38/38	0/3/3/3

All (72) 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
4	V	802	ANP	PB-O3A	8.78	1.70	1.59
4	R	802	ANP	PB-O3A	8.78	1.70	1.59
4	W	802	ANP	PB-O3A	8.76	1.70	1.59
4	T	802	ANP	PB-O3A	8.72	1.69	1.59
4	Y	802	ANP	PB-O3A	8.72	1.69	1.59
4	U	802	ANP	PB-O3A	8.69	1.69	1.59
4	a	802	ANP	PB-O3A	8.65	1.69	1.59
4	Q	802	ANP	PB-O3A	8.62	1.69	1.59
4	Z	802	ANP	PG-N3B	6.39	1.80	1.63
4	S	802	ANP	PG-N3B	6.38	1.80	1.63
4	X	802	ANP	PG-N3B	6.37	1.80	1.63
4	T	802	ANP	PG-N3B	6.36	1.80	1.63
4	Q	802	ANP	PG-N3B	6.36	1.80	1.63
4	b	802	ANP	PG-N3B	6.35	1.80	1.63
4	W	802	ANP	PG-N3B	6.35	1.79	1.63
4	U	802	ANP	PG-N3B	6.34	1.79	1.63
4	Y	802	ANP	PG-N3B	6.34	1.79	1.63
4	a	802	ANP	PG-N3B	6.34	1.79	1.63
4	R	802	ANP	PG-N3B	6.33	1.79	1.63
4	V	802	ANP	PG-N3B	6.31	1.79	1.63
4	b	802	ANP	PG-O1G	4.69	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	U	802	ANP	PG-O1G	4.68	1.53	1.46
4	Z	802	ANP	PG-O1G	4.68	1.53	1.46
4	T	802	ANP	PG-O1G	4.67	1.53	1.46
4	X	802	ANP	PG-O1G	4.66	1.53	1.46
4	a	802	ANP	PG-O1G	4.66	1.53	1.46
4	R	802	ANP	PG-O1G	4.65	1.53	1.46
4	Q	802	ANP	PG-O1G	4.62	1.53	1.46
4	W	802	ANP	PG-O1G	4.61	1.53	1.46
4	S	802	ANP	PG-O1G	4.60	1.53	1.46
4	Y	802	ANP	PG-O1G	4.58	1.53	1.46
4	V	802	ANP	PG-O1G	4.56	1.53	1.46
4	Q	802	ANP	PB-O1B	2.72	1.50	1.46
4	V	802	ANP	PB-O1B	2.72	1.50	1.46
4	b	802	ANP	PB-O1B	2.71	1.50	1.46
4	X	802	ANP	PB-O1B	2.69	1.50	1.46
4	Y	802	ANP	PB-O1B	2.69	1.50	1.46
4	T	802	ANP	PB-O1B	2.69	1.50	1.46
4	a	802	ANP	PB-O1B	2.68	1.50	1.46
4	Z	802	ANP	PB-O1B	2.67	1.50	1.46
4	S	802	ANP	PB-O1B	2.66	1.50	1.46
4	U	802	ANP	PB-O1B	2.65	1.50	1.46
4	W	802	ANP	PB-O1B	2.65	1.50	1.46
4	R	802	ANP	PB-O1B	2.64	1.50	1.46
4	Y	802	ANP	C8-N7	-2.36	1.30	1.34
4	U	802	ANP	C8-N7	-2.34	1.30	1.34
4	b	802	ANP	C8-N7	-2.33	1.30	1.34
4	W	802	ANP	C8-N7	-2.33	1.30	1.34
4	a	802	ANP	C8-N7	-2.31	1.30	1.34
4	X	802	ANP	C8-N7	-2.31	1.30	1.34
4	Q	802	ANP	C8-N7	-2.29	1.30	1.34
4	R	802	ANP	C8-N7	-2.28	1.30	1.34
4	T	802	ANP	C8-N7	-2.27	1.30	1.34
4	Z	802	ANP	C8-N7	-2.27	1.30	1.34
4	V	802	ANP	C8-N7	-2.27	1.30	1.34
4	S	802	ANP	C8-N7	-2.23	1.30	1.34
4	Q	802	ANP	PB-O2B	-2.12	1.51	1.56
4	R	802	ANP	PB-O2B	-2.12	1.51	1.56
4	X	802	ANP	PB-O2B	-2.11	1.51	1.56
4	Z	802	ANP	PB-O2B	-2.11	1.51	1.56
4	S	802	ANP	PB-O2B	-2.10	1.51	1.56
4	U	802	ANP	PB-O2B	-2.10	1.51	1.56
4	T	802	ANP	PB-O2B	-2.10	1.51	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	V	802	ANP	PB-O2B	-2.09	1.51	1.56
4	W	802	ANP	PB-O2B	-2.09	1.51	1.56
4	b	802	ANP	PB-O2B	-2.09	1.51	1.56
4	a	802	ANP	PB-O2B	-2.08	1.51	1.56
4	Y	802	ANP	PB-O2B	-2.08	1.51	1.56

All (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
4	Z	802	ANP	O2B-PB-O1B	4.68	119.90	109.87
4	X	802	ANP	O2B-PB-O1B	4.67	119.89	109.87
4	T	802	ANP	O2B-PB-O1B	4.66	119.86	109.87
4	W	802	ANP	O2B-PB-O1B	4.66	119.86	109.87
4	S	802	ANP	O2B-PB-O1B	4.66	119.86	109.87
4	Y	802	ANP	O2B-PB-O1B	4.62	119.79	109.87
4	a	802	ANP	O2B-PB-O1B	4.62	119.78	109.87
4	Q	802	ANP	O1G-PG-N3B	-4.23	105.55	111.77
4	S	802	ANP	O1G-PG-N3B	-4.21	105.57	111.77
4	W	802	ANP	O1G-PG-N3B	-4.13	105.69	111.77
4	V	802	ANP	O1G-PG-N3B	-4.10	105.73	111.77
4	T	802	ANP	O1G-PG-N3B	-4.08	105.76	111.77
4	a	802	ANP	O1G-PG-N3B	-4.07	105.77	111.77
4	X	802	ANP	O1G-PG-N3B	-4.07	105.78	111.77
4	Y	802	ANP	O1G-PG-N3B	-4.07	105.78	111.77
4	U	802	ANP	O1G-PG-N3B	-4.04	105.82	111.77
4	R	802	ANP	O1G-PG-N3B	-4.04	105.83	111.77
4	b	802	ANP	O1G-PG-N3B	-4.03	105.83	111.77
4	Z	802	ANP	O1G-PG-N3B	-3.97	105.92	111.77
4	V	802	ANP	O2G-PG-O3G	2.62	114.64	107.59
4	Y	802	ANP	O2G-PG-O3G	2.61	114.61	107.59
4	R	802	ANP	O2G-PG-O3G	2.60	114.57	107.59
4	W	802	ANP	O2G-PG-O3G	2.59	114.54	107.59
4	U	802	ANP	O2G-PG-O3G	2.58	114.51	107.59
4	T	802	ANP	O2G-PG-O3G	2.57	114.49	107.59
4	Q	802	ANP	O2G-PG-O3G	2.56	114.48	107.59
4	b	802	ANP	O2G-PG-O3G	2.56	114.47	107.59
4	a	802	ANP	O2G-PG-O3G	2.56	114.47	107.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	X	802	ANP	O2G-PG-O3G	2.56	114.46	107.59
4	S	802	ANP	O2G-PG-O3G	2.55	114.45	107.59
4	Z	802	ANP	O2G-PG-O3G	2.54	114.43	107.59

There are no chirality outliers.

All (29) torsion outliers are listed below:

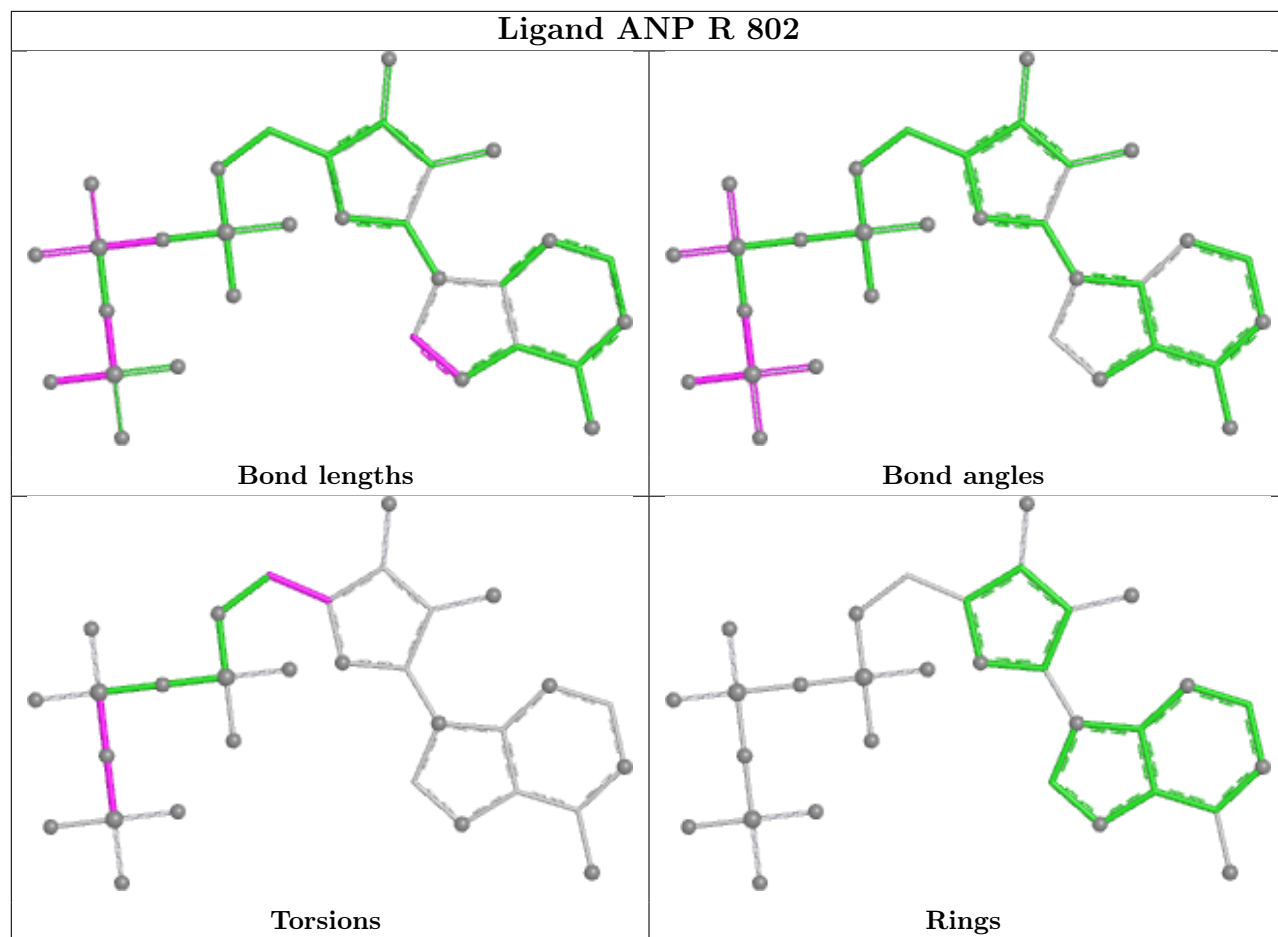
Mol	Chain	Res	Type	Atoms
4	Q	802	ANP	PB-N3B-PG-O1G
4	Q	802	ANP	PG-N3B-PB-O1B
4	R	802	ANP	PB-N3B-PG-O1G
4	S	802	ANP	PB-N3B-PG-O1G
4	S	802	ANP	PG-N3B-PB-O1B
4	T	802	ANP	PB-N3B-PG-O1G
4	T	802	ANP	PG-N3B-PB-O1B
4	U	802	ANP	PB-N3B-PG-O1G
4	U	802	ANP	PG-N3B-PB-O1B
4	V	802	ANP	PG-N3B-PB-O1B
4	W	802	ANP	PB-N3B-PG-O1G
4	W	802	ANP	PG-N3B-PB-O1B
4	X	802	ANP	PB-N3B-PG-O1G
4	Y	802	ANP	PB-N3B-PG-O1G
4	Y	802	ANP	PG-N3B-PB-O1B
4	Z	802	ANP	PB-N3B-PG-O1G
4	a	802	ANP	PB-N3B-PG-O1G
4	a	802	ANP	PG-N3B-PB-O1B
4	b	802	ANP	PB-N3B-PG-O1G
4	V	802	ANP	C3'-C4'-C5'-O5'
4	X	802	ANP	PG-N3B-PB-O1B
4	Z	802	ANP	PG-N3B-PB-O1B
4	b	802	ANP	PG-N3B-PB-O1B
4	V	802	ANP	O4'-C4'-C5'-O5'
4	U	802	ANP	C3'-C4'-C5'-O5'
4	V	802	ANP	PA-O3A-PB-O1B
4	Z	802	ANP	PA-O3A-PB-O1B
4	R	802	ANP	PG-N3B-PB-O3A
4	R	802	ANP	C3'-C4'-C5'-O5'

