



## wwPDB EM Validation Summary Report ⓘ

Mar 5, 2025 – 02:20 AM EST

PDB ID : 9B4I  
EMDB ID : EMD-44181  
Title : Filament of D-TLKIVWI, a D-peptide that disaggregates Alzheimer's Paired Helical Filaments, determined by Cryo-EM  
Authors : Hou, K.; Ge, P.; Sawaya, M.R.; Eisenberg, D.S.  
Deposited on : 2024-03-20  
Resolution : 3.60 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev117  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.41.4

# 1 Overall quality at a glance ⓘ












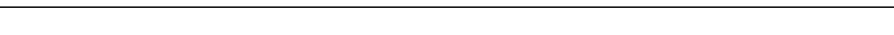


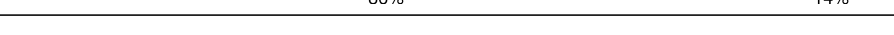

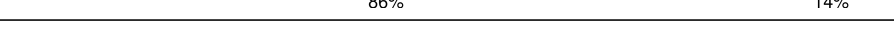
The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.60 Å.











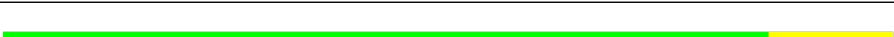


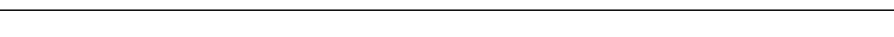
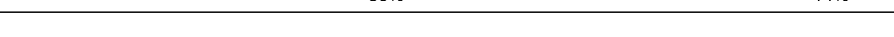
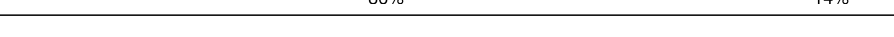



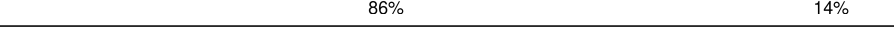





There are no overall percentile quality scores available for this entry.

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  $\geq 3$ , 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	0	7	 86%14%
1	1	7	 86%14%
1	2	7	 14%86%14%
1	3	7	 86%14%
1	4	7	 86%14%
1	5	7	 86%14%
1	6	7	 29%86%14%
1	7	7	 29%86%14%
1	8	7	 86%14%
1	9	7	 71%29%
1	A	7	 86%14%
1	B	7	 86%14%
1	C	7	 86%14%
1	D	7	 86%14%
1	E	7	 71%29%
1	F	7	 86%14%
1	G	7	 86%14%















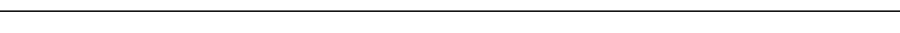
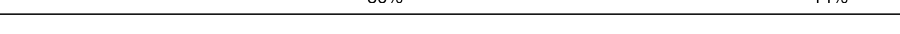


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Mol	Chain	Length	Quality of chain
1	H	7	
1	I	7	
1	J	7	
1	K	7	
1	L	7	
1	M	7	
1	N	7	
1	O	7	
1	P	7	
1	Q	7	
1	R	7	
1	S	7	
1	T	7	
1	U	7	
1	V	7	
1	W	7	
1	X	7	
1	Y	7	
1	Z	7	
1	a	7	
1	b	7	
1	c	7	
1	d	7	
1	e	7	
1	f	7	

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Mol	Chain	Length	Quality of chain
1	g	7	 86%14%
1	h	7	 86%14%
1	i	7	 86%14%
1	j	7	 86%14%
1	k	7	 71%29%
1	l	7	 86%14%
1	m	7	 86%14%
1	n	7	 14%86%14%
1	o	7	 86%14%
1	p	7	 86%14%
1	q	7	 29%86%14%
1	r	7	 14%86%14%
1	s	7	 86%14%
1	t	7	 86%14%
1	u	7	 86%14%
1	v	7	 86%14%
1	w	7	 29%86%14%
1	x	7	 29%86%14%

