wwPDB EM Validation Summary Report (i)

Dec 12, 2022 – 05:00 PM EST

PDB ID	:	3J6Q
EMDB ID	:	EMD-5926
Title	:	Identification of the active sites in the methyltransferases of a transcribing dsRNA virus
Authors	:	Zhu, B.; Yang, C.; Liu, H.; Cheng, L.; Song, F.; Zeng, S.; Huang, X.; Ji, G.; Zhu, P.
Deposited on	:	2014-03-20
Resolution	:	3.80 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 (i) 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 (1)) were used in the production of this report:

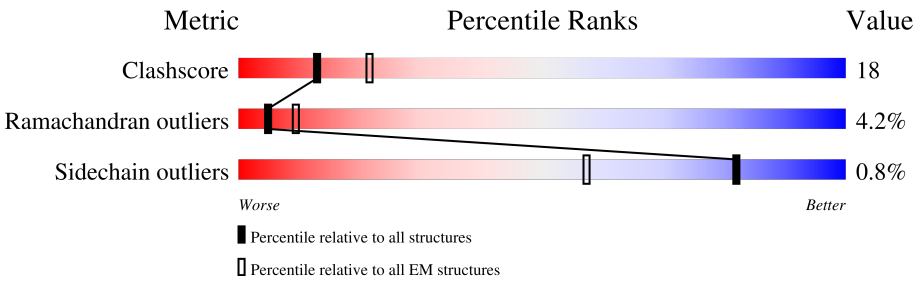
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1058	17% 80% 16% •
1	B	1058	18% 80% 16% •
1	C	1058	17% 80% 16% •
1	D	1058	17% 81% 16% •
1	E	1058	18% 81% 16% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	GPL	B	234	-	-	X	-
2	SAH	A	1101	-	-	X	-
2	SAH	A	1102	-	-	X	-
2	SAH	B	1101	-	-	X	-
2	SAH	B	1102	-	-	X	-
2	SAH	C	1101	-	-	X	-
2	SAH	C	1102	-	-	X	-
2	SAH	D	1101	-	-	X	-
2	SAH	D	1102	-	-	X	-
2	SAH	E	1101	-	-	X	-
2	SAH	E	1102	-	-	X	-

2 Entry composition (i)

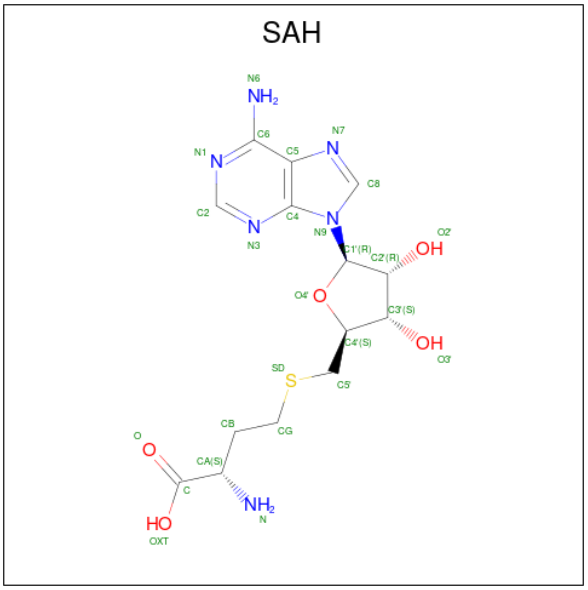
There are 2 unique types of molecules in this entry. The entry contains 42575 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Structural protein VP3.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
1	A	1058	8463	5358	1463	1596	1	45	0	0
1	B	1058	8463	5358	1463	1596	1	45	0	0
1	C	1058	8463	5358	1463	1596	1	45	0	0
1	D	1058	8463	5358	1463	1596	1	45	0	0
1	E	1058	8463	5358	1463	1596	1	45	0	0

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
2	A	1	52	28	12	10	2	0

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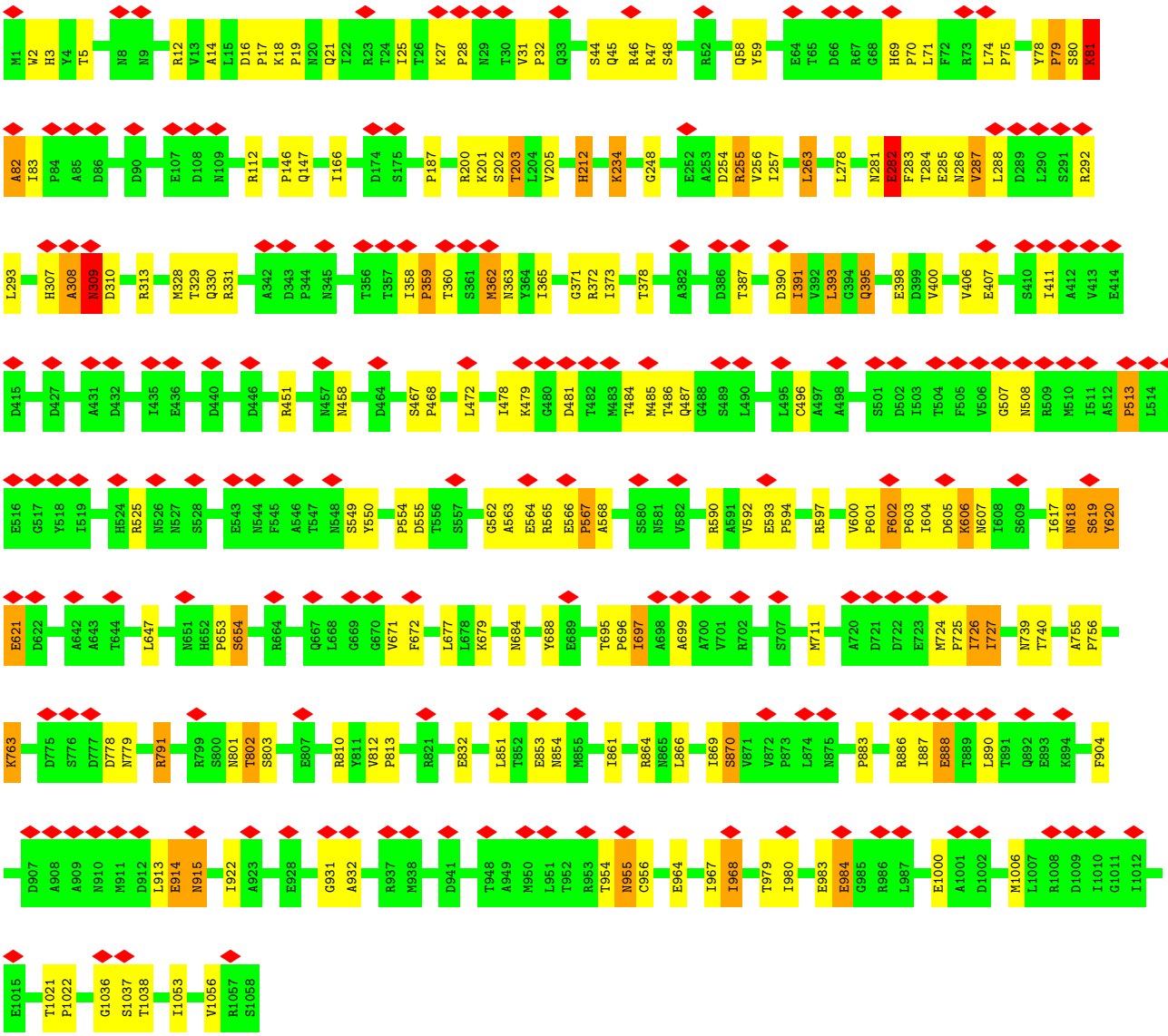
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
2	A	1	52	28	12	10	2	0
2	B	1	52	28	12	10	2	0
2	B	1	52	28	12	10	2	0
2	C	1	52	28	12	10	2	0
2	C	1	52	28	12	10	2	0
2	D	1	52	28	12	10	2	0
2	D	1	52	28	12	10	2	0
2	E	1	52	28	12	10	2	0
2	E	1	52	28	12	10	2	0

3 Residue-property plots (i)

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.