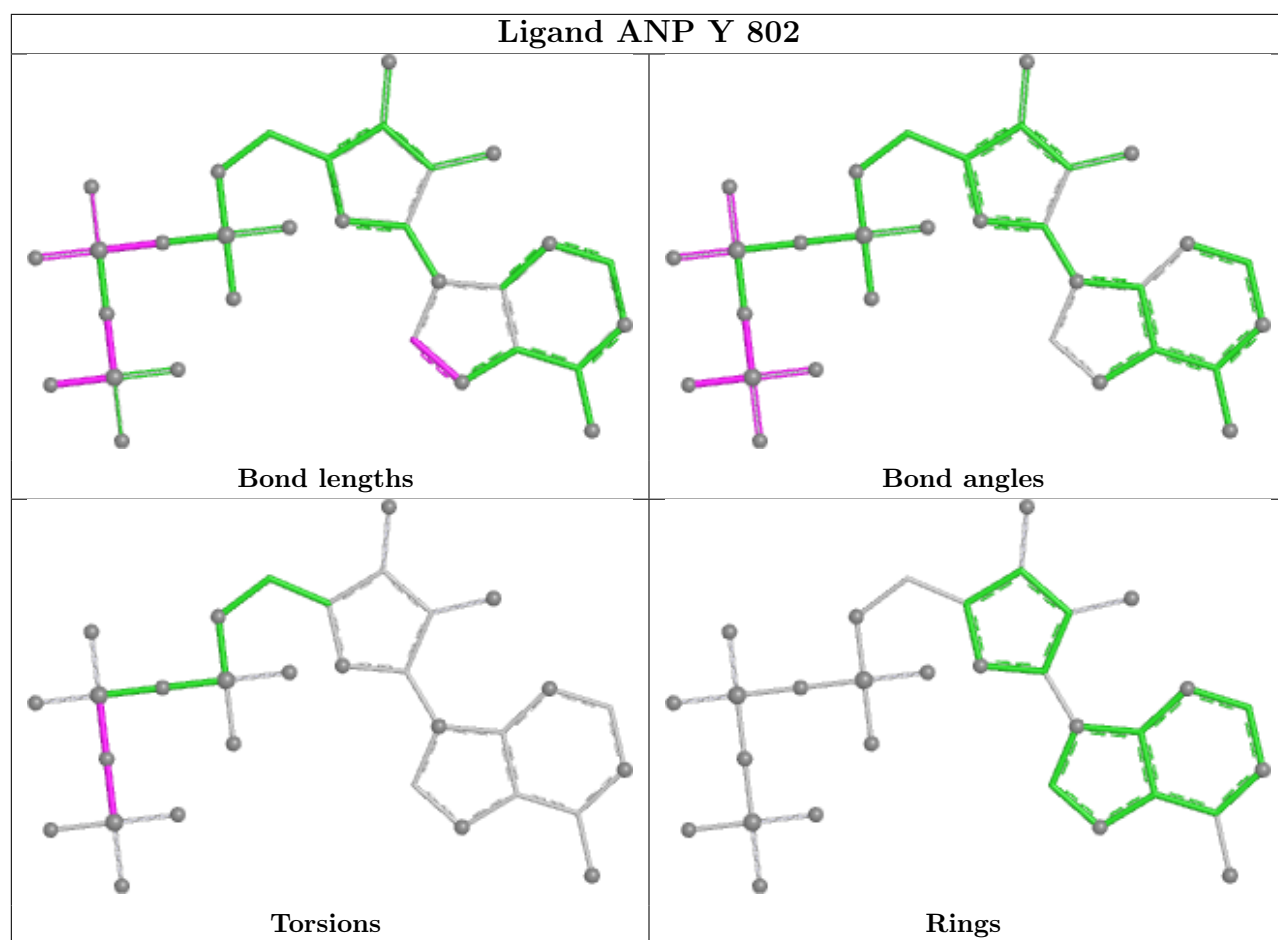
There are no ring outliers.

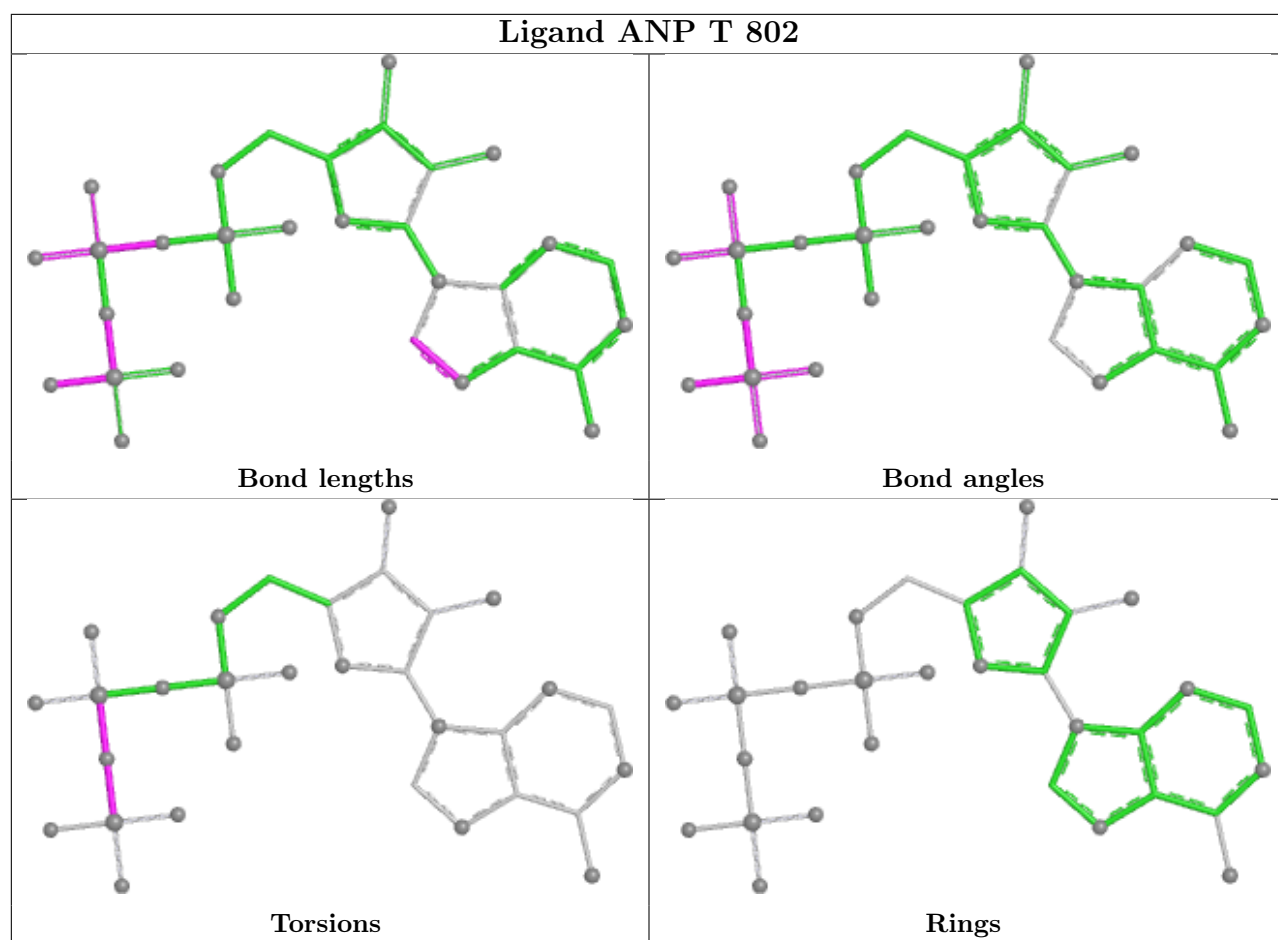
12 monomers are involved in 28 short contacts:

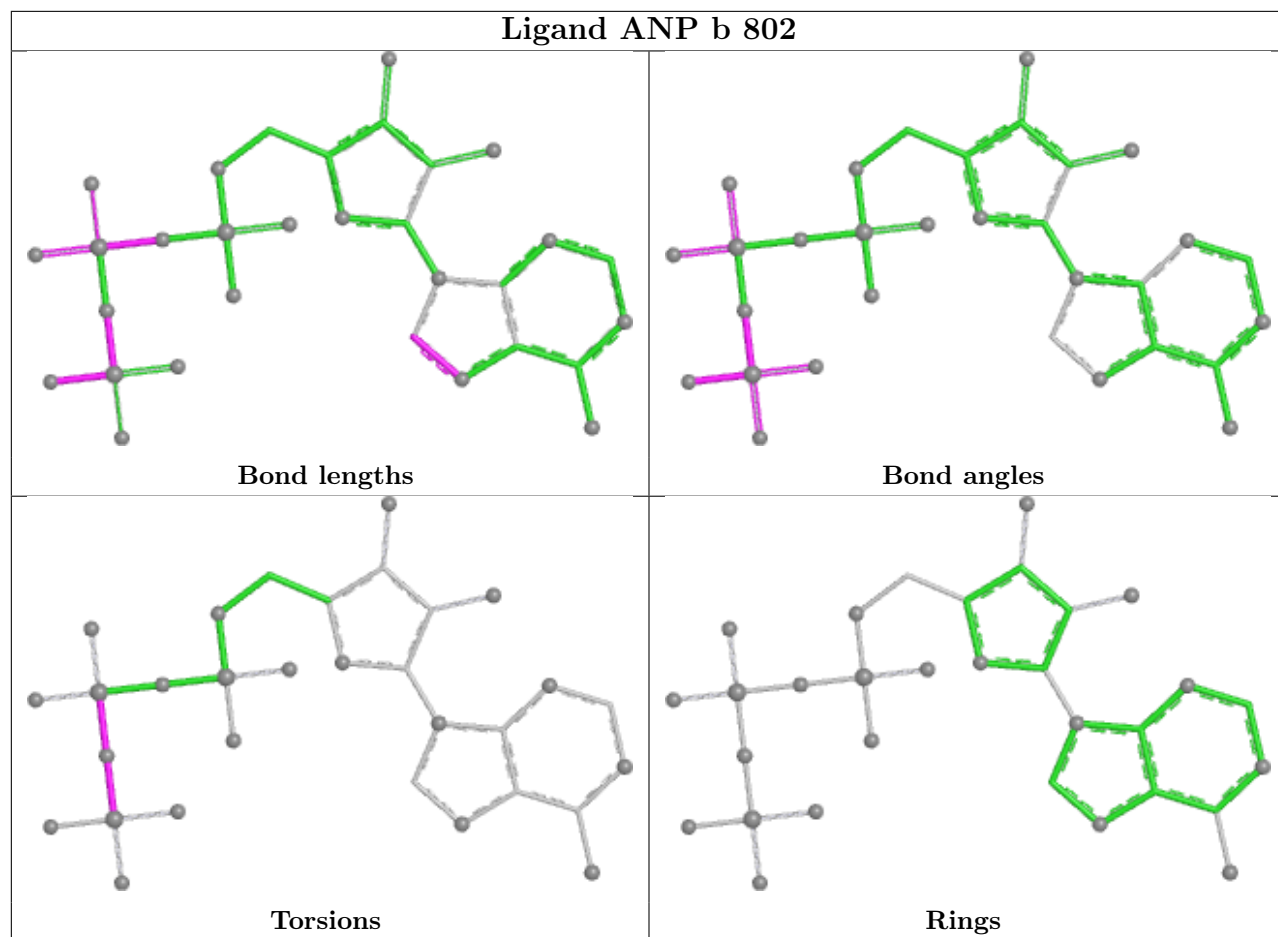
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	R	802	ANP	2	0
4	Y	802	ANP	2	0
4	T	802	ANP	2	0
4	b	802	ANP	2	0
4	U	802	ANP	2	0
4	X	802	ANP	2	0
4	a	802	ANP	2	0
4	S	802	ANP	4	0
4	V	802	ANP	3	0
4	W	802	ANP	2	0
4	Z	802	ANP	2	0
4	Q	802	ANP	3	0