## 2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 3720 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 (with D amino acids) called DTH-DLE-DLY-DIL-DVA-DTR-DIL.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	7	Total	C	N	O	0	0
			62	44	9	9		
1	B	7	Total	C	N	O	0	0
			62	44	9	9		
1	C	7	Total	C	N	O	0	0
			62	44	9	9		
1	D	7	Total	C	N	O	0	0
			62	44	9	9		
1	E	7	Total	C	N	O	0	0
			62	44	9	9		
1	F	7	Total	C	N	O	0	0
			62	44	9	9		
1	G	7	Total	C	N	O	0	0
			62	44	9	9		
1	H	7	Total	C	N	O	0	0
			62	44	9	9		
1	I	7	Total	C	N	O	0	0
			62	44	9	9		
1	J	7	Total	C	N	O	0	0
			62	44	9	9		
1	K	7	Total	C	N	O	0	0
			62	44	9	9		
1	L	7	Total	C	N	O	0	0
			62	44	9	9		
1	M	7	Total	C	N	O	0	0
			62	44	9	9		
1	N	7	Total	C	N	O	0	0
			62	44	9	9		
1	O	7	Total	C	N	O	0	0
			62	44	9	9		
1	P	7	Total	C	N	O	0	0
			62	44	9	9		
1	Q	7	Total	C	N	O	0	0
			62	44	9	9		

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	R	7	Total 62	C 44	N 9	O 9	0	0
1	S	7	Total 62	C 44	N 9	O 9	0	0
1	T	7	Total 62	C 44	N 9	O 9	0	0
1	U	7	Total 62	C 44	N 9	O 9	0	0
1	V	7	Total 62	C 44	N 9	O 9	0	0
1	W	7	Total 62	C 44	N 9	O 9	0	0
1	X	7	Total 62	C 44	N 9	O 9	0	0
1	Y	7	Total 62	C 44	N 9	O 9	0	0
1	Z	7	Total 62	C 44	N 9	O 9	0	0
1	0	7	Total 62	C 44	N 9	O 9	0	0
1	1	7	Total 62	C 44	N 9	O 9	0	0
1	2	7	Total 62	C 44	N 9	O 9	0	0
1	3	7	Total 62	C 44	N 9	O 9	0	0
1	4	7	Total 62	C 44	N 9	O 9	0	0
1	5	7	Total 62	C 44	N 9	O 9	0	0
1	6	7	Total 62	C 44	N 9	O 9	0	0
1	7	7	Total 62	C 44	N 9	O 9	0	0
1	8	7	Total 62	C 44	N 9	O 9	0	0
1	9	7	Total 62	C 44	N 9	O 9	0	0
1	a	7	Total 62	C 44	N 9	O 9	0	0
1	b	7	Total 62	C 44	N 9	O 9	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	c	7	Total 62	C 44	N 9	O 9	0	0
1	d	7	Total 62	C 44	N 9	O 9	0	0
1	e	7	Total 62	C 44	N 9	O 9	0	0
1	f	7	Total 62	C 44	N 9	O 9	0	0
1	g	7	Total 62	C 44	N 9	O 9	0	0
1	h	7	Total 62	C 44	N 9	O 9	0	0
1	i	7	Total 62	C 44	N 9	O 9	0	0
1	j	7	Total 62	C 44	N 9	O 9	0	0
1	k	7	Total 62	C 44	N 9	O 9	0	0
1	l	7	Total 62	C 44	N 9	O 9	0	0
1	m	7	Total 62	C 44	N 9	O 9	0	0
1	n	7	Total 62	C 44	N 9	O 9	0	0
1	o	7	Total 62	C 44	N 9	O 9	0	0
1	p	7	Total 62	C 44	N 9	O 9	0	0
1	q	7	Total 62	C 44	N 9	O 9	0	0
1	r	7	Total 62	C 44	N 9	O 9	0	0
1	s	7	Total 62	C 44	N 9	O 9	0	0
1	t	7	Total 62	C 44	N 9	O 9	0	0
1	u	7	Total 62	C 44	N 9	O 9	0	0
1	v	7	Total 62	C 44	N 9	O 9	0	0
1	w	7	Total 62	C 44	N 9	O 9	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	x	7	Total	C	N	O	0	0
			62	44	9	9		