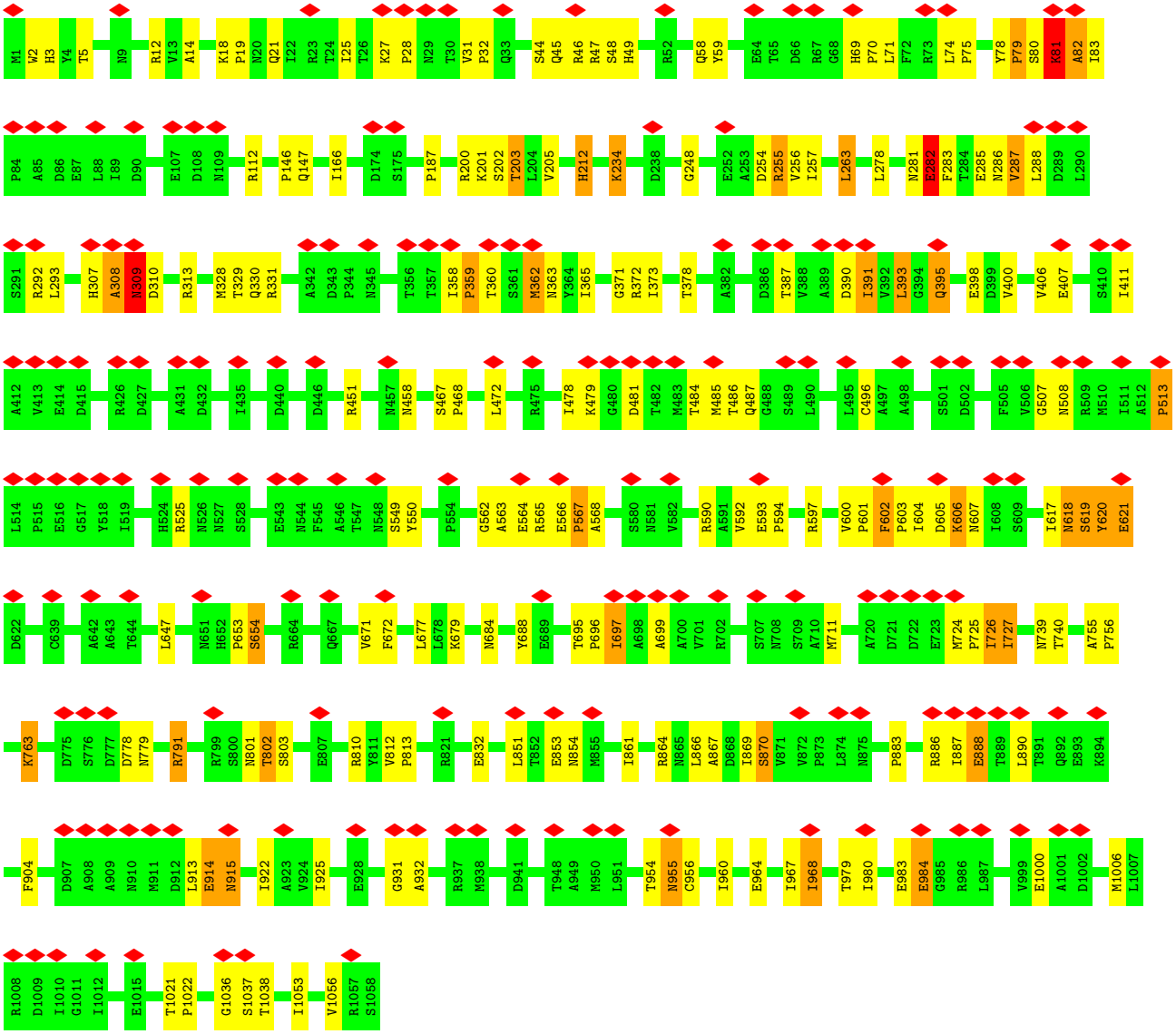
- Molecule 1: Structural protein VP3

Chain A: 17% 80% 16%



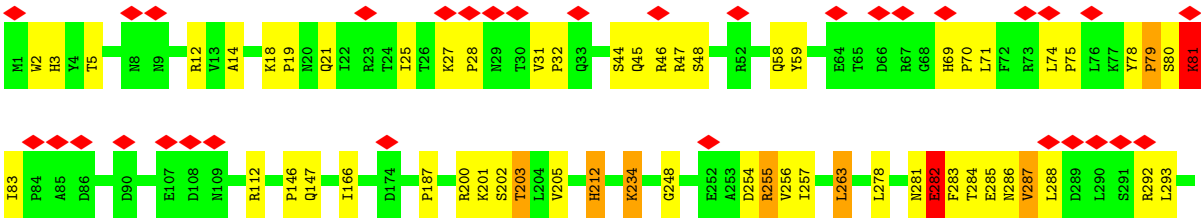
- Molecule 1: Structural protein VP3

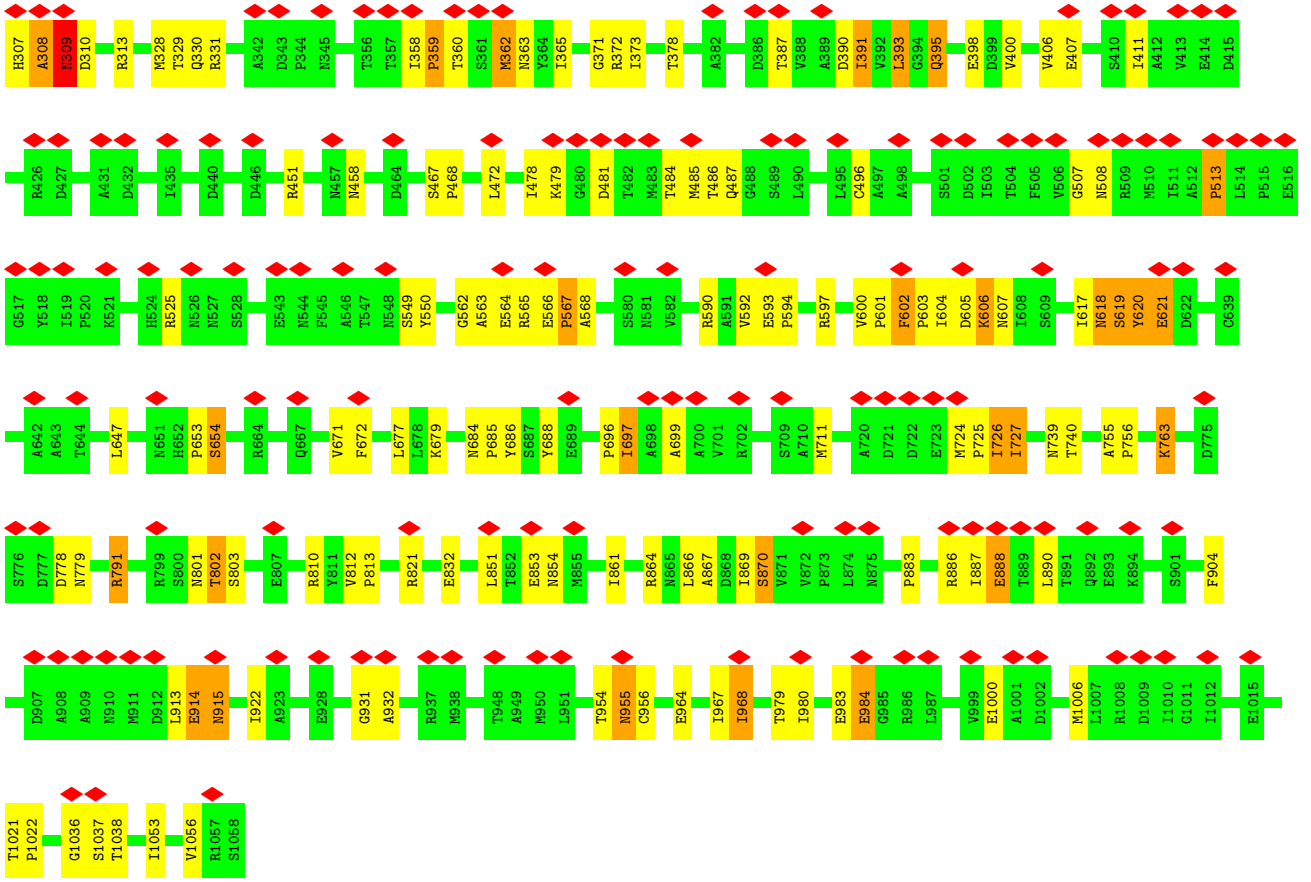
Chain B:



- Molecule 1: Structural protein VP3

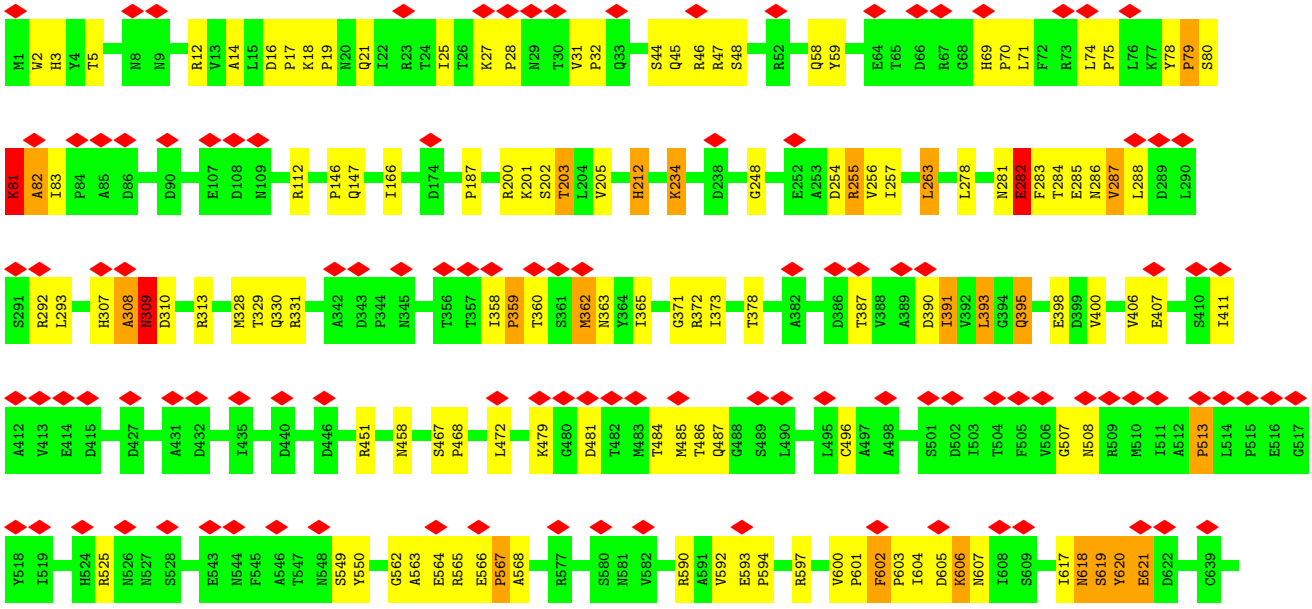
Chain C:

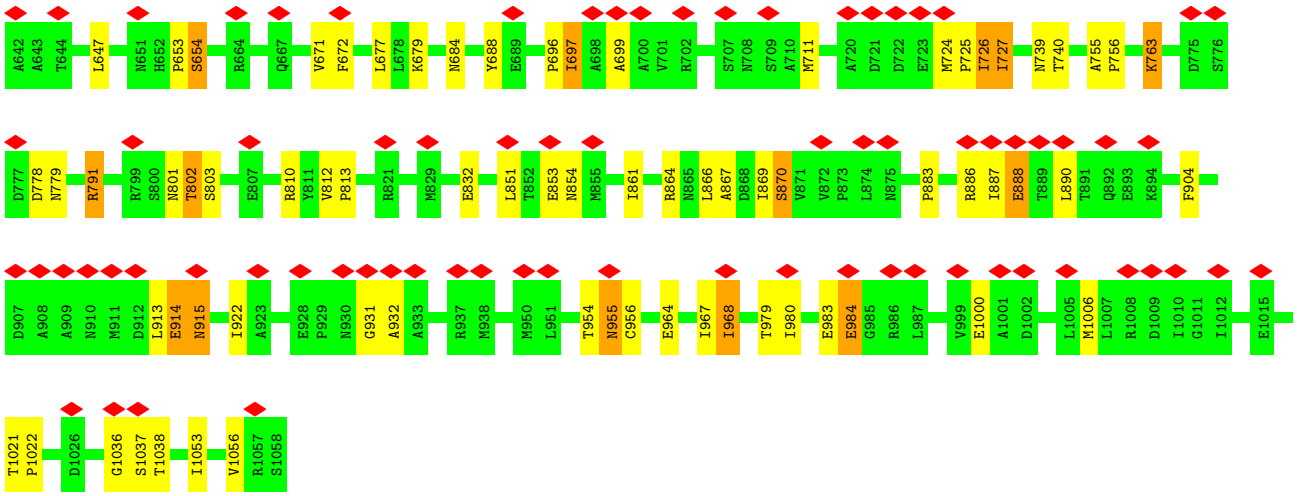




- Molecule 1: Structural protein VP3

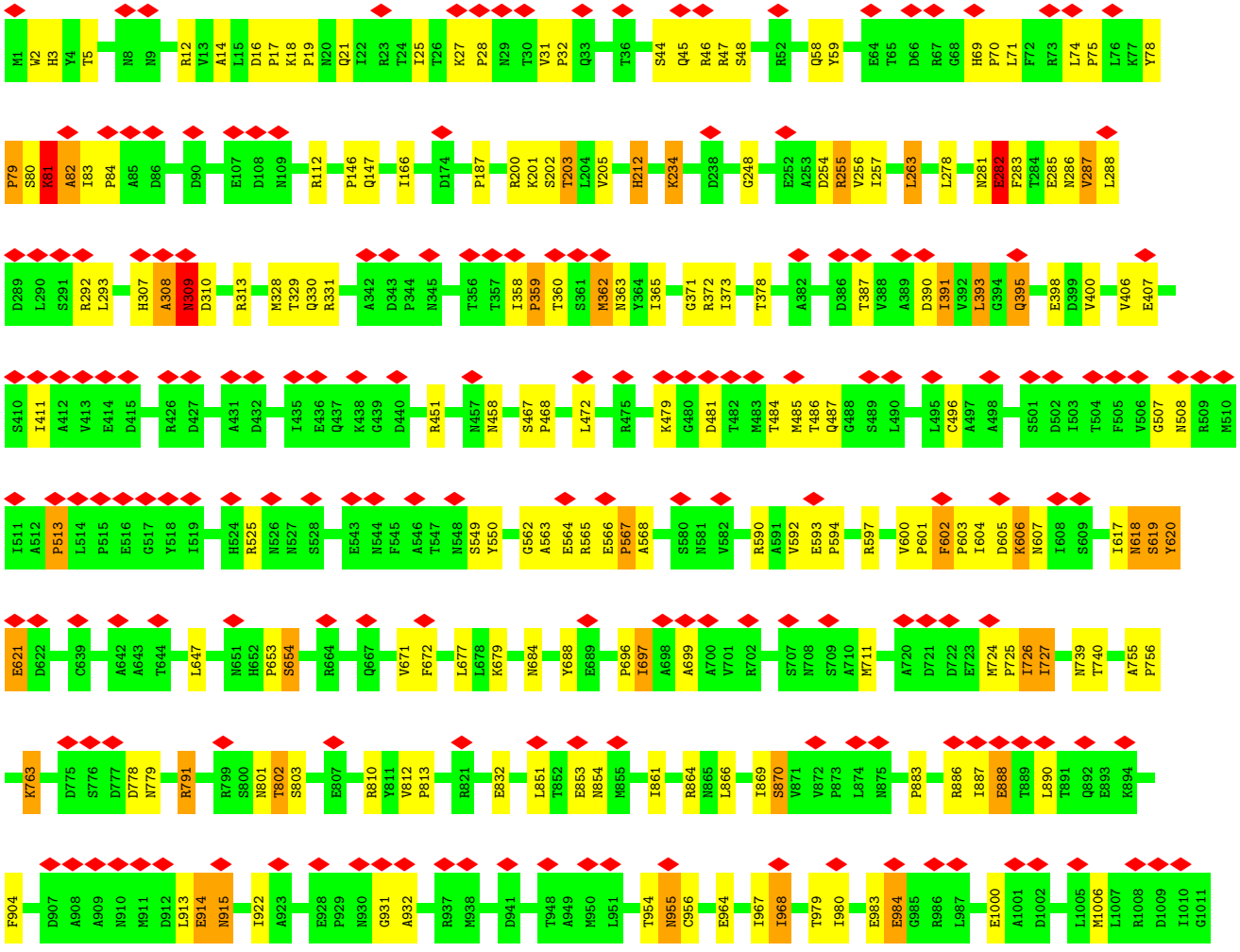
Chain D:

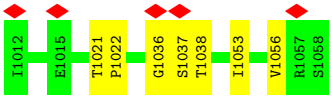




- Molecule 1: Structural protein VP3

Chain E:




I1012
E1015
T1021
P1022
G1036
S1037
T1038
I1053
V1056
R1057
S1058

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	30000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	EMAN	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	Not provided	
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	125390	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor
Maximum map value	114.122	Depositor
Minimum map value	-104.620	Depositor
Average map value	1.202	Depositor
Map value standard deviation	10.389	Depositor
Recommended contour level	20.0	Depositor
Map size (Å)	746.304, 746.304, 374.348	wwPDB
Map dimensions	624, 624, 313	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.196, 1.196, 1.196	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.61	3/8615 (0.0%)	0.55	2/11731 (0.0%)
1	B	0.62	3/8615 (0.0%)	0.55	2/11731 (0.0%)
1	C	0.62	3/8615 (0.0%)	0.55	2/11731 (0.0%)
1	D	0.62	3/8615 (0.0%)	0.54	2/11731 (0.0%)
1	E	0.62	3/8615 (0.0%)	0.55	2/11731 (0.0%)
All	All	0.62	15/43075 (0.0%)	0.55	10/58655 (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
1	A	0	5
1	B	0	5
1	C	0	5
1	D	0	5
1	E	0	5
All	All	0	25

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	513	PRO	N-CD	6.56	1.57	1.47
1	D	513	PRO	N-CD	6.55	1.57	1.47
1	B	513	PRO	N-CD	6.54	1.57	1.47
1	A	513	PRO	N-CD	6.54	1.57	1.47
1	C	513	PRO	N-CD	6.47	1.56	1.47

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	79	PRO	CA-N-CD	-5.23	104.17	111.50
1	C	79	PRO	CA-N-CD	-5.23	104.18	111.50
1	A	79	PRO	CA-N-CD	-5.22	104.19	111.50
1	D	79	PRO	CA-N-CD	-5.21	104.20	111.50
1	B	79	PRO	CA-N-CD	-5.19	104.23	111.50

There are no chirality outliers.

5 of 25 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	308	ALA	Peptide
1	A	309	ASN	Peptide
1	A	362	MET	Peptide
1	A	71	LEU	Peptide
1	A	81	LYS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8463	0	8411	385	0
1	B	8463	0	8411	400	0
1	C	8463	0	8411	390	0
1	D	8463	0	8411	385	0
1	E	8463	0	8411	385	0
2	A	52	0	38	28	0
2	B	52	0	38	29	0
2	C	52	0	38	29	0
2	D	52	0	38	28	0
2	E	52	0	38	29	0
All	All	42575	0	42245	1567	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 18.

The worst 5 of 1567 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:A:395:GLN:CG	1:B:112:ARG:NH2	1.75	1.48
1:B:395:GLN:CG	1:C:112:ARG:NH2	1.77	1.48
1:C:395:GLN:CG	1:D:112:ARG:NH2	1.74	1.46
1:A:112:ARG:NH2	1:E:395:GLN:CG	1.74	1.45
1:D:395:GLN:CG	1:E:112:ARG:NH2	1.76	1.45

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1055/1058 (100%)	889 (84%)	122 (12%)	44 (4%)	3 26
1	B	1055/1058 (100%)	889 (84%)	122 (12%)	44 (4%)	3 26
1	C	1055/1058 (100%)	887 (84%)	123 (12%)	45 (4%)	2 26
1	D	1055/1058 (100%)	887 (84%)	124 (12%)	44 (4%)	3 26
1	E	1055/1058 (100%)	887 (84%)	124 (12%)	44 (4%)	3 26
All	All	5275/5290 (100%)	4439 (84%)	615 (12%)	221 (4%)	5 26

5 of 221 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	212	HIS
1	A	282	GLU
1	A	287	VAL
1	A	309	ASN
1	A	330	GLN

5.3.2 Protein sidechains (i)

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	942/942 (100%)	934 (99%)	8 (1%)	81 89
1	B	942/942 (100%)	934 (99%)	8 (1%)	81 89
1	C	942/942 (100%)	934 (99%)	8 (1%)	81 89
1	D	942/942 (100%)	934 (99%)	8 (1%)	81 89
1	E	942/942 (100%)	934 (99%)	8 (1%)	81 89
All	All	4710/4710 (100%)	4670 (99%)	40 (1%)	82 89

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	620	TYR
1	E	525	ARG
1	D	763	LYS
1	E	282	GLU
1	E	763	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	45	GLN
1	D	45	GLN
1	C	45	GLN
1	B	45	GLN
1	D	21	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

5 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	GPL	C	234	1	29,34,35	2.59	2 (6%)	29,49,51	1.33	4 (13%)
1	GPL	E	234	1	29,34,35	2.59	2 (6%)	29,49,51	1.34	4 (13%)
1	GPL	A	234	1	29,34,35	2.58	2 (6%)	29,49,51	1.33	4 (13%)
1	GPL	D	234	1	29,34,35	2.56	2 (6%)	29,49,51	1.33	4 (13%)
1	GPL	B	234	1	29,34,35	2.57	2 (6%)	29,49,51	1.34	4 (13%)

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	GPL	C	234	1	-	9/15/37/39	0/3/3/3
1	GPL	E	234	1	-	9/15/37/39	0/3/3/3
1	GPL	A	234	1	-	9/15/37/39	0/3/3/3
1	GPL	D	234	1	-	9/15/37/39	0/3/3/3
1	GPL	B	234	1	-	9/15/37/39	0/3/3/3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	234	GPL	P-NZ	12.85	1.75	1.61
1	A	234	GPL	P-NZ	12.84	1.75	1.61
1	E	234	GPL	P-NZ	12.81	1.75	1.61
1	B	234	GPL	P-NZ	12.77	1.75	1.61
1	D	234	GPL	P-NZ	12.73	1.75	1.61

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	234	GPL	C3'-C2'-C1'	3.59	106.39	100.98
1	B	234	GPL	C3'-C2'-C1'	3.56	106.34	100.98
1	D	234	GPL	C3'-C2'-C1'	3.55	106.32	100.98
1	A	234	GPL	C3'-C2'-C1'	3.54	106.31	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	234	GPL	C3'-C2'-C1'	3.53	106.29	100.98

There are no chirality outliers.

5 of 45 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	234	GPL	C5'-O5'-P-O2P
1	A	234	GPL	N-CA-CB-CG
1	A	234	GPL	C-CA-CB-CG
1	B	234	GPL	C5'-O5'-P-O2P
1	B	234	GPL	N-CA-CB-CG

There are no ring outliers.