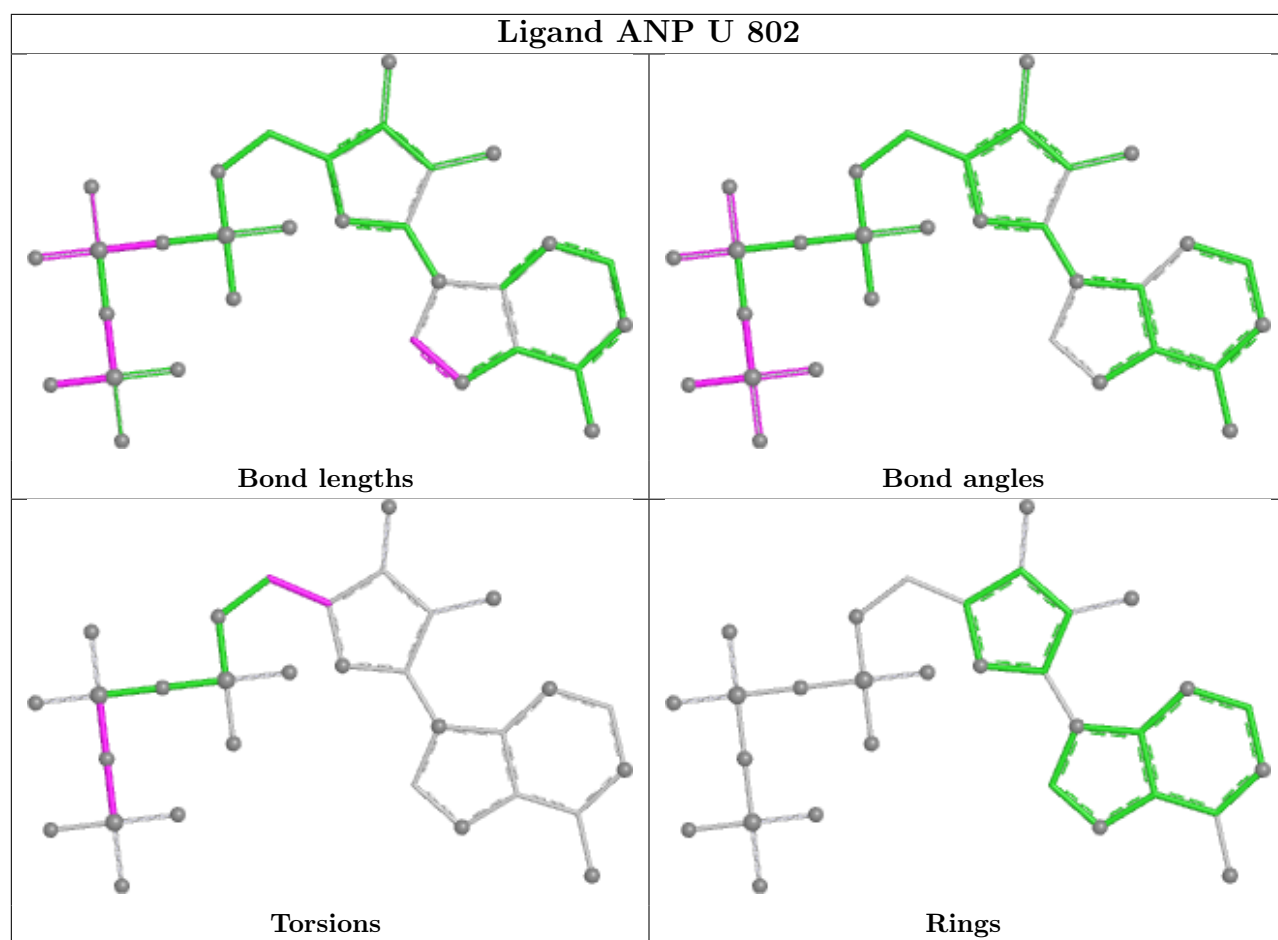
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