### 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: DTH-DLE-DLY-DIL-DVA-DTR-DIL

Chain A:  86% 14%



- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL

Chain B:  86% 14%



- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL

Chain C:  86% 14%



- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL

Chain D:  86% 14%




- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL

Chain E:  71% 29%




- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL

Chain F:  86% 14%



- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL

Chain G:  86% 14%




- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL

Chain H:  71% 29%




- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL

Chain I:  86% 14%




- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL

Chain J:  14% 86% 14%




- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL

Chain K:  86% 14%




- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL

Chain L:  86% 14%

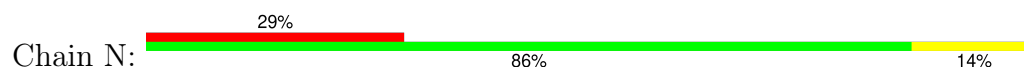


- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL

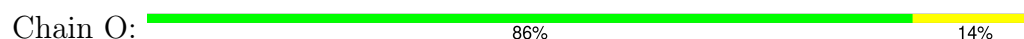
Chain M:  29% 86% 14%



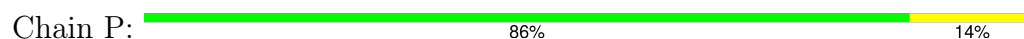
- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL



- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL



- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL



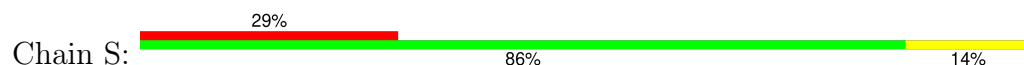
- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL



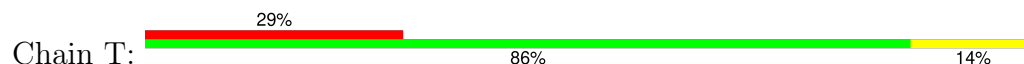
- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL



- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL




- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL






- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL

Chain U:  86% 14%




- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL

Chain V:  86% 14%




- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL

Chain W:  86% 14%




- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL

Chain X:  86% 14%




- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL

Chain Y:  86% 14%




- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL

Chain Z:  86% 14%




- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL

Chain 0:  86% 14%




- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL

Chain 1:  86% 14%




- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL

Chain 2:  14% 86% 14%




- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL

Chain 3:  86% 14%




- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL

Chain 4:  86% 14%




- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL

Chain 5:  86% 14%




- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL

Chain 6:  29% 86% 14%




- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL

Chain 7:  29% 86% 14%



- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL

Chain 8:  86% 14%




- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL

Chain 9:  71% 29%




- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL

Chain a:  86% 14%




- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL

Chain b:  86% 14%




- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL

Chain c:  29% 86% 14%




- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL

Chain d:  14% 86% 14%




- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL

Chain e:  86% 14%




- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL

Chain f:  86% 14%




- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL

Chain g:  86% 14%




- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL

Chain h:  86% 14%




- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL

Chain i:  86% 14%



- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL

Chain j:  86% 14%




- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL

Chain k:  71% 29%




- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL

Chain l:  86% 14%




- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL

Chain m:  86% 14%




- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL

Chain n:  14% 86% 14%




- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL

Chain o:  86% 14%




- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL

Chain p:  86% 14%




- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL

Chain q:  29% 86% 14%




- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL

Chain r:  14% 86% 14%



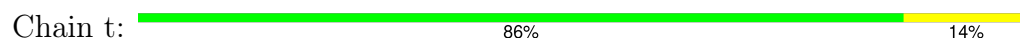
- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL

Chain s:  86% 14%

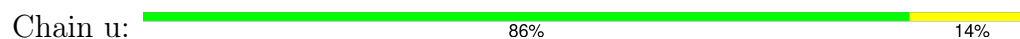




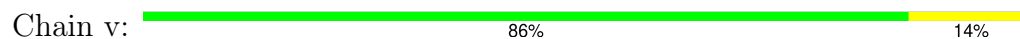
- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL



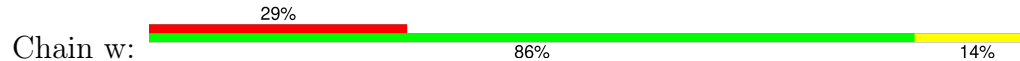
- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL



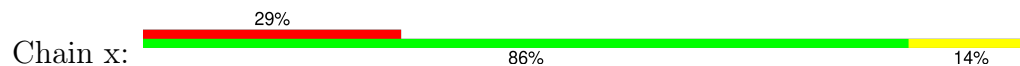
- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL



- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL



- Molecule 1: DTH-DLE-DLY-DIL-DVA-DTR-DIL



## 4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=1.604, 1.604°, rise=9.659, 9.659 Å, axial sym=C1, C1	Depositor
Number of segments used	26250	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{Å}^2$ )	50	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	26.094	Depositor
Minimum map value	-15.689	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	5.21	Depositor
Map size (Å)	300.8, 300.8, 300.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.93999994, 0.93999994, 0.93999994	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: DLE, DTR, DIL, DLY, DTH, DVA

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

### 5.3 Torsion angles [i](#)

#### 5.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

#### 5.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

#### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

420 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	DLY	m	3	1	7,8,9	0.51	0	3,8,10	0.38	0
1	DLE	8	2	1	5,7,8	0.58	0	6,8,10	0.38	0
1	DTH	g	1	1	5,6,7	0.48	0	5,7,9	0.79	0
1	DTH	L	1	1	5,6,7	0.50	0	5,7,9	0.83	0
1	DTH	a	1	1	5,6,7	0.49	0	5,7,9	0.87	0
1	DTR	t	6	1	13,15,16	0.76	0	11,20,22	0.99	0
1	DTH	x	1	1	5,6,7	0.49	0	5,7,9	0.79	0
1	DVA	t	5	1	4,6,7	0.62	0	6,7,9	0.91	0
1	DLE	7	2	1	5,7,8	0.57	0	6,8,10	0.19	0
1	DIL	2	7	1	8,8,8	0.86	1 (12%)	9,10,10	1.12	1 (11%)
1	DTR	I	6	1	13,15,16	0.76	0	11,20,22	0.95	0
1	DVA	R	5	1	4,6,7	0.66	0	6,7,9	0.92	0
1	DVA	I	5	1	4,6,7	0.60	0	6,7,9	0.97	0
1	DIL	L	7	1	8,8,8	0.85	1 (12%)	9,10,10	1.21	2 (22%)
1	DIL	f	4	1	6,7,8	0.53	0	4,8,10	0.91	0
1	DLE	F	2	1	5,7,8	0.57	0	6,8,10	0.15	0
1	DLY	S	3	1	7,8,9	0.50	0	3,8,10	0.35	0
1	DIL	4	7	1	8,8,8	0.83	1 (12%)	9,10,10	1.13	1 (11%)