5 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	234	GPL	8	0
1	E	234	GPL	8	0
1	A	234	GPL	8	0
1	D	234	GPL	8	0
1	B	234	GPL	9	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SAH	E	1101	-	24,28,28	1.03	1 (4%)	25,40,40	1.39	3 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SAH	D	1102	-	24,28,28	1.02	1 (4%)	25,40,40	1.38	3 (12%)
2	SAH	D	1101	-	24,28,28	1.03	1 (4%)	25,40,40	1.38	3 (12%)
2	SAH	B	1101	-	24,28,28	1.02	1 (4%)	25,40,40	1.39	3 (12%)
2	SAH	B	1102	-	24,28,28	1.02	1 (4%)	25,40,40	1.38	3 (12%)
2	SAH	A	1101	-	24,28,28	1.03	1 (4%)	25,40,40	1.38	3 (12%)
2	SAH	A	1102	-	24,28,28	1.02	1 (4%)	25,40,40	1.38	3 (12%)
2	SAH	C	1102	-	24,28,28	1.01	1 (4%)	25,40,40	1.37	3 (12%)
2	SAH	E	1102	-	24,28,28	1.03	1 (4%)	25,40,40	1.38	3 (12%)
2	SAH	C	1101	-	24,28,28	1.03	1 (4%)	25,40,40	1.38	3 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SAH	E	1101	-	-	4/11/31/31	0/3/3/3
2	SAH	D	1102	-	-	1/11/31/31	0/3/3/3
2	SAH	D	1101	-	-	5/11/31/31	0/3/3/3
2	SAH	B	1101	-	-	4/11/31/31	0/3/3/3
2	SAH	B	1102	-	-	1/11/31/31	0/3/3/3
2	SAH	A	1101	-	-	5/11/31/31	0/3/3/3
2	SAH	A	1102	-	-	1/11/31/31	0/3/3/3
2	SAH	C	1102	-	-	1/11/31/31	0/3/3/3
2	SAH	E	1102	-	-	1/11/31/31	0/3/3/3
2	SAH	C	1101	-	-	5/11/31/31	0/3/3/3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1101	SAH	C5-C4	2.52	1.47	1.40
2	D	1101	SAH	C5-C4	2.47	1.47	1.40
2	A	1101	SAH	C5-C4	2.46	1.47	1.40
2	E	1101	SAH	C5-C4	2.45	1.47	1.40
2	B	1101	SAH	C5-C4	2.43	1.47	1.40

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1102	SAH	N3-C2-N1	-3.37	123.41	128.68
2	D	1102	SAH	N3-C2-N1	-3.33	123.47	128.68
2	E	1102	SAH	N3-C2-N1	-3.31	123.50	128.68
2	B	1102	SAH	N3-C2-N1	-3.30	123.52	128.68
2	C	1102	SAH	N3-C2-N1	-3.30	123.52	128.68

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

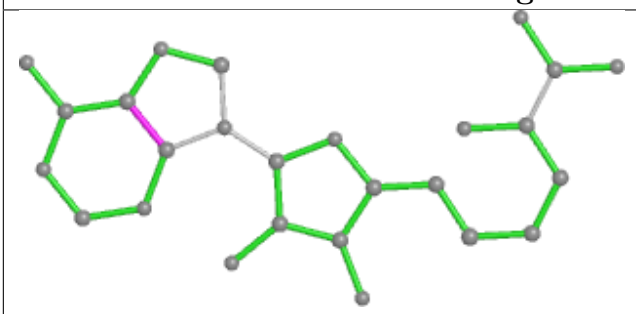
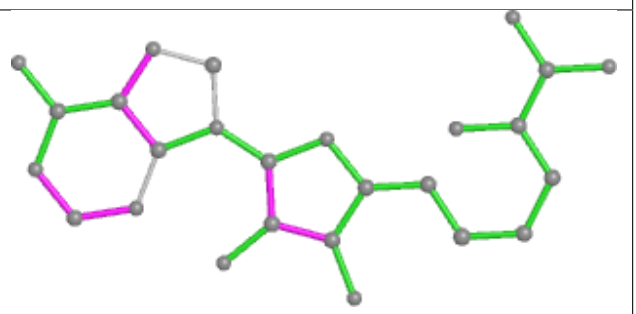
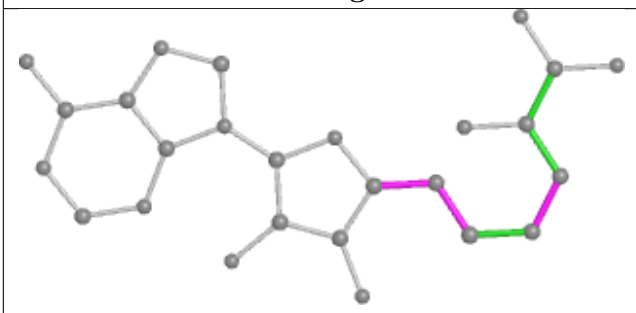
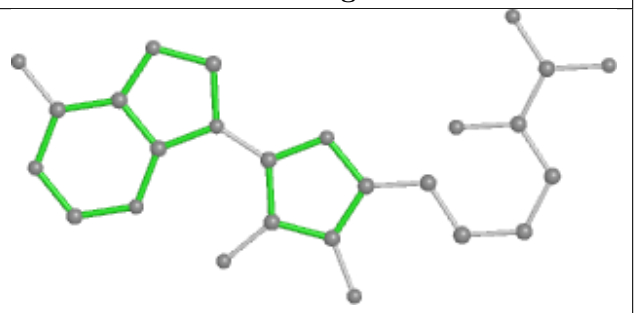
Mol	Chain	Res	Type	Atoms
2	A	1101	SAH	CA-CB-CG-SD
2	A	1101	SAH	O4'-C4'-C5'-SD
2	A	1101	SAH	C3'-C4'-C5'-SD
2	B	1101	SAH	CA-CB-CG-SD
2	B	1101	SAH	O4'-C4'-C5'-SD

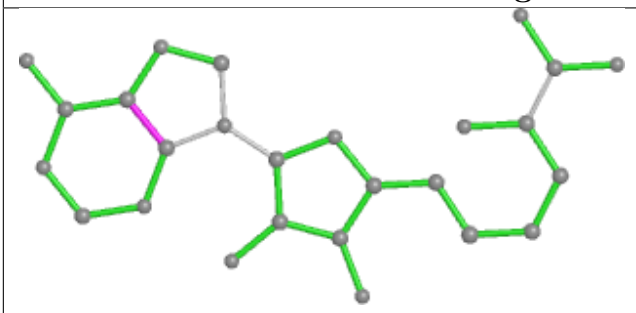
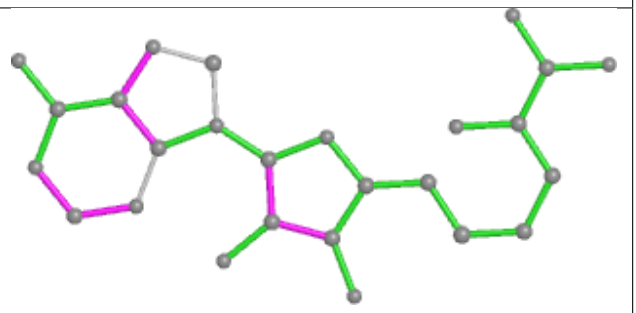
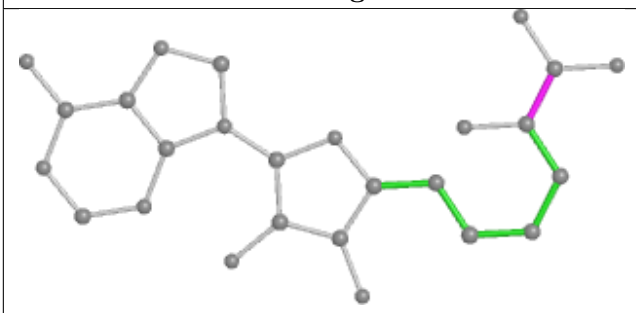
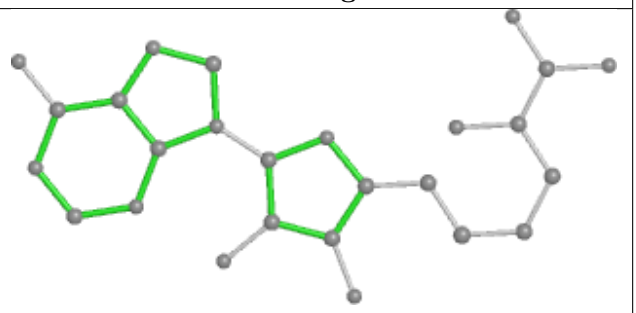
There are no ring outliers.

10 monomers are involved in 143 short contacts:

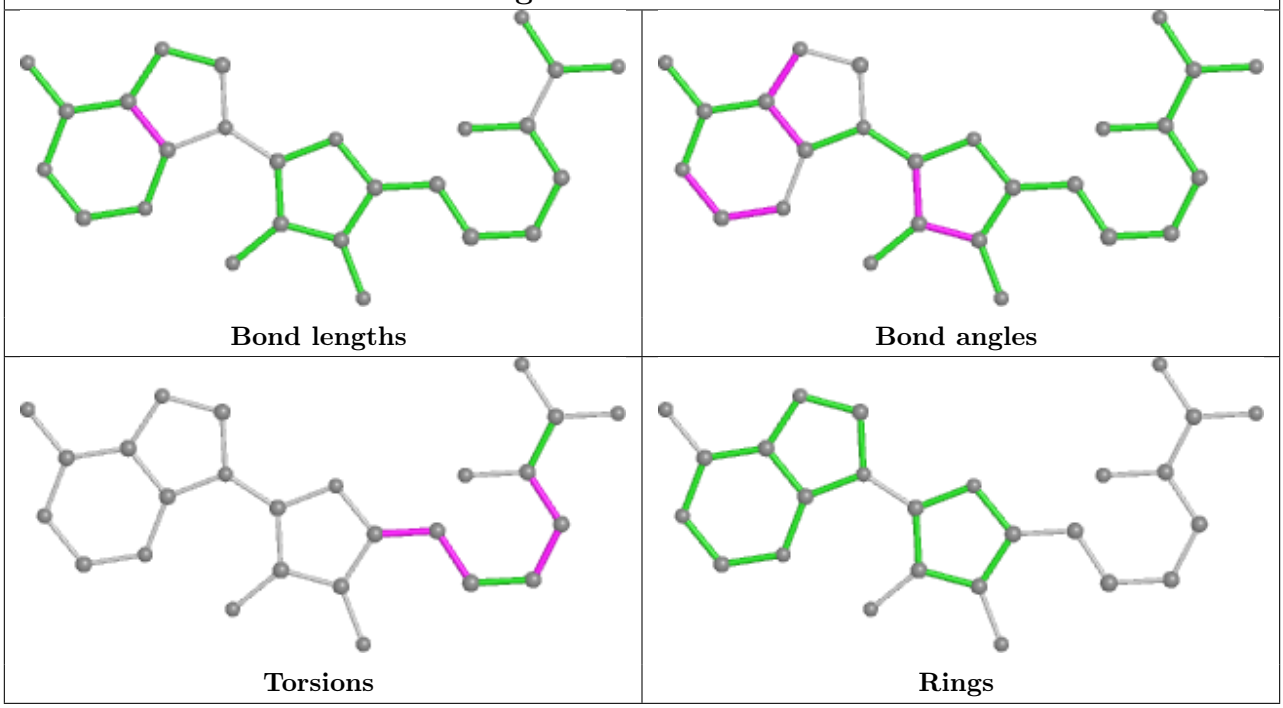
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1101	SAH	14	0
2	D	1102	SAH	14	0
2	D	1101	SAH	14	0
2	B	1101	SAH	14	0
2	B	1102	SAH	15	0
2	A	1101	SAH	14	0
2	A	1102	SAH	14	0
2	C	1102	SAH	14	0
2	E	1102	SAH	15	0
2	C	1101	SAH	15	0

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 then 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.