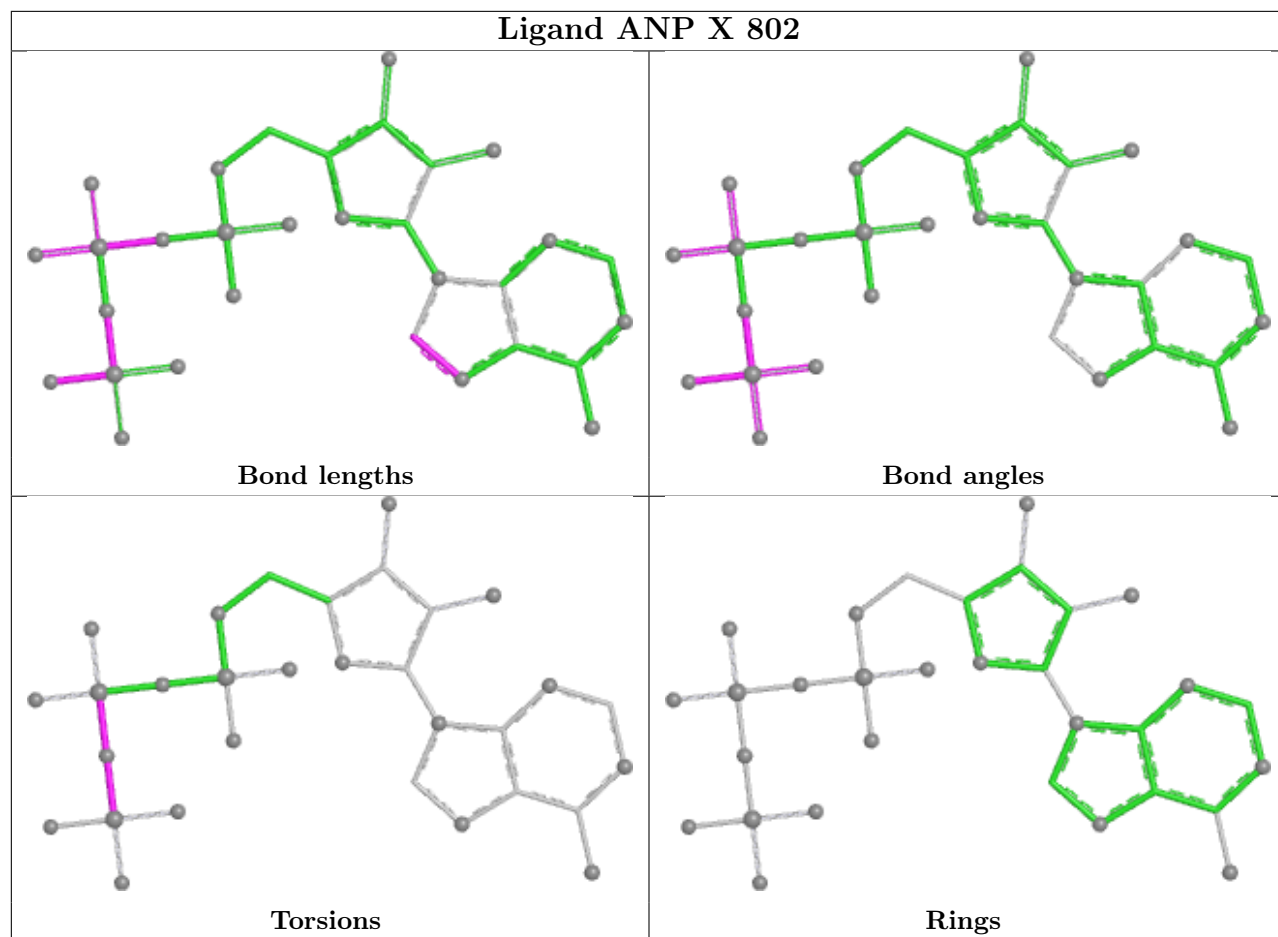


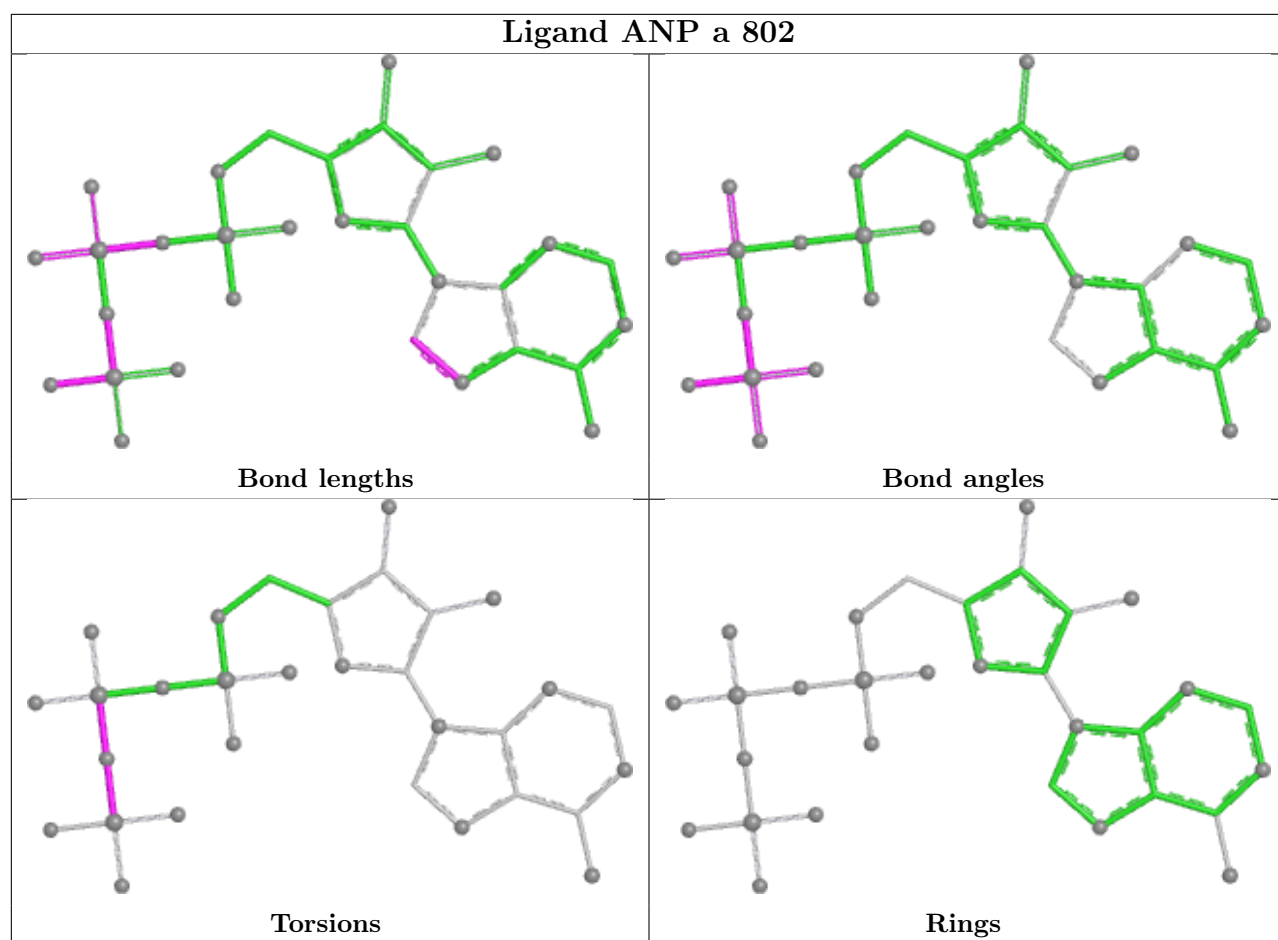


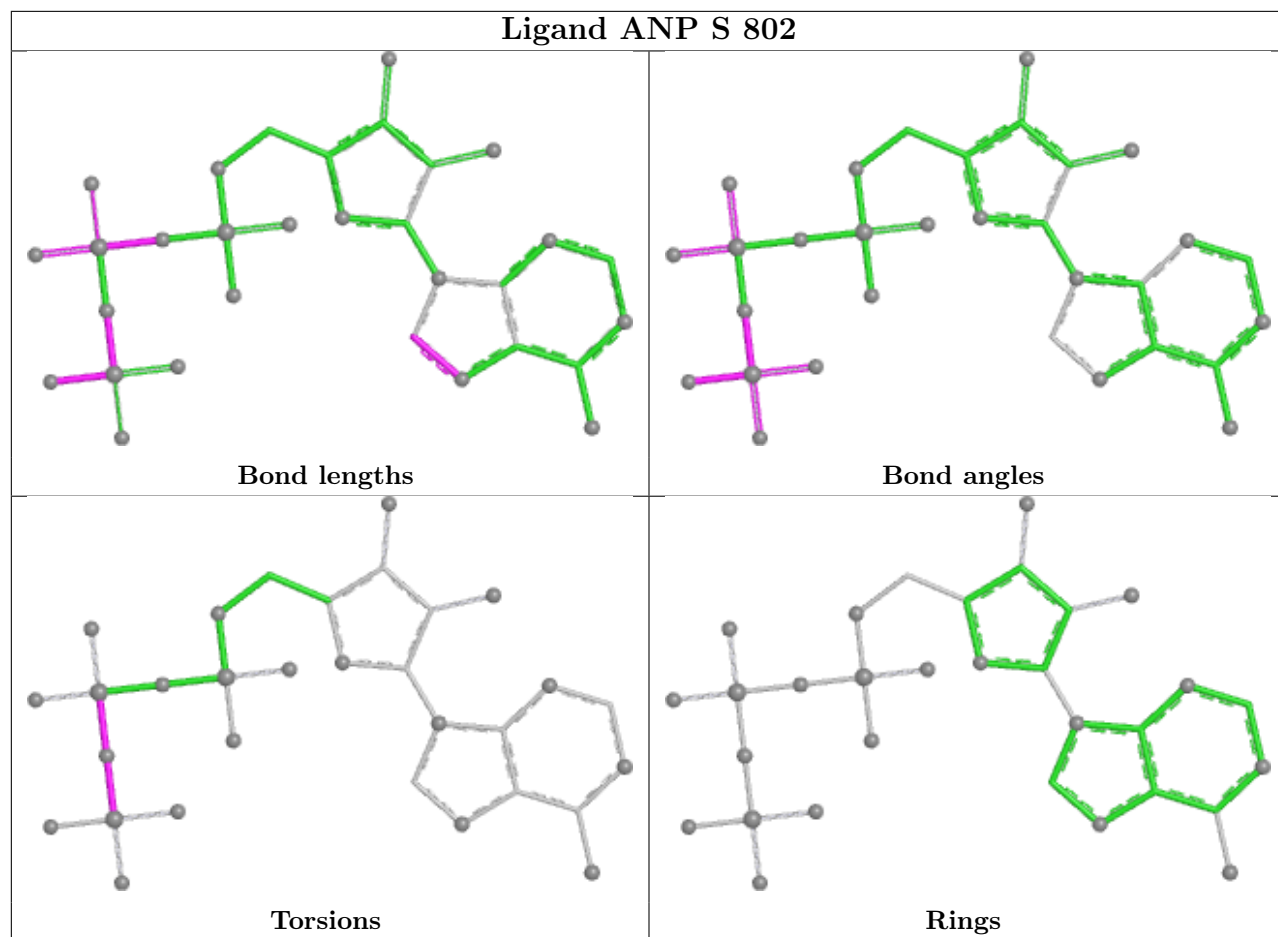


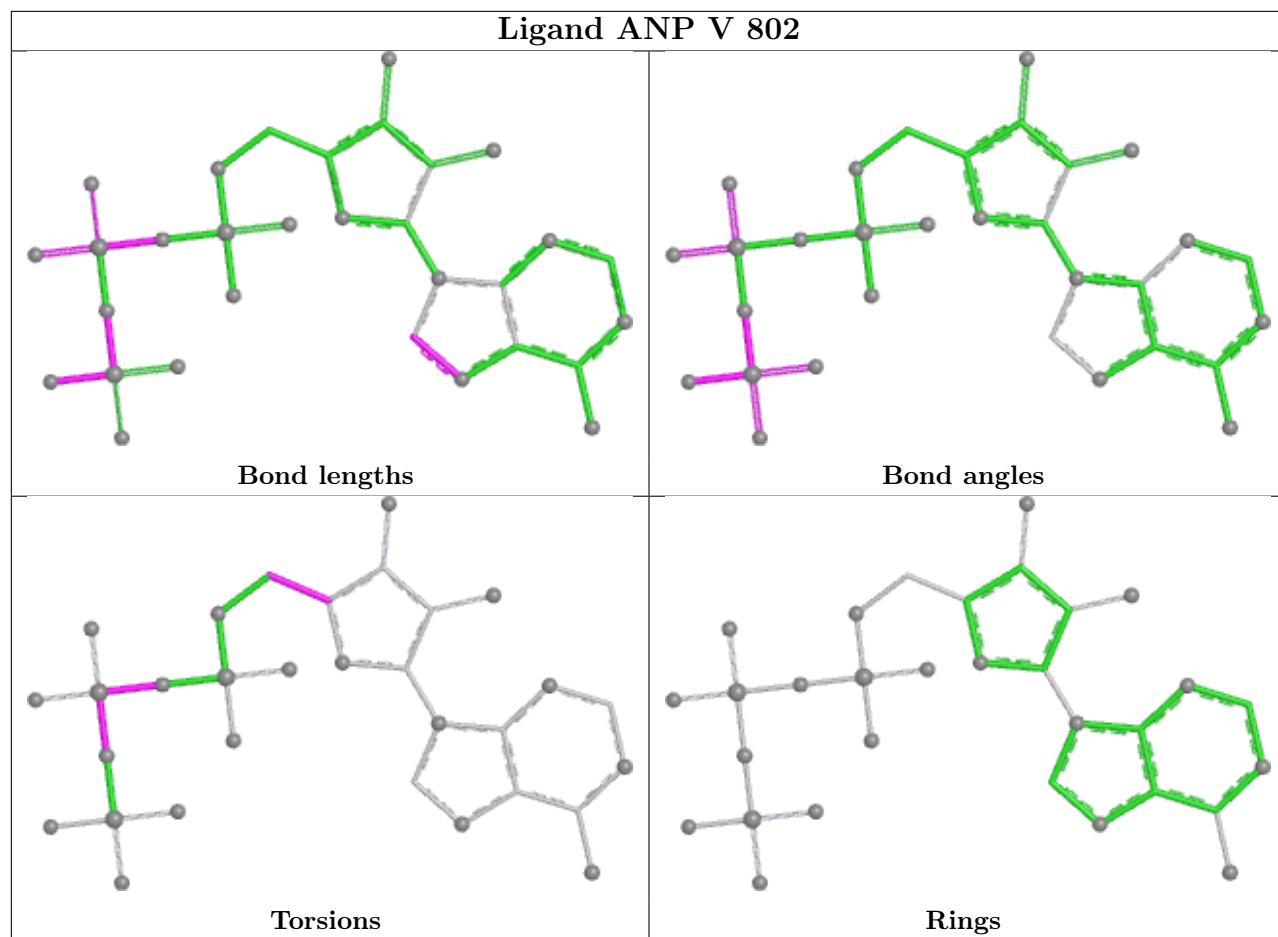


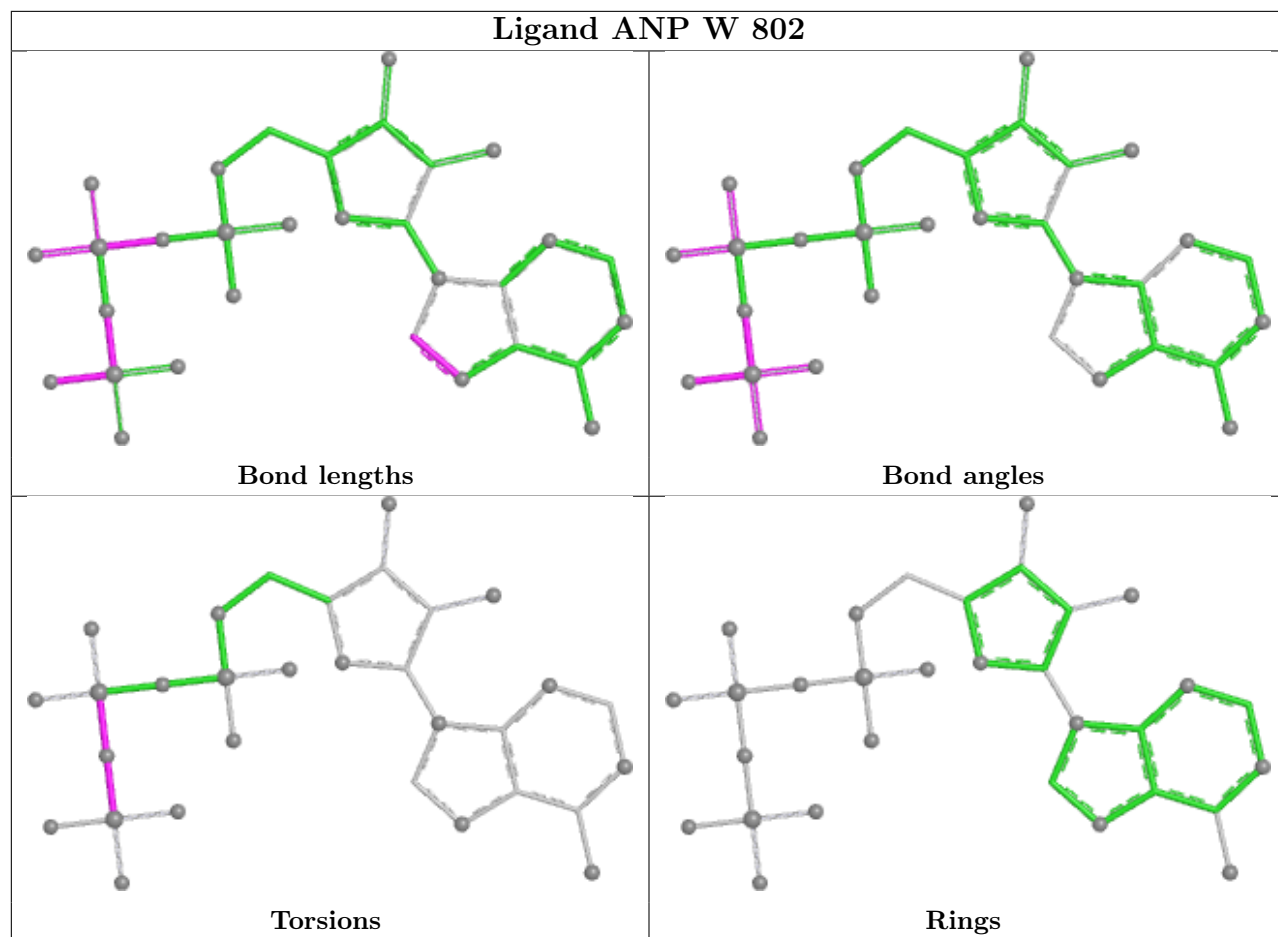


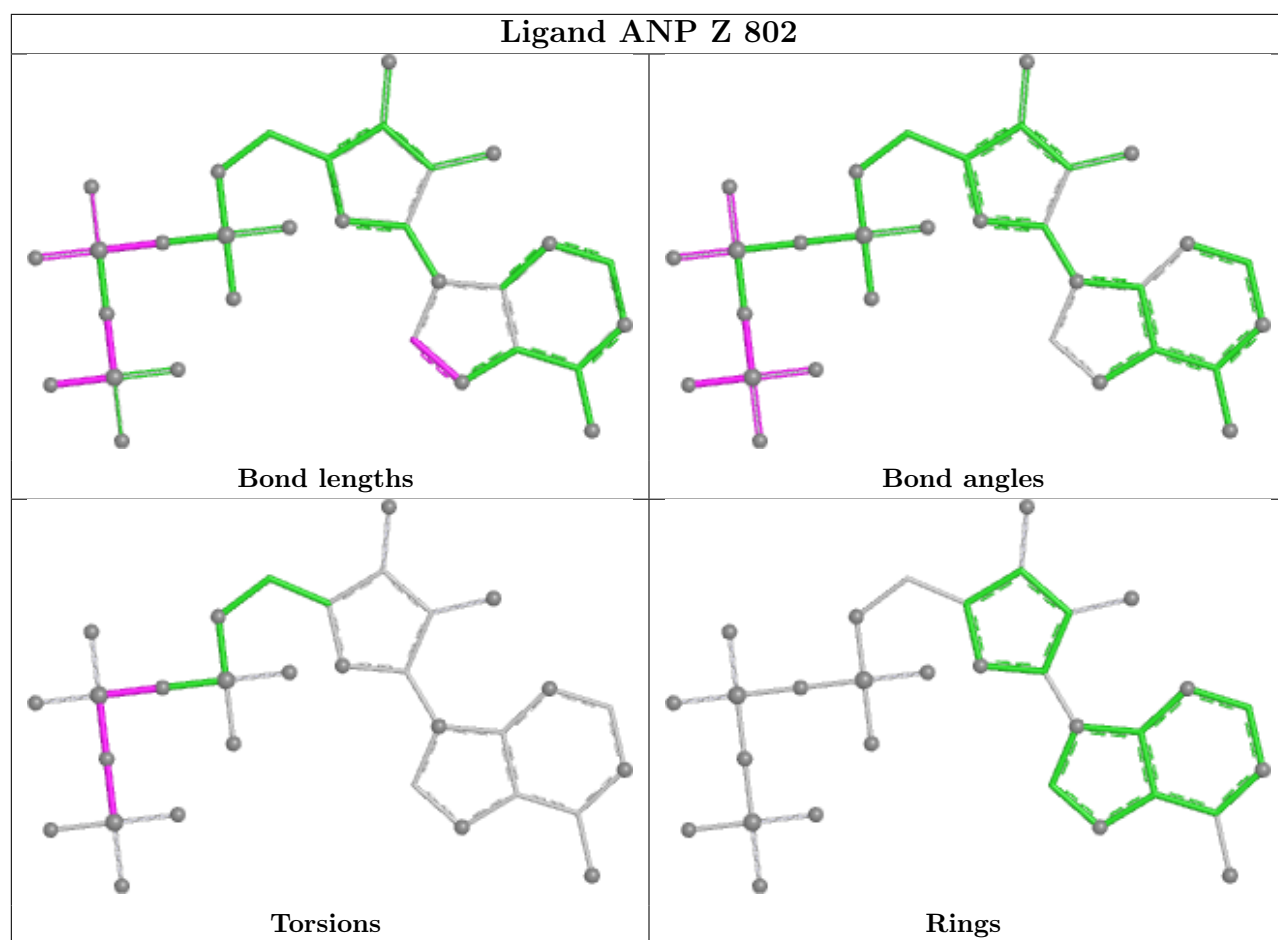


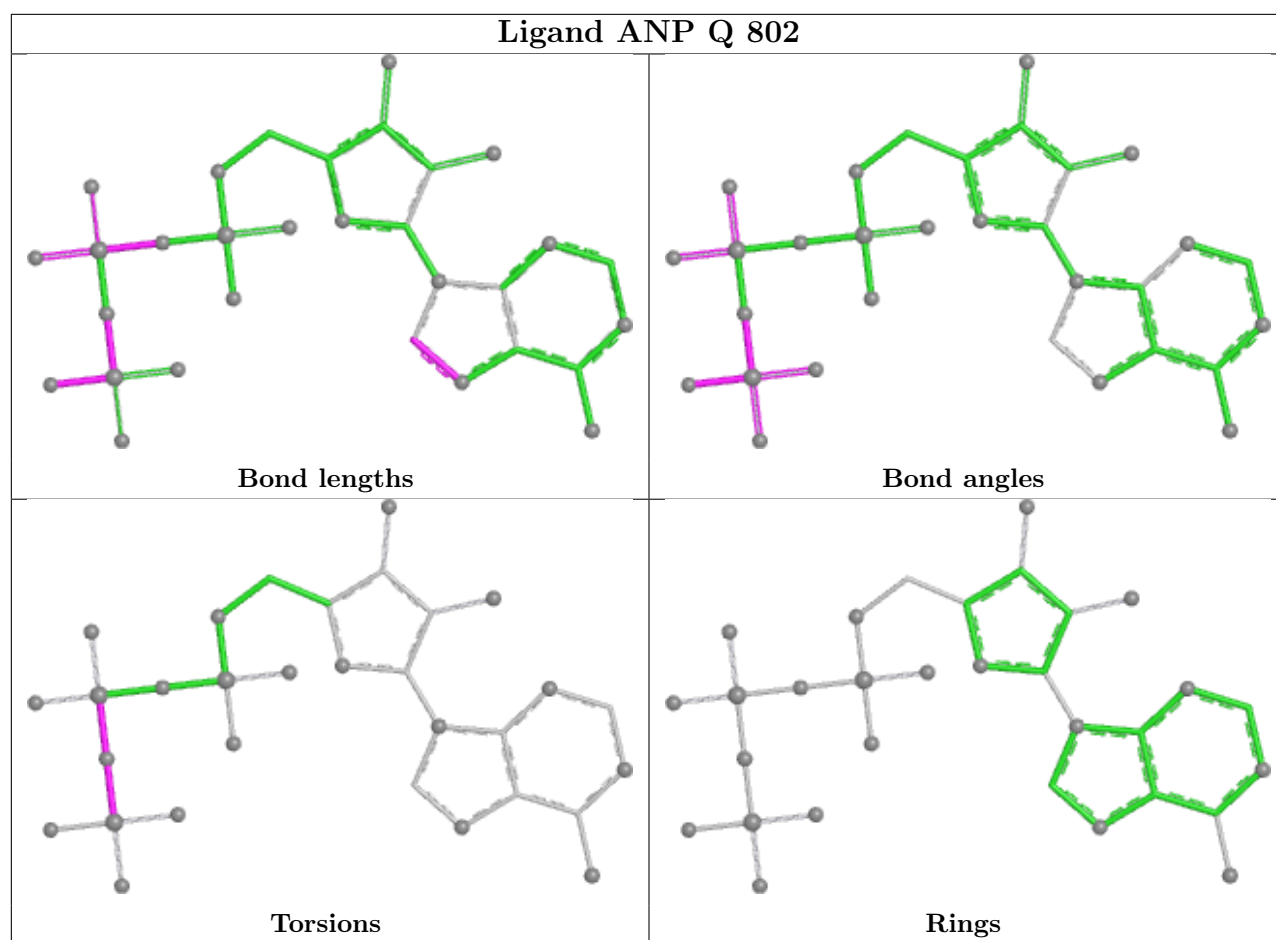












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

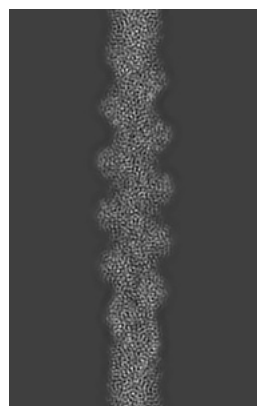
6 Map visualisation [i](#)

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.

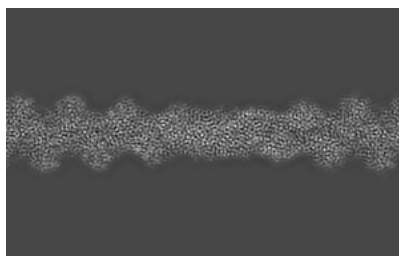
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