1	DLE	B	2	1	5,7,8	0.57	0	6,8,10	0.20	0
1	DIL	3	7	1	8,8,8	0.81	1 (12%)	9,10,10	1.15	2 (22%)
1	DLE	V	2	1	5,7,8	0.55	0	6,8,10	0.20	0
1	DLY	b	3	1	7,8,9	0.52	0	3,8,10	0.31	0
1	DLY	q	3	1	7,8,9	0.50	0	3,8,10	0.47	0
1	DTR	B	6	1	13,15,16	0.76	0	11,20,22	0.97	0
1	DVA	B	5	1	4,6,7	0.62	0	6,7,9	0.94	0
1	DLE	X	2	1	5,7,8	0.56	0	6,8,10	0.47	0
1	DLY	a	3	1	7,8,9	0.49	0	3,8,10	0.33	0
1	DLY	p	3	1	7,8,9	0.50	0	3,8,10	0.49	0
1	DVA	G	5	1	4,6,7	0.60	0	6,7,9	0.94	0
1	DLY	P	3	1	7,8,9	0.50	0	3,8,10	0.29	0
1	DTR	x	6	1	13,15,16	0.73	0	11,20,22	0.97	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	DLE	r	2	1	5,7,8	0.58	0	6,8,10	0.20	0
1	DVA	x	5	1	4,6,7	0.61	0	6,7,9	0.90	0
1	DLY	x	3	1	7,8,9	0.52	0	3,8,10	0.42	0
1	DIL	w	4	1	6,7,8	0.53	0	4,8,10	0.93	0
1	DIL	t	7	1	8,8,8	0.89	1 (12%)	9,10,10	1.14	2 (22%)
1	DLE	d	2	1	5,7,8	0.57	0	6,8,10	0.18	0
1	DIL	f	7	1	8,8,8	0.88	1 (12%)	9,10,10	1.09	1 (11%)
1	DVA	D	5	1	4,6,7	0.62	0	6,7,9	0.92	0
1	DTH	F	1	1	5,6,7	0.49	0	5,7,9	0.79	0
1	DTH	i	1	1	5,6,7	0.49	0	5,7,9	0.78	0
1	DIL	H	4	1	6,7,8	0.54	0	4,8,10	0.92	0
1	DTH	l	1	1	5,6,7	0.48	0	5,7,9	0.78	0
1	DIL	d	7	1	8,8,8	0.82	1 (12%)	9,10,10	1.16	1 (11%)
1	DTR	F	6	1	13,15,16	0.75	0	11,20,22	0.99	0
1	DIL	P	7	1	8,8,8	0.89	1 (12%)	9,10,10	1.15	2 (22%)
1	DIL	S	4	1	6,7,8	0.54	0	4,8,10	0.93	0
1	DIL	I	4	1	6,7,8	0.54	0	4,8,10	0.90	0
1	DLY	k	3	1	7,8,9	0.51	0	3,8,10	0.41	0
1	DTH	Y	1	1	5,6,7	0.51	0	5,7,9	0.78	0
1	DIL	w	7	1	8,8,8	0.83	1 (12%)	9,10,10	1.14	1 (11%)
1	DIL	u	7	1	8,8,8	0.84	1 (12%)	9,10,10	1.18	1 (11%)
1	DVA	l	5	1	4,6,7	0.63	0	6,7,9	0.95	0
1	DTH	9	1	1	5,6,7	0.49	0	5,7,9	0.87	0
1	DLE	i	2	1	5,7,8	0.59	0	6,8,10	0.19	0
1	DIL	u	4	1	6,7,8	0.52	0	4,8,10	0.90	0
1	DIL	E	4	1	6,7,8	0.52	0	4,8,10	0.89	0
1	DLE	f	2	1	5,7,8	0.56	0	6,8,10	0.20	0
1	DTH	b	1	1	5,6,7	0.48	0	5,7,9	0.86	0
1	DTR	G	6	1	13,15,16	0.75	0	11,20,22	0.96	0
1	DLE	2	2	1	5,7,8	0.58	0	6,8,10	0.25	0
1	DIL	U	4	1	6,7,8	0.53	0	4,8,10	0.89	0
1	DTR	W	6	1	13,15,16	0.73	0	11,20,22	0.98	0
1	DLY	4	3	1	7,8,9	0.52	0	3,8,10	0.32	0