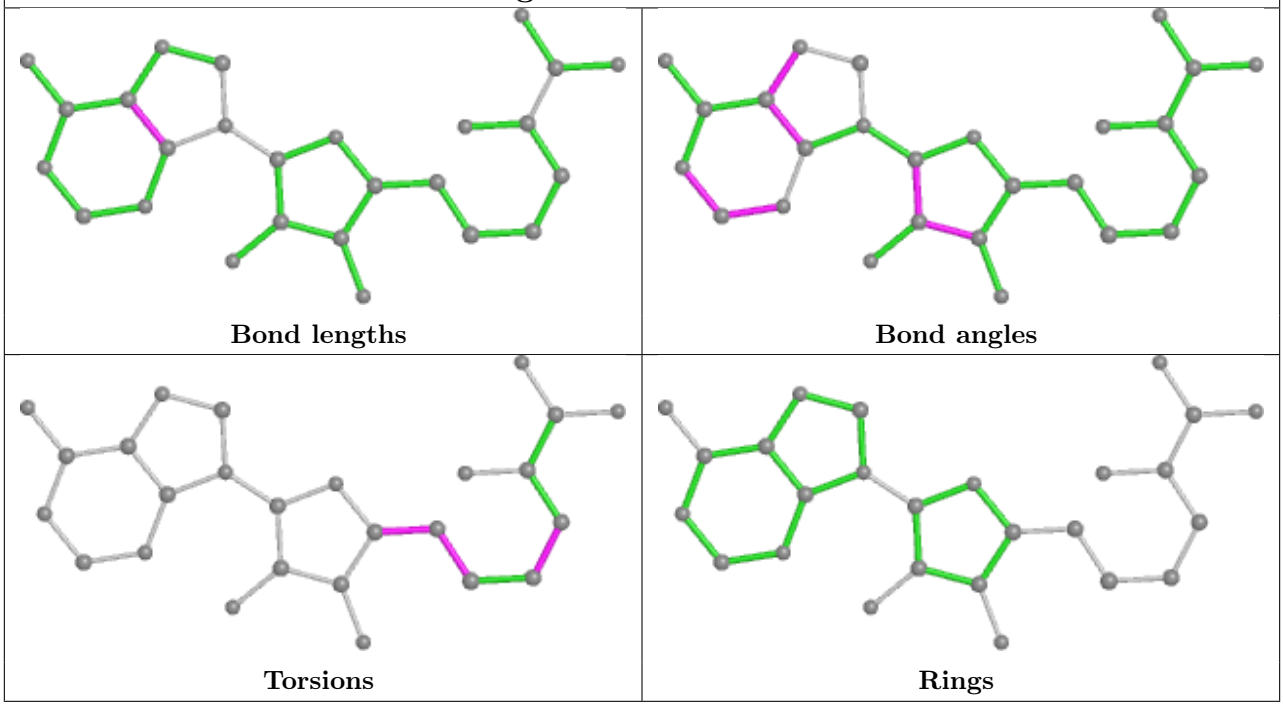
Ligand SAH E 1101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SAH D 1102	
 Bond lengths	 Bond angles
 Torsions	 Rings