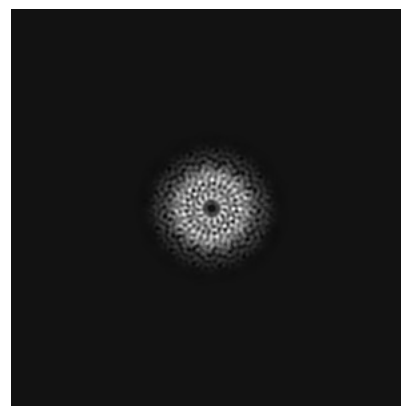
6.1.1 Primary map



X

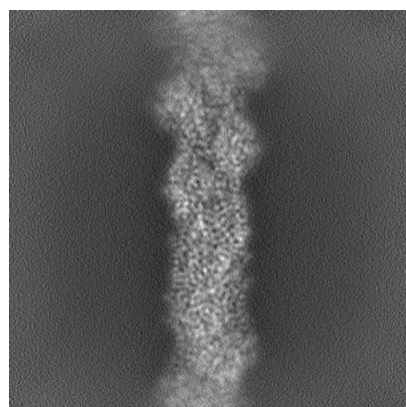


Y

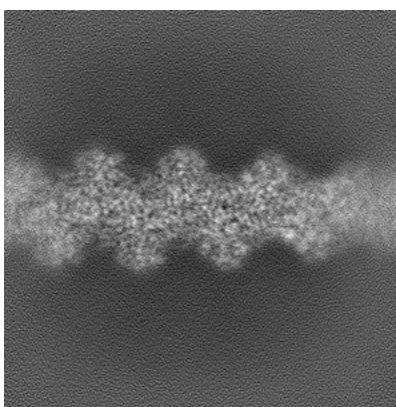


Z

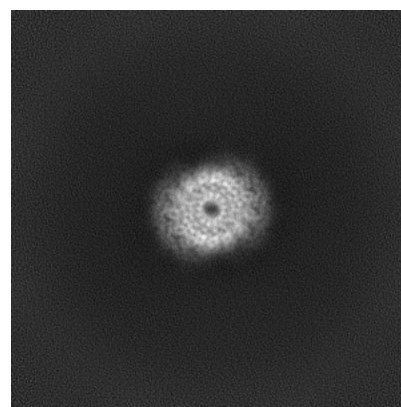
6.1.2 Raw map



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

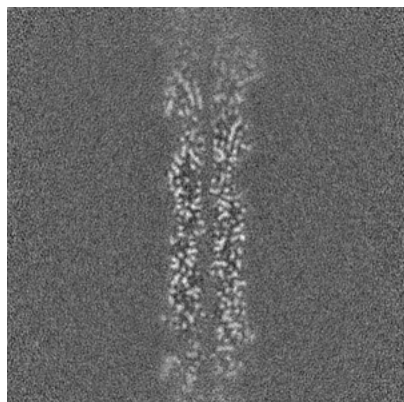


Y Index: 160

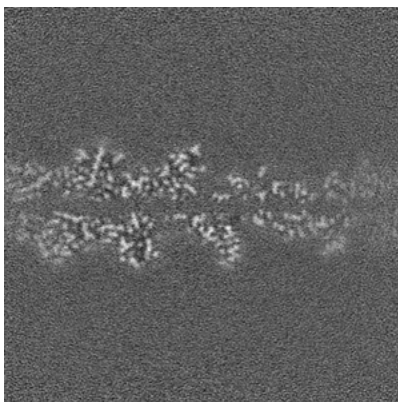


Z Index: 256

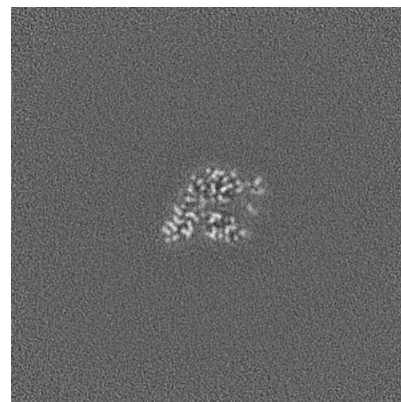
6.2.2 Raw map



X Index: 160



Y Index: 160

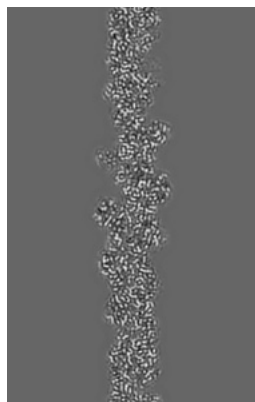


Z Index: 160

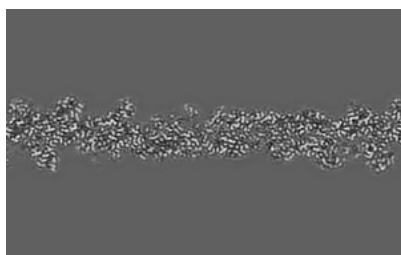
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

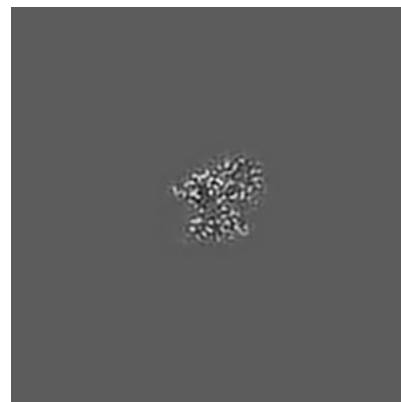
6.3.1 Primary map



X Index: 152

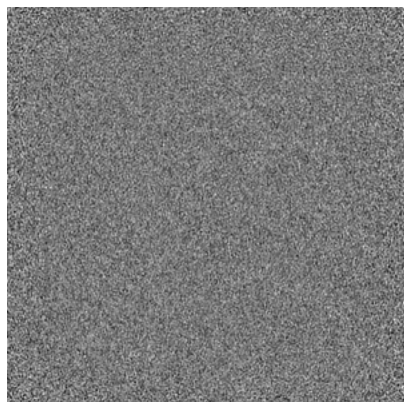


Y Index: 170

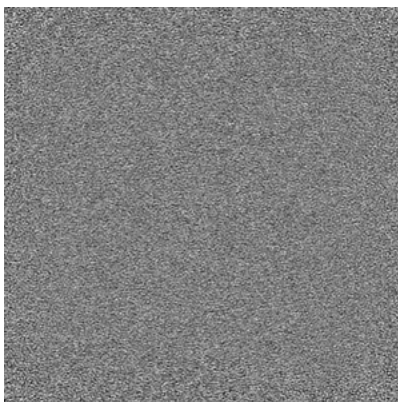


Z Index: 143

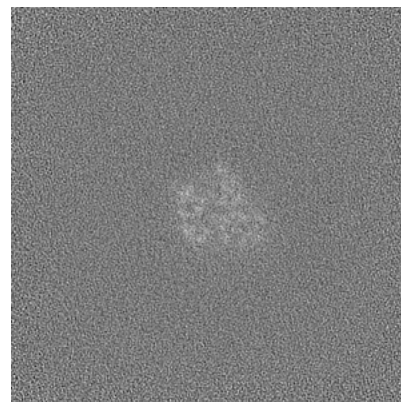
6.3.2 Raw map



X Index: 0



Y Index: 0

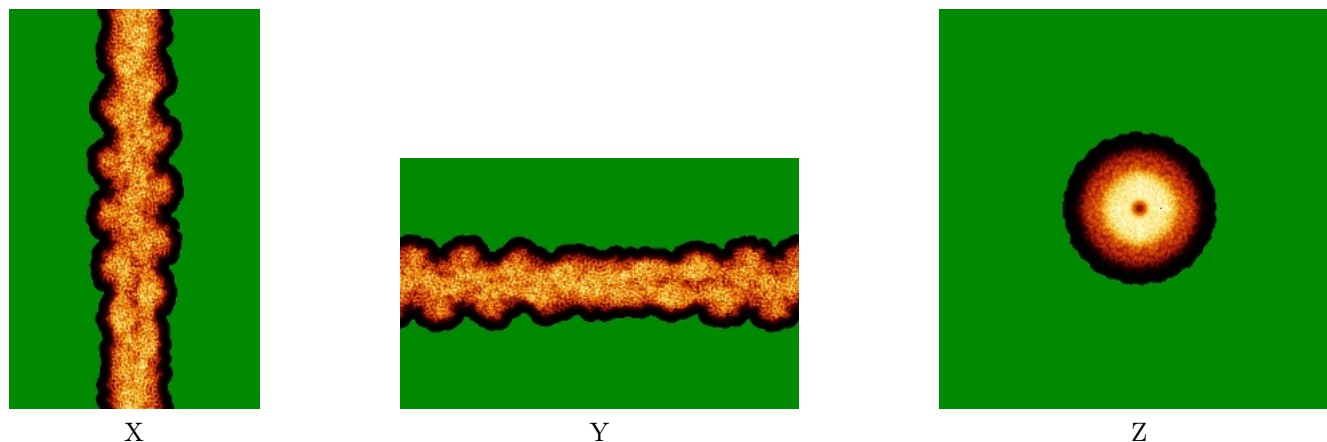


Z Index: 0

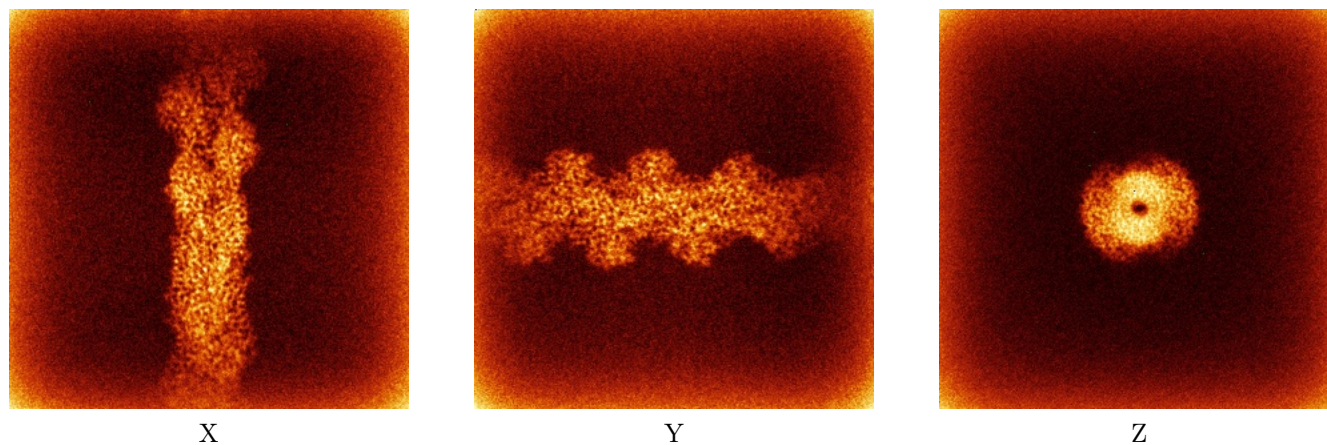
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



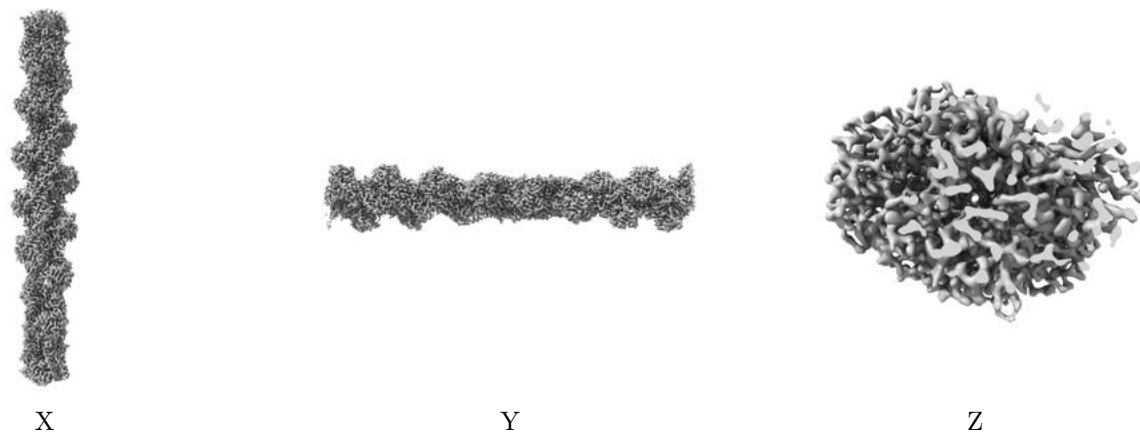
6.4.2 Raw map



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.