1	DLY	v	3	1	7,8,9	0.51	0	3,8,10	0.30	0
1	DTR	2	6	1	13,15,16	0.75	0	11,20,22	0.97	0
1	DVA	2	5	1	4,6,7	0.62	0	6,7,9	0.99	0
1	DVA	Q	5	1	4,6,7	0.62	0	6,7,9	0.89	0
1	DTH	n	1	1	5,6,7	0.49	0	5,7,9	0.88	0
1	DLY	K	3	1	7,8,9	0.52	0	3,8,10	0.31	0
1	DIL	C	4	1	6,7,8	0.51	0	4,8,10	0.91	0
1	DLY	i	3	1	7,8,9	0.52	0	3,8,10	0.41	0
1	DLY	d	3	1	7,8,9	0.51	0	3,8,10	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	DLY	V	3	1	7,8,9	0.50	0	3,8,10	0.40	0
1	DTR	j	6	1	13,15,16	0.74	0	11,20,22	1.00	0
1	DLY	Z	3	1	7,8,9	0.51	0	3,8,10	0.38	0
1	DVA	j	5	1	4,6,7	0.61	0	6,7,9	0.98	0
1	DTR	O	6	1	13,15,16	0.74	0	11,20,22	0.95	0
1	DTH	Z	1	1	5,6,7	0.50	0	5,7,9	0.78	0
1	DTR	c	6	1	13,15,16	0.74	0	11,20,22	0.96	0
1	DVA	c	5	1	4,6,7	0.63	0	6,7,9	0.98	0
1	DTH	N	1	1	5,6,7	0.51	0	5,7,9	0.78	0
1	DLY	w	3	1	7,8,9	0.51	0	3,8,10	0.35	0
1	DVA	H	5	1	4,6,7	0.62	0	6,7,9	0.96	0
1	DLE	M	2	1	5,7,8	0.59	0	6,8,10	0.16	0
1	DLY	O	3	1	7,8,9	0.52	0	3,8,10	0.41	0
1	DLE	H	2	1	5,7,8	0.57	0	6,8,10	0.23	0
1	DLY	n	3	1	7,8,9	0.53	0	3,8,10	0.38	0
1	DTR	M	6	1	13,15,16	0.74	0	11,20,22	0.96	0
1	DTH	3	1	1	5,6,7	0.46	0	5,7,9	0.86	0
1	DVA	W	5	1	4,6,7	0.60	0	6,7,9	0.96	0
1	DVA	M	5	1	4,6,7	0.58	0	6,7,9	0.89	0
1	DIL	Z	7	1	8,8,8	0.84	1 (12%)	9,10,10	1.17	1 (11%)
1	DTH	P	1	1	5,6,7	0.48	0	5,7,9	0.86	0
1	DTH	h	1	1	5,6,7	0.48	0	5,7,9	0.91	0
1	DTH	0	1	1	5,6,7	0.50	0	5,7,9	0.79	0
1	DTR	e	6	1	13,15,16	0.78	0	11,20,22	0.97	0
1	DIL	4	4	1	6,7,8	0.52	0	4,8,10	0.90	0
1	DTR	6	6	1	13,15,16	0.73	0	11,20,22	0.97	0
1	DTH	A	1	1	5,6,7	0.51	0	5,7,9	0.82	0
1	DLY	2	3	1	7,8,9	0.52	0	3,8,10	0.40	0
1	DLE	J	2	1	5,7,8	0.57	0	6,8,10	0.43	0
1	DIL	m	4	1	6,7,8	0.52	0	4,8,10	0.90	0
1	DLY	9	3	1	7,8,9	0.49	0	3,8,10	0.30	0
1	DLE	k	2	1	5,7,8	0.57	0	6,8,10	0.18	0
1	DLE	u	2	1	5,7,8	0.58	0	6,8,10	0.30	0
1	DLE	E	2	1	5,7,8	0.58	0	6,8,10	0.19	0
1	DTR	0	6	1	13,15,16	0.73	0	11,20,22	0.97	0
1	DIL	I	7	1	8,8,8	0.88	1 (12%)	9,10,10	1.14	1 (11%)
1	DIL	J	7	1	8,8,8	0.83	1 (12%)	9,10,10	1.13	1 (11%)
1	DVA	O	5	1	4,6,7	0.63	0	6,7,9	0.90	0