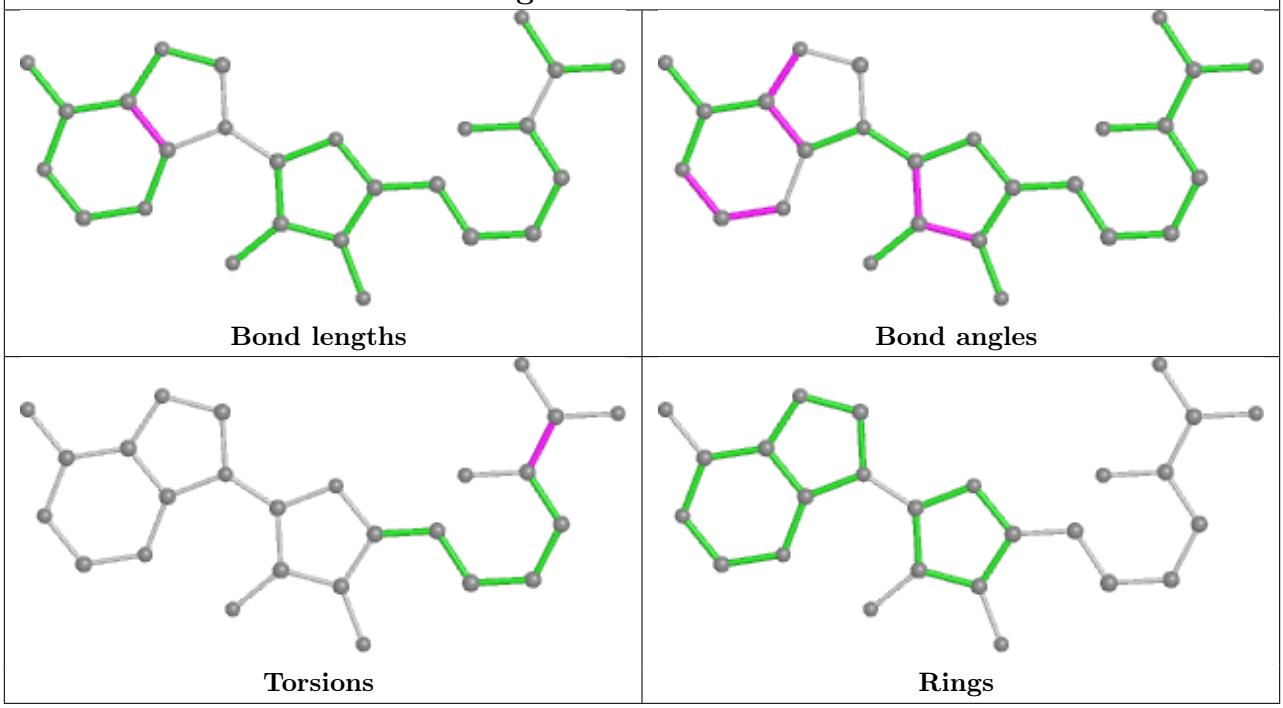
Ligand SAH D 1101



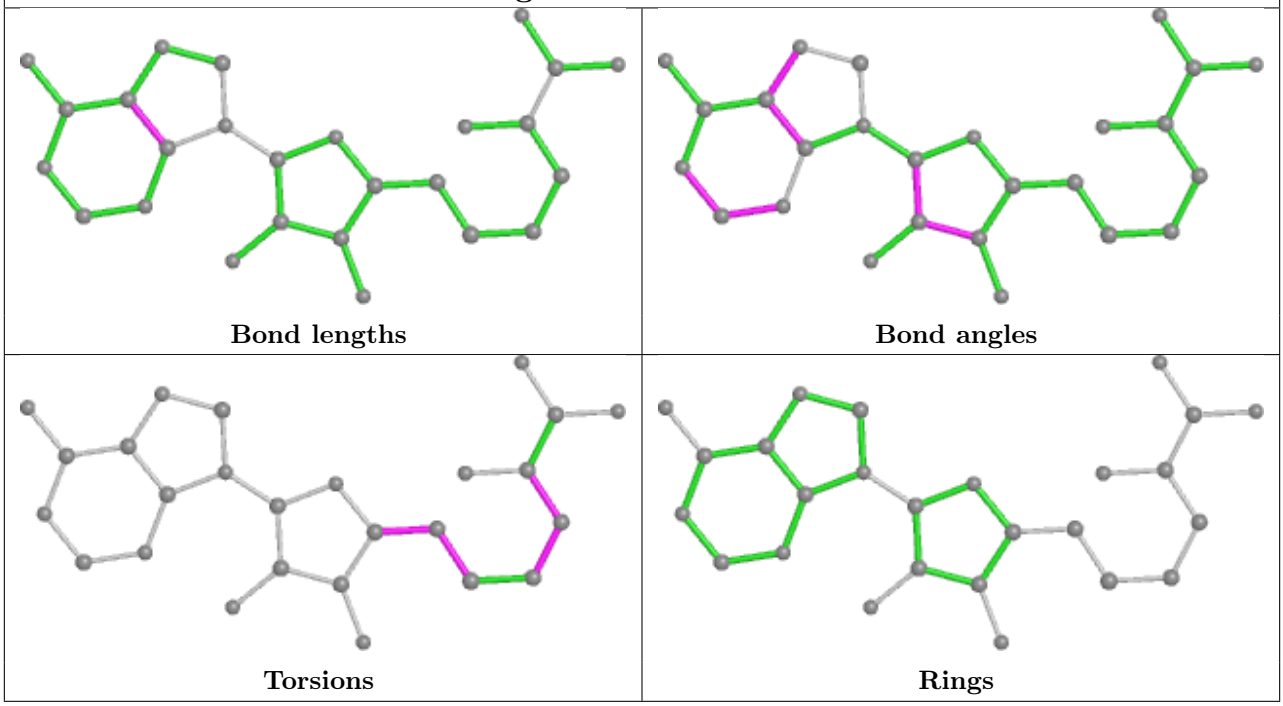
Ligand SAH B 1101

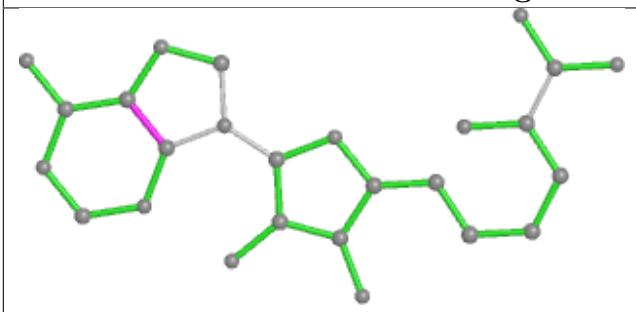
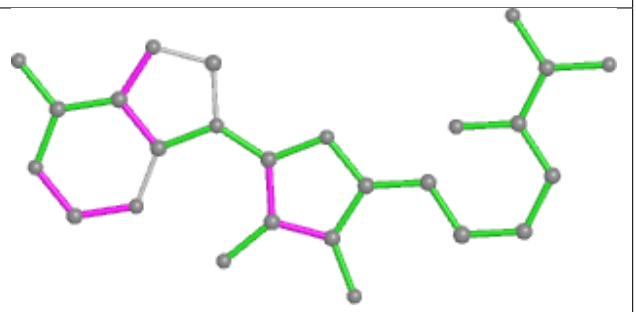
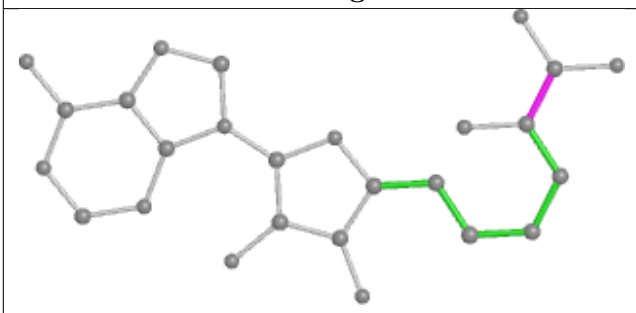
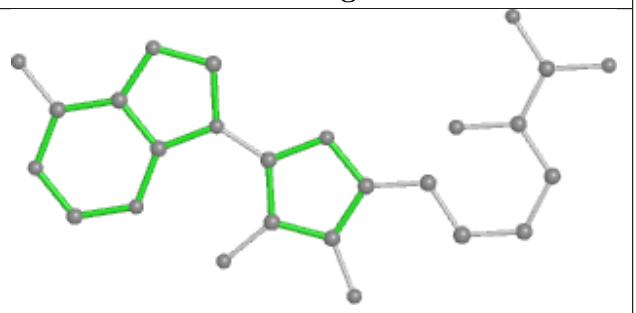


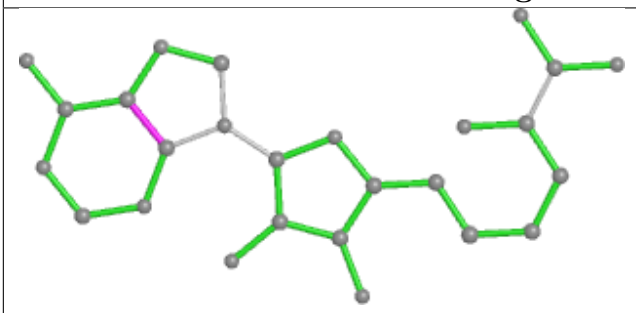
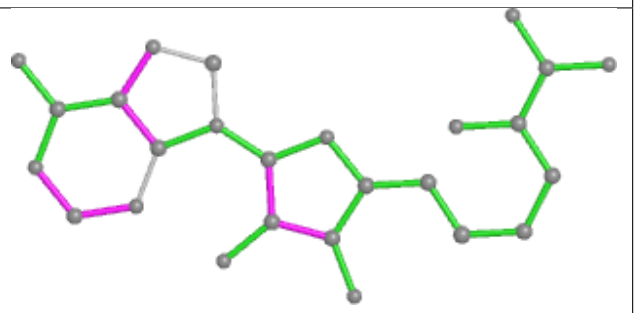
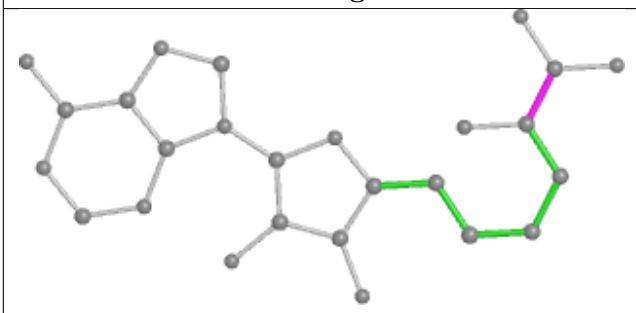
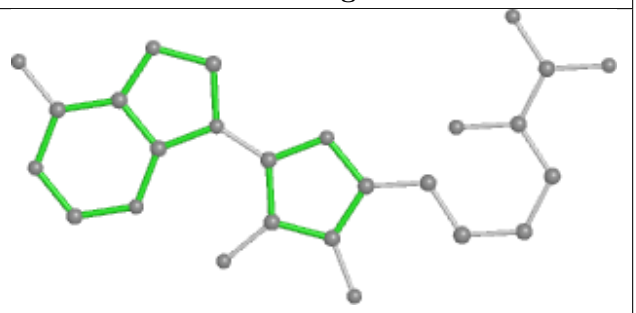
Ligand SAH B 1102



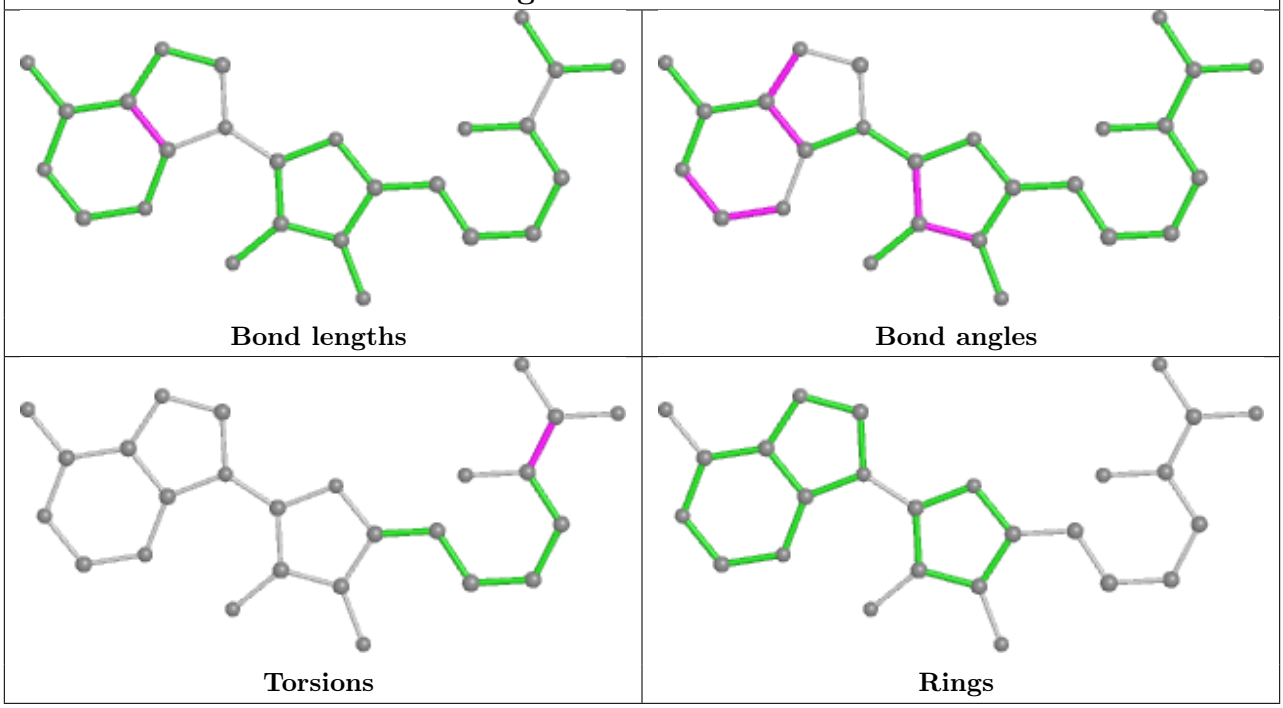
Ligand SAH A 1101



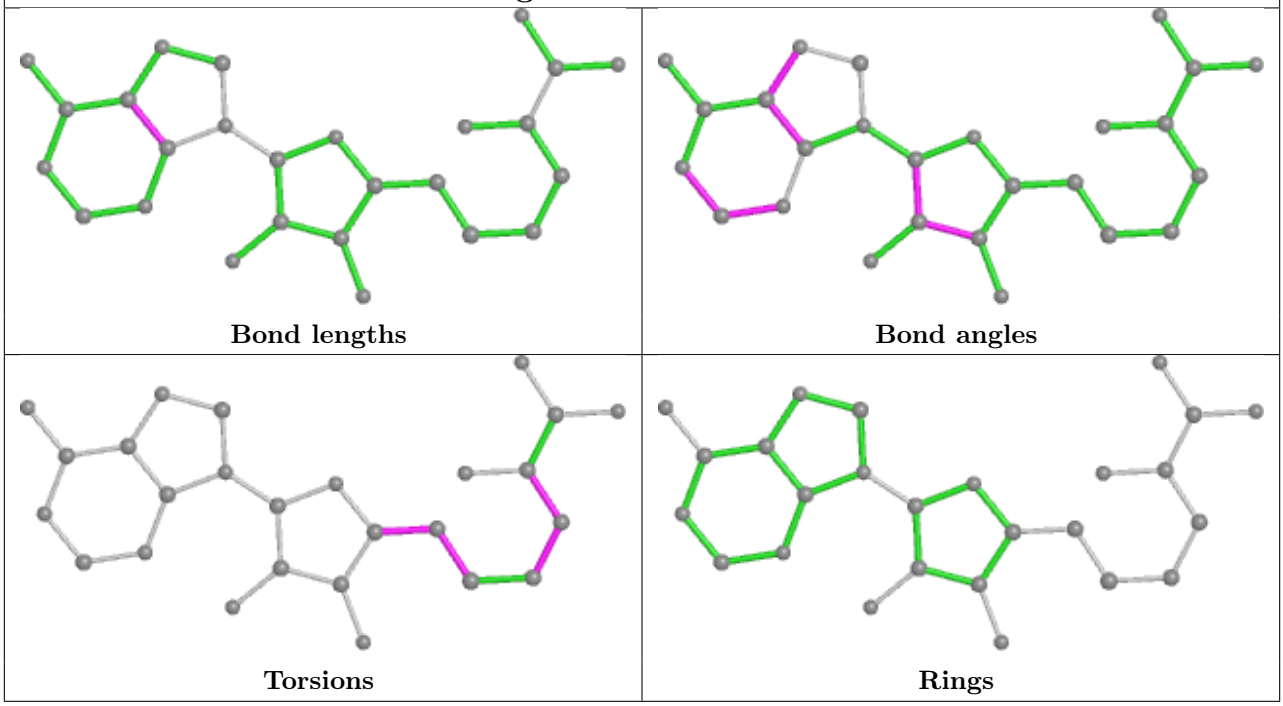
Ligand SAH A 1102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SAH C 1102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SAH E 1102



Ligand SAH C 1101



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.