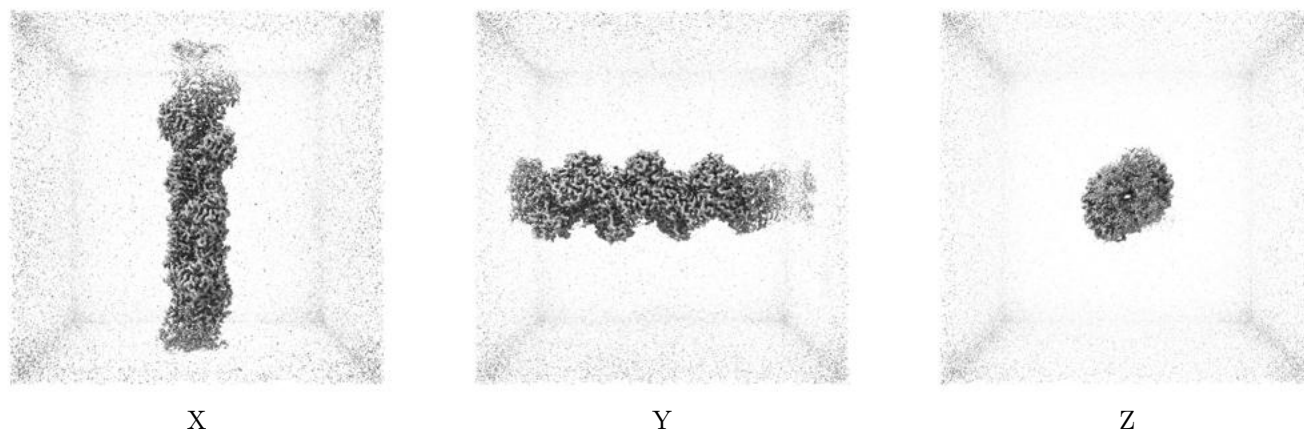
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.307. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

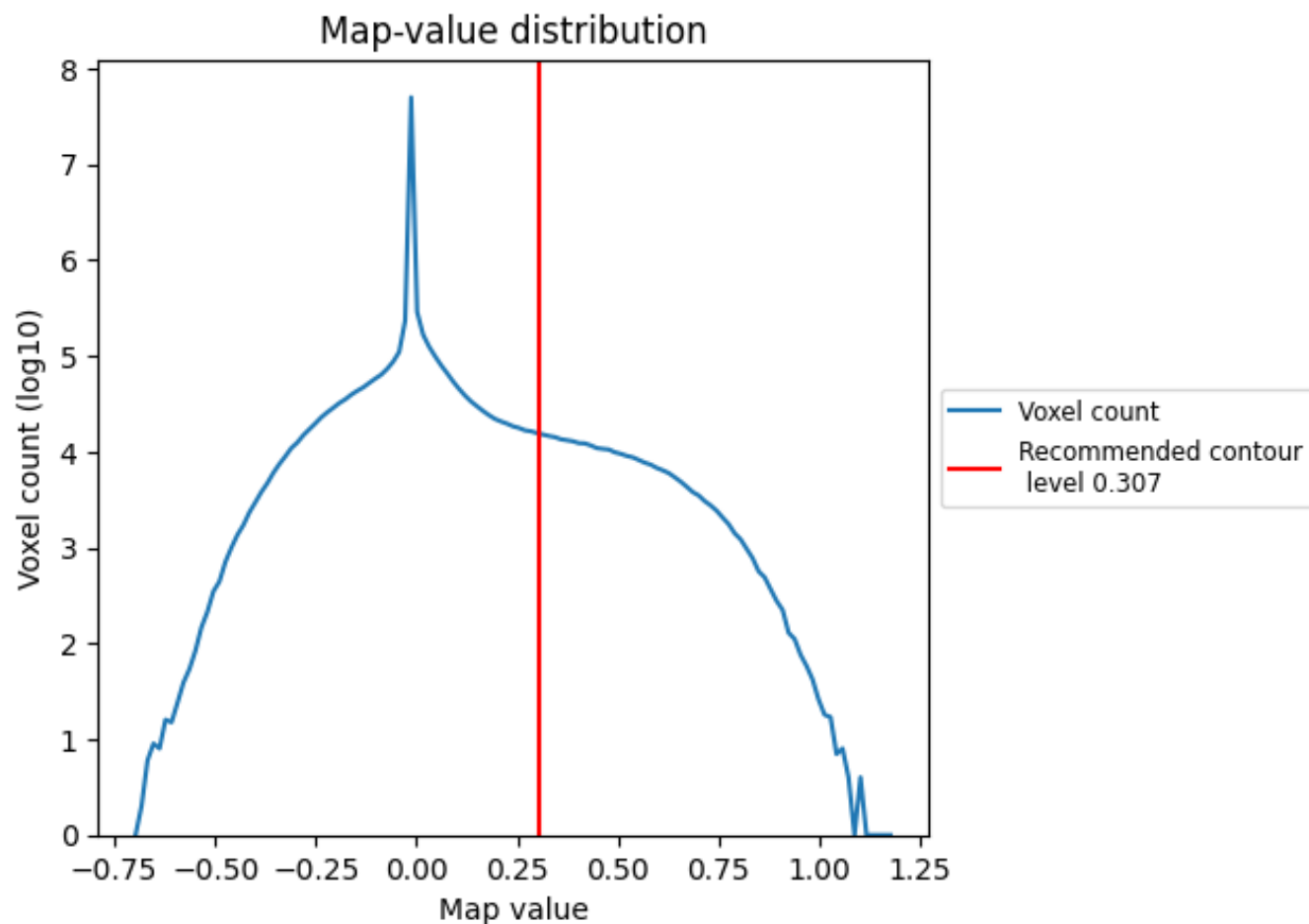
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

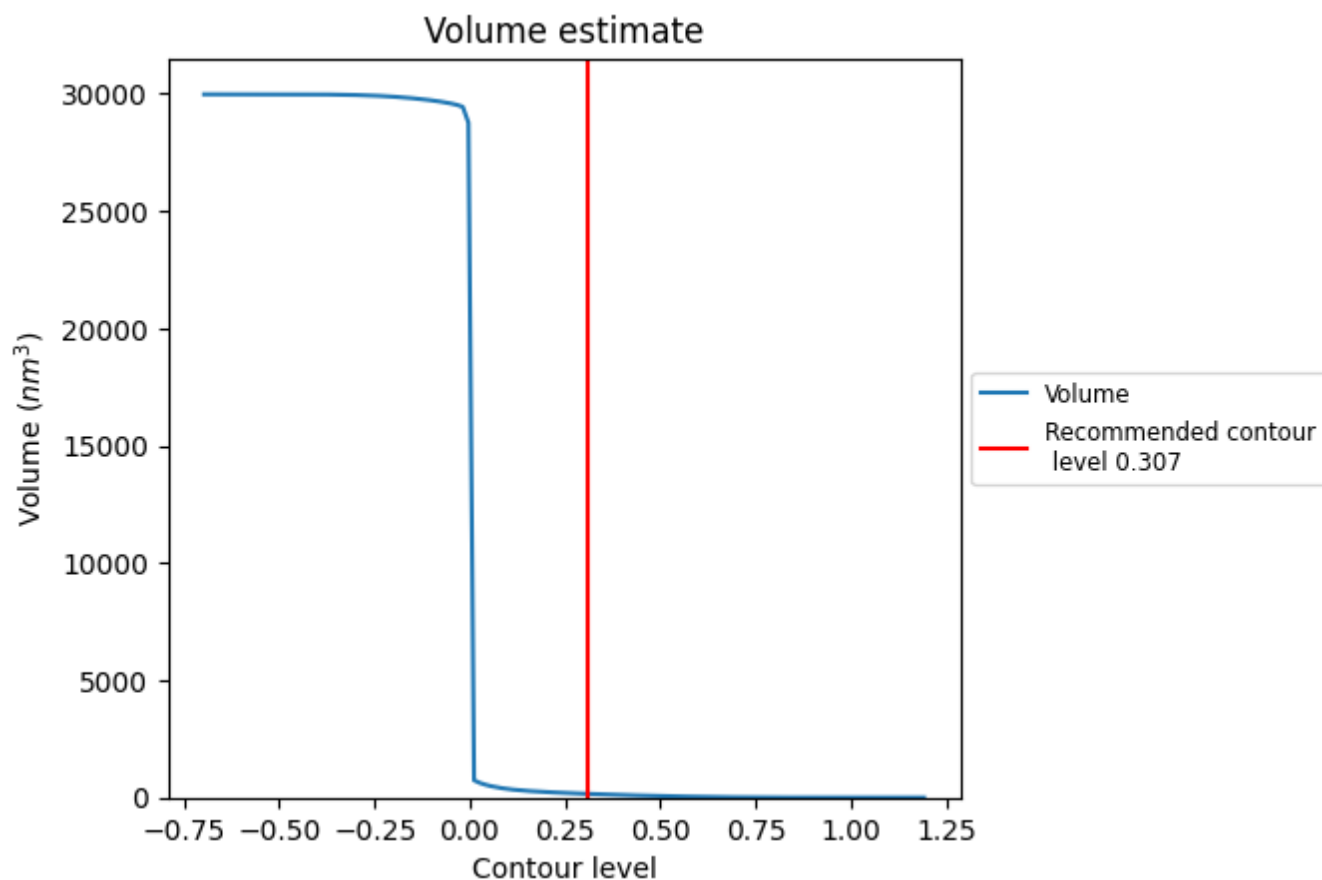
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 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.

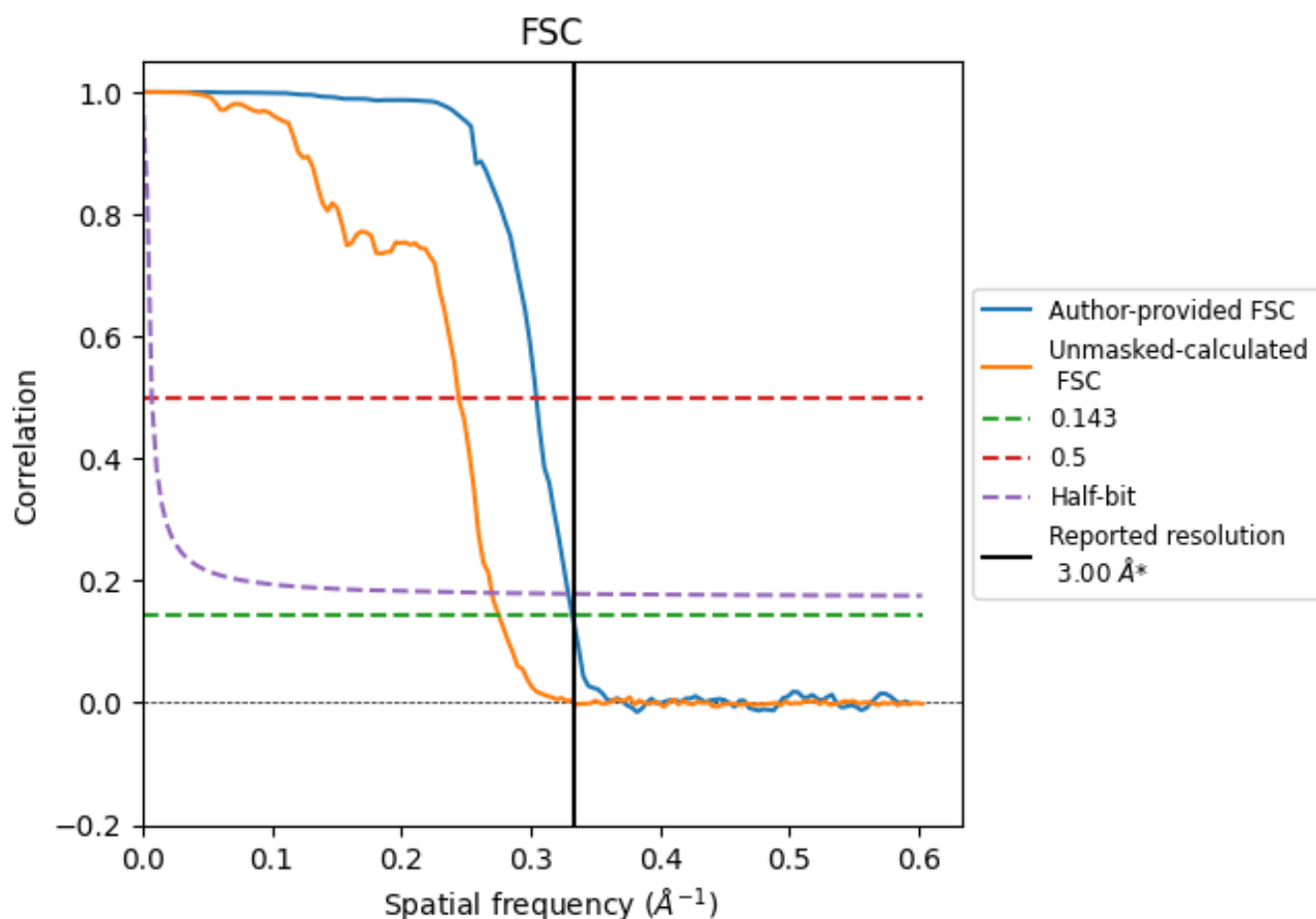
7.3 Rotationally averaged power spectrum [i](#)