1	DIL	6	4	1	6,7,8	0.51	0	4,8,10	0.84	0
1	DTH	E	1	1	5,6,7	0.50	0	5,7,9	0.77	0
1	DVA	o	5	1	4,6,7	0.61	0	6,7,9	0.93	0
1	DIL	O	4	1	6,7,8	0.52	0	4,8,10	0.89	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	DTR	Z	6	1	13,15,16	0.75	0	11,20,22	0.97	0
1	DTR	N	6	1	13,15,16	0.74	0	11,20,22	0.99	0
1	DTH	q	1	1	5,6,7	0.52	0	5,7,9	0.80	0
1	DLY	A	3	1	7,8,9	0.51	0	3,8,10	0.22	0
1	DLY	s	3	1	7,8,9	0.51	0	3,8,10	0.41	0
1	DTH	R	1	1	5,6,7	0.48	0	5,7,9	0.85	0
1	DIL	g	7	1	8,8,8	0.83	1 (12%)	9,10,10	1.15	1 (11%)
1	DLE	D	2	1	5,7,8	0.56	0	6,8,10	0.47	0
1	DIL	x	7	1	8,8,8	0.83	1 (12%)	9,10,10	1.16	1 (11%)
1	DIL	p	4	1	6,7,8	0.50	0	4,8,10	0.88	0
1	DLE	I	2	1	5,7,8	0.58	0	6,8,10	0.25	0
1	DIL	L	4	1	6,7,8	0.51	0	4,8,10	0.91	0
1	DIL	a	4	1	6,7,8	0.52	0	4,8,10	0.89	0
1	DTR	k	6	1	13,15,16	0.74	0	11,20,22	0.99	1 (9%)
1	DTR	R	6	1	13,15,16	0.75	0	11,20,22	0.98	0
1	DTH	l	1	1	5,6,7	0.52	0	5,7,9	0.76	0
1	DTR	E	6	1	13,15,16	0.73	0	11,20,22	0.99	1 (9%)
1	DVA	E	5	1	4,6,7	0.62	0	6,7,9	0.93	0
1	DLY	J	3	1	7,8,9	0.51	0	3,8,10	0.38	0
1	DVA	4	5	1	4,6,7	0.63	0	6,7,9	0.93	0
1	DVA	v	5	1	4,6,7	0.65	0	6,7,9	0.93	0
1	DIL	X	4	1	6,7,8	0.52	0	4,8,10	0.90	0
1	DVA	3	5	1	4,6,7	0.62	0	6,7,9	0.93	0
1	DLE	v	2	1	5,7,8	0.56	0	6,8,10	0.24	0
1	DVA	A	5	1	4,6,7	0.64	0	6,7,9	0.93	0
1	DTH	d	1	1	5,6,7	0.51	0	5,7,9	0.79	0
1	DLE	g	2	1	5,7,8	0.57	0	6,8,10	0.35	0
1	DVA	T	5	1	4,6,7	0.61	0	6,7,9	0.88	0
1	DLE	a	2	1	5,7,8	0.57	0	6,8,10	0.32	0
1	DTR	C	6	1	13,15,16	0.74	0	11,20,22	0.98	0
1	DVA	0	5	1	4,6,7	0.61	0	6,7,9	0.93	0
1	DVA	C	5	1	4,6,7	0.60	0	6,7,9	0.96	0
1	DLY	U	3	1	7,8,9	0.51	0	3,8,10	0.23	0
1	DLE	m	2	1	5,7,8	0.58	0	6,8,10	0.24	0
1	DLE	C	2	1	5,7,8	0.57	0	6,8,10	0.37	0
1	DLE	t	2	1	5,7,8	0.57	0	6,8,10	0.31	0
1	DIL	m	7	1	8,8,8	0.88	1 (12%)	9,10,10	1.13	1 (11%)
1	DTH	7	1	1	5,6,7	0.51	0	5,7,9	0.77	0
1	DTH	p	1	1	5,6,7	0.49	0	5,7,9	0.84	0
1	DIL	Q	7	1	8,8,8	0.84	1 (12%)	9,10,10	1.16	1 (11%)
1	DTH	5	1	1	5,6,7	0.48	0	5,7,9	0.80	0
1	DLY	D	3	1	7,8,9	0.54	0	3,8,10	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	DTR	8	6	1	13,15,16	0.74	0	11,20,22	0.97	0