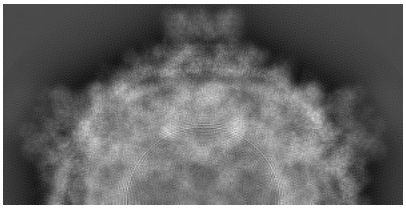
6 Map visualisation (i)

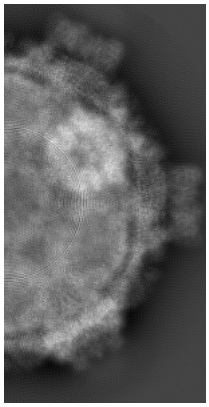
This section contains visualisations of the EMDB entry EMD-5926. These allow visual inspection of the internal detail of the map and identification of artifacts.

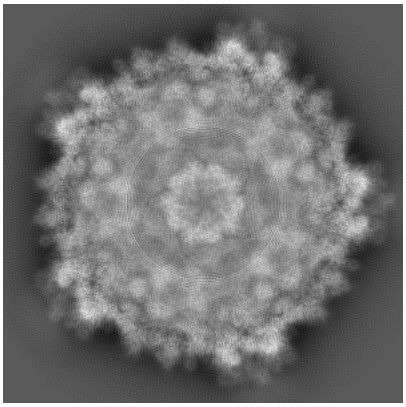
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map


X

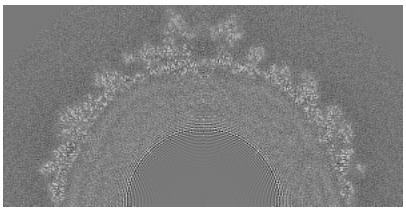

Y

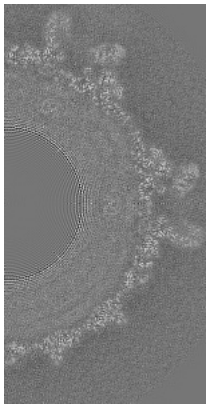

Z

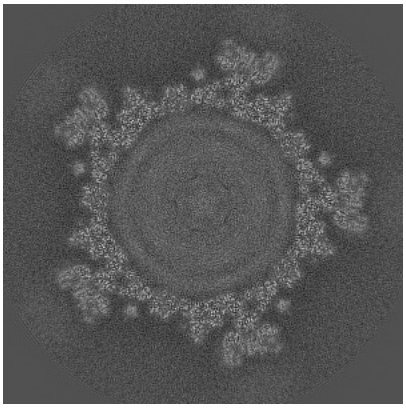
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map


X Index: 312

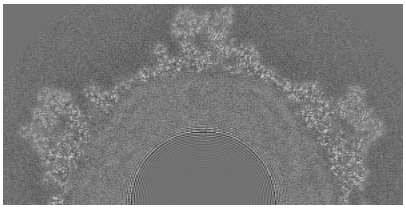

Y Index: 312


Z Index: 156

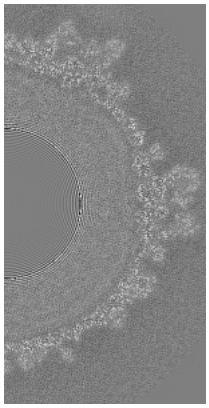
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

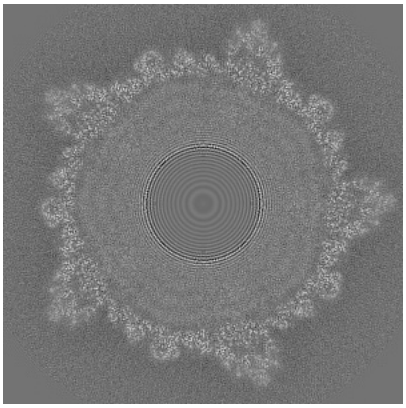
6.3.1 Primary map



X Index: 352



Y Index: 337

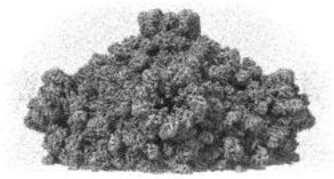


Z Index: 81

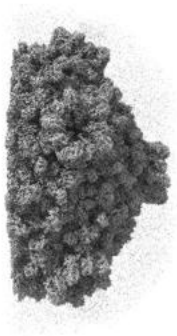
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

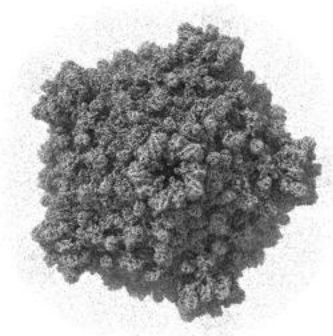
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 20.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

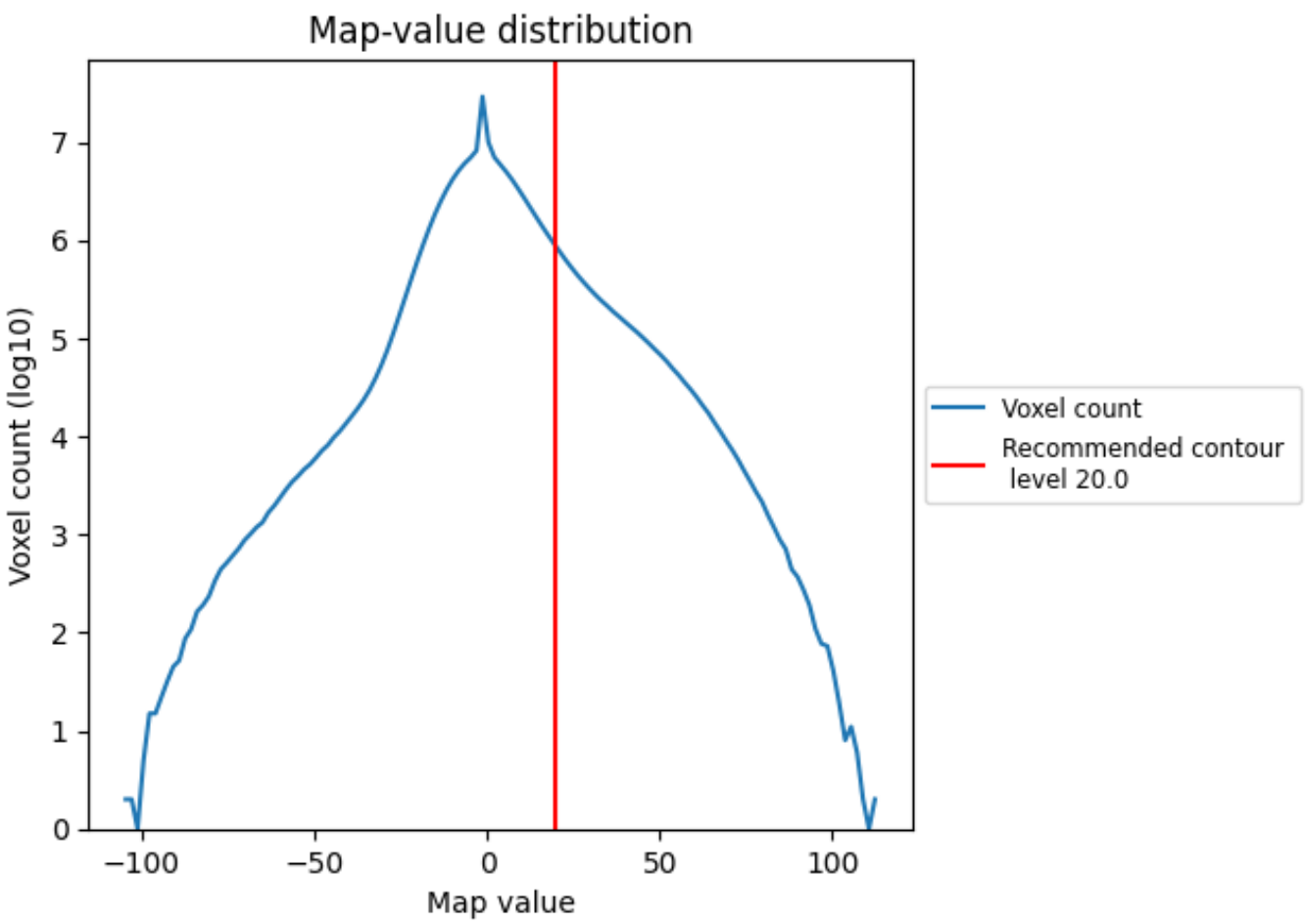
6.5 Mask visualisation (i)