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](#)

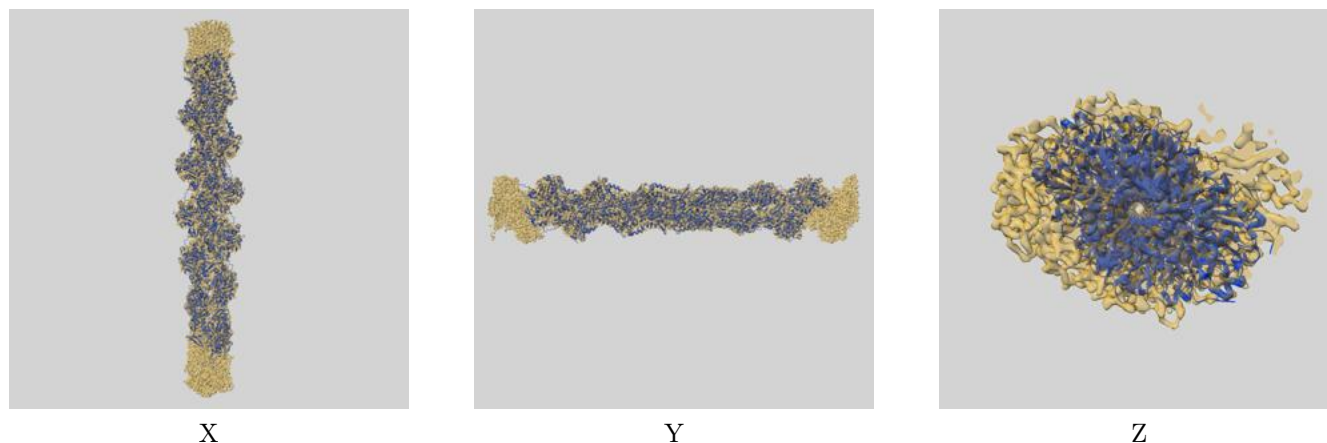
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.01	3.29	3.04
Unmasked-calculated*	3.63	4.09	3.70

*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](#)

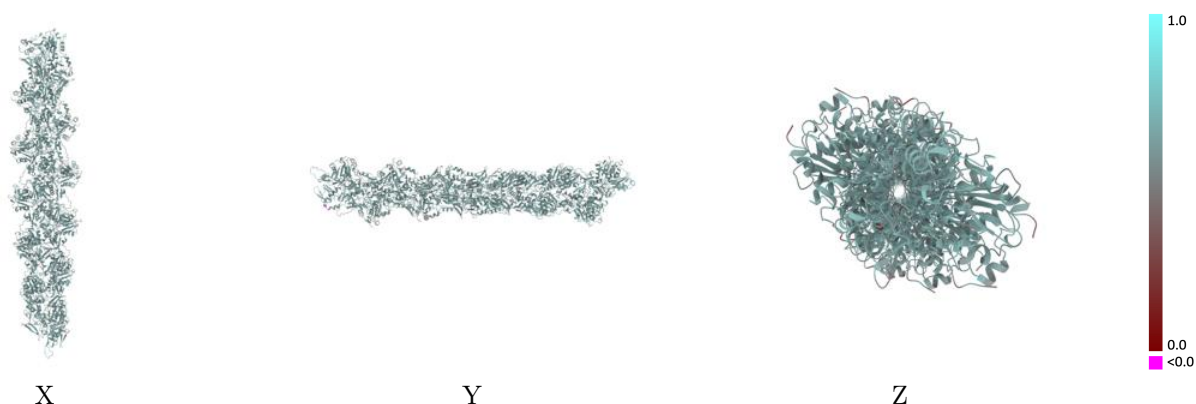
This section contains information regarding the fit between EMDB map EMD-71108 and PDB model 9P1I. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



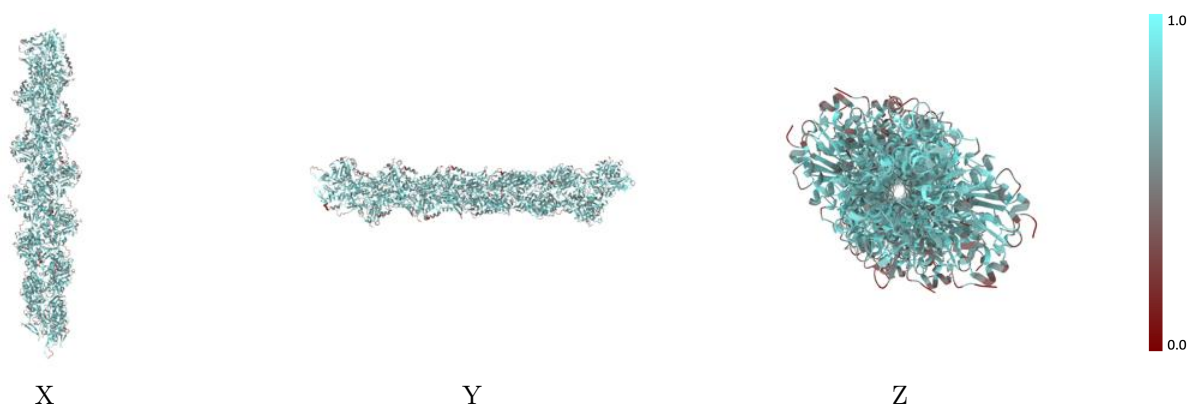
The images above show the 3D surface view of the map at the recommended contour level 0.307 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



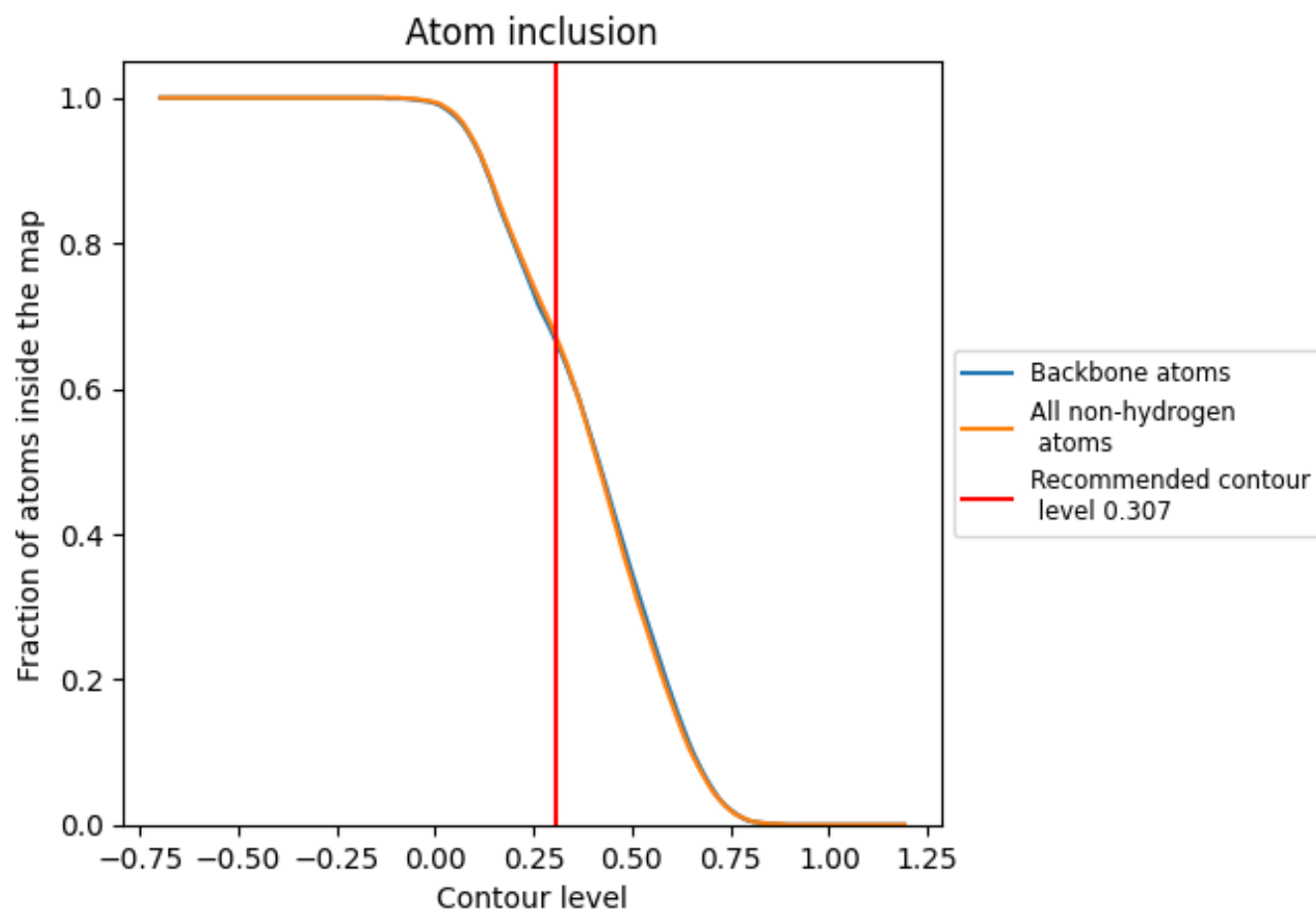
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	<div><div></div></div> 0.6710	<div><div></div></div> 0.5890
Q	<div><div></div></div> 0.6940	<div><div></div></div> 0.5930
R	<div><div></div></div> 0.6900	<div><div></div></div> 0.5940
S	<div><div></div></div> 0.6920	<div><div></div></div> 0.5920
T	<div><div></div></div> 0.6930	<div><div></div></div> 0.5940
U	<div><div></div></div> 0.6930	<div><div></div></div> 0.5940
V	<div><div></div></div> 0.6940	<div><div></div></div> 0.5950
W	<div><div></div></div> 0.6890	<div><div></div></div> 0.5930
X	<div><div></div></div> 0.6960	<div><div></div></div> 0.5920
Y	<div><div></div></div> 0.6910	<div><div></div></div> 0.5930
Z	<div><div></div></div> 0.6910	<div><div></div></div> 0.5940
a	<div><div></div></div> 0.6920	<div><div></div></div> 0.5940
b	<div><div></div></div> 0.6900	<div><div></div></div> 0.5920
c	<div><div></div></div> 0.5850	<div><div></div></div> 0.5570
d	<div><div></div></div> 0.5650	<div><div></div></div> 0.5550
e	<div><div></div></div> 0.5680	<div><div></div></div> 0.5600
f	<div><div></div></div> 0.5560	<div><div></div></div> 0.5550
g	<div><div></div></div> 0.5880	<div><div></div></div> 0.5610
h	<div><div></div></div> 0.5620	<div><div></div></div> 0.5570
i	<div><div></div></div> 0.5650	<div><div></div></div> 0.5530
j	<div><div></div></div> 0.5790	<div><div></div></div> 0.5600
k	<div><div></div></div> 0.5590	<div><div></div></div> 0.5590
l	<div><div></div></div> 0.5880	<div><div></div></div> 0.5600
m	<div><div></div></div> 0.5790	<div><div></div></div> 0.5480
n	<div><div></div></div> 0.5850	<div><div></div></div> 0.5550

1.0

0.0

<0.0