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

7 Map analysis (i)

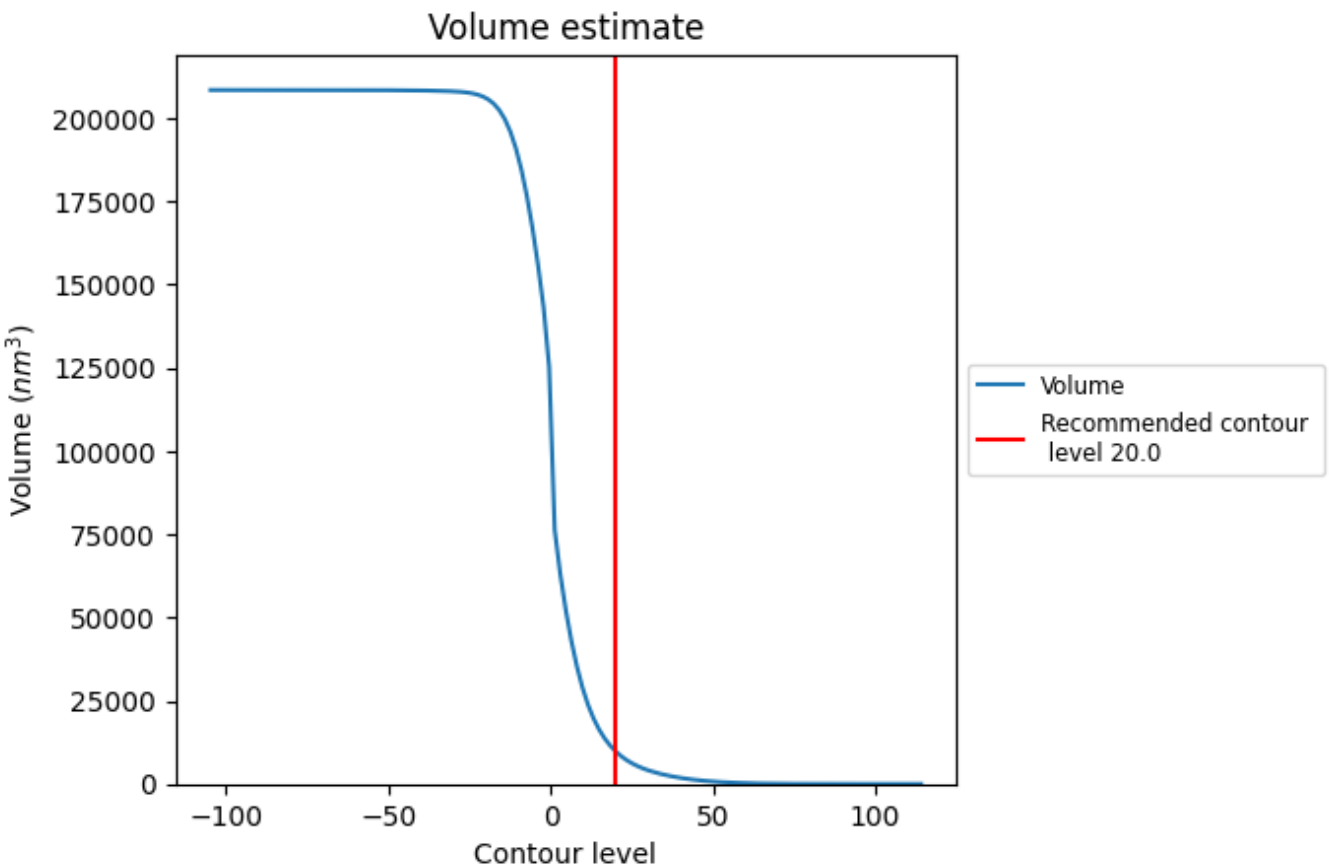
This section contains the results of statistical analysis of the map.

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 9897 nm^3; this corresponds to an approximate mass of 8940 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)

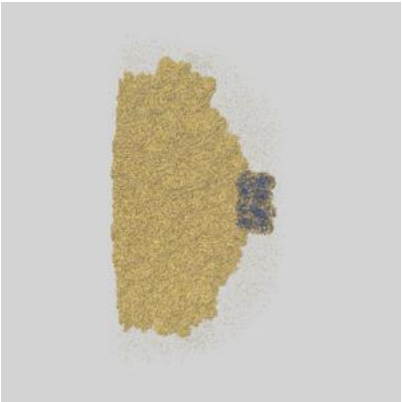
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit (i)

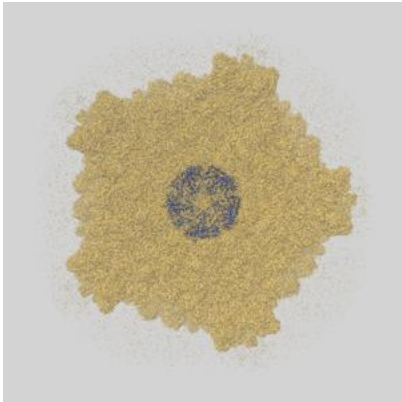
This section contains information regarding the fit between EMDB map EMD-5926 and PDB model 3J6Q. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay (i)

X



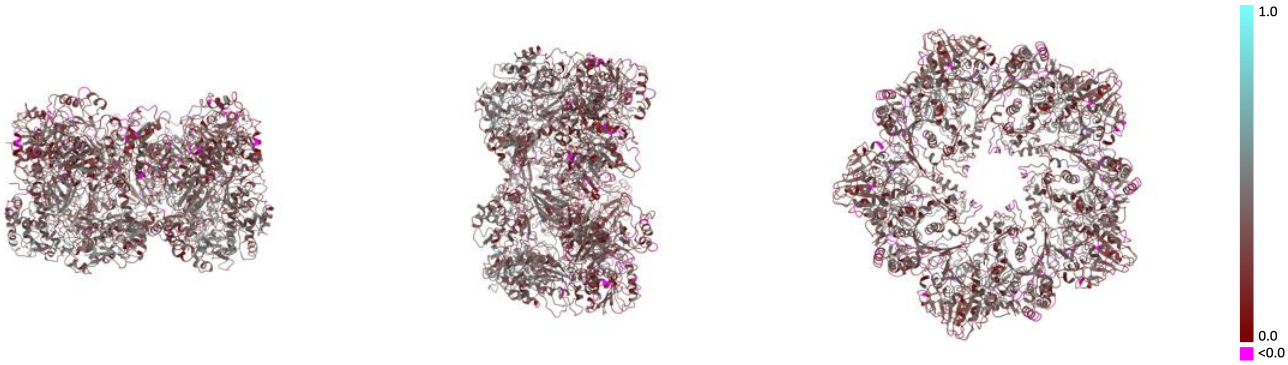
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 20.0 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.

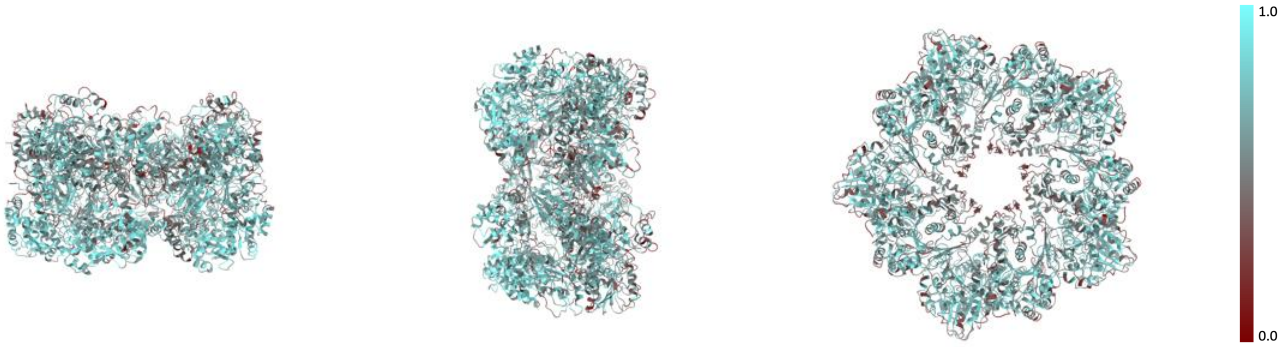
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

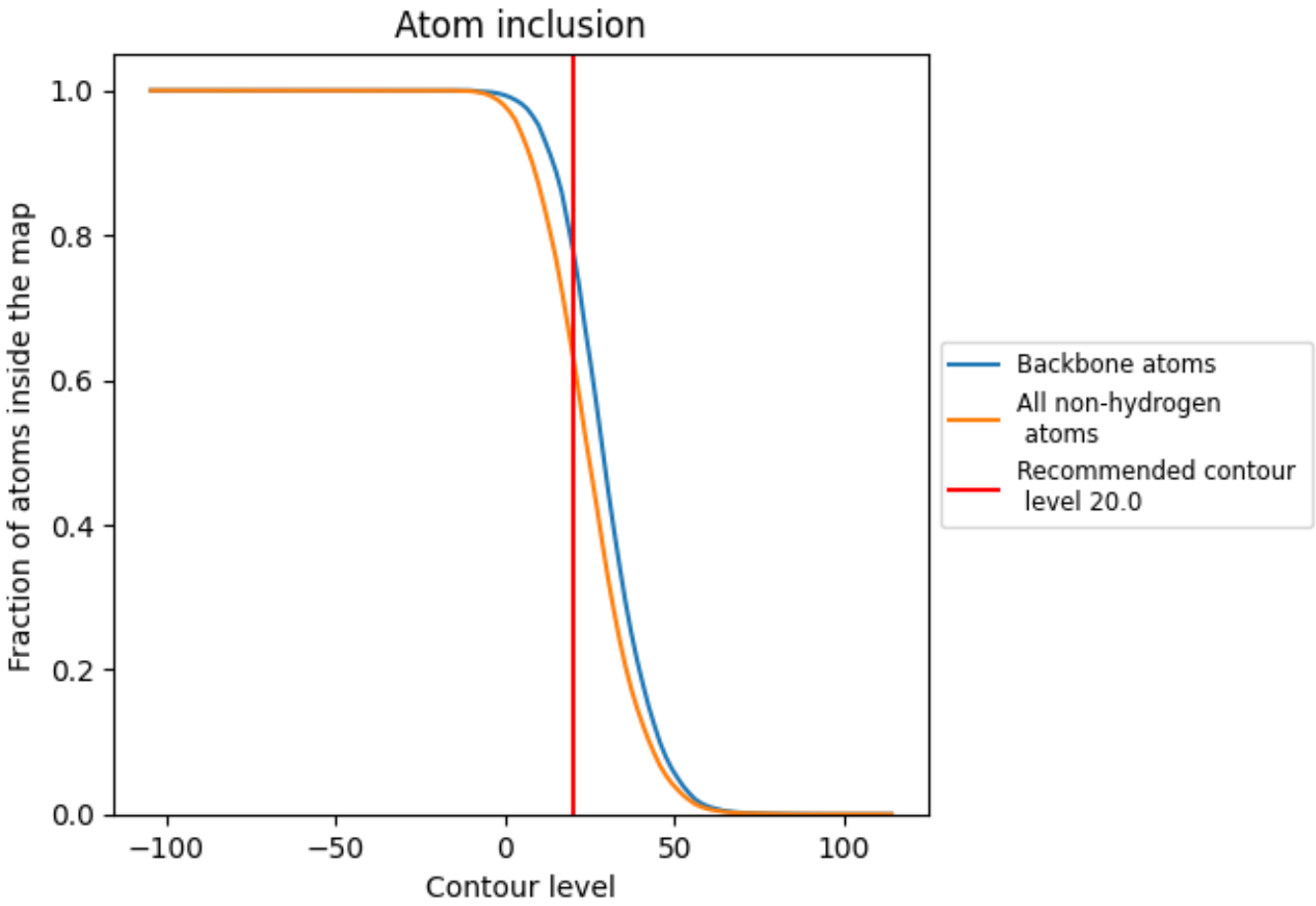
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (20.0).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 63% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (20.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6336	0.3160
A	0.6335	0.3160
B	0.6335	0.3150
C	0.6334	0.3150
D	0.6342	0.3160
E	0.6335	0.3160