1	DLY	6	3	1	7,8,9	0.51	0	3,8,10	0.47	0
1	DTH	K	1	1	5,6,7	0.48	0	5,7,9	0.84	0
1	DIL	l	4	1	6,7,8	0.53	0	4,8,10	0.92	0
1	DIL	B	4	1	6,7,8	0.53	0	4,8,10	0.91	0
1	DTR	7	6	1	13,15,16	0.74	0	11,20,22	0.99	0
1	DIL	j	7	1	8,8,8	0.84	1 (12%)	9,10,10	1.16	1 (11%)
1	DIL	V	4	1	6,7,8	0.51	0	4,8,10	0.91	0
1	DVA	b	5	1	4,6,7	0.65	0	6,7,9	0.91	0
1	DTR	g	6	1	13,15,16	0.74	0	11,20,22	0.98	0
1	DVA	g	5	1	4,6,7	0.60	0	6,7,9	0.95	0
1	DTR	P	6	1	13,15,16	0.75	0	11,20,22	0.98	0
1	DVA	m	5	1	4,6,7	0.61	0	6,7,9	1.01	0
1	DVA	h	5	1	4,6,7	0.64	0	6,7,9	0.92	0
1	DTH	k	1	1	5,6,7	0.50	0	5,7,9	0.78	0
1	DIL	k	4	1	6,7,8	0.54	0	4,8,10	0.88	0
1	DLY	T	3	1	7,8,9	0.52	0	3,8,10	0.40	0
1	DLY	h	3	1	7,8,9	0.52	0	3,8,10	0.24	0
1	DIL	9	4	1	6,7,8	0.50	0	4,8,10	0.90	0
1	DLY	L	3	1	7,8,9	0.51	0	3,8,10	0.48	0
1	DTR	1	6	1	13,15,16	0.75	0	11,20,22	0.98	0
1	DIL	M	7	1	8,8,8	0.83	1 (12%)	9,10,10	1.24	2 (22%)
1	DTH	8	1	1	5,6,7	0.48	0	5,7,9	0.84	0
1	DTH	U	1	1	5,6,7	0.49	0	5,7,9	0.83	0
1	DTR	D	6	1	13,15,16	0.75	0	11,20,22	0.97	0
1	DIL	b	4	1	6,7,8	0.52	0	4,8,10	0.90	0
1	DIL	j	4	1	6,7,8	0.53	0	4,8,10	0.90	0
1	DLY	o	3	1	7,8,9	0.52	0	3,8,10	0.33	0
1	DLY	Q	3	1	7,8,9	0.50	0	3,8,10	0.33	0
1	DLY	5	3	1	7,8,9	0.50	0	3,8,10	0.49	0
1	DIL	n	4	1	6,7,8	0.52	0	4,8,10	0.88	0
1	DIL	6	7	1	8,8,8	0.83	1 (12%)	9,10,10	1.24	2 (22%)
1	DTR	d	6	1	13,15,16	0.75	0	11,20,22	0.96	0
1	DLE	O	2	1	5,7,8	0.58	0	6,8,10	0.41	0
1	DLE	c	2	1	5,7,8	0.57	0	6,8,10	0.18	0
1	DIL	g	4	1	6,7,8	0.52	0	4,8,10	0.92	0
1	DVA	P	5	1	4,6,7	0.61	0	6,7,9	0.92	0
1	DLE	o	2	1	5,7,8	0.58	0	6,8,10	0.29	0
1	DIL	Z	4	1	6,7,8	0.53	0	4,8,10	0.91	0
1	DTH	S	1	1	5,6,7	0.52	0	5,7,9	0.76	0
1	DTH	V	1	1	5,6,7	0.46	0	5,7,9	0.81	0
1	DIL	r	4	1	6,7,8	0.53	0	4,8,10	0.94	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	DIL	O	7	1	8,8,8	0.87	1 (12%)	9,10,10	1.11	1 (11%)
1	DLY	t	3	1	7,8,9	0.49	0	3,8,10	0.29	0
1	DIL	5	4	1	6,7,8	0.51	0	4,8,10	0.90	0
1	DTH	I	1	1	5,6,7	0.52	0	5,7,9	0.80	0
1	DLE	W	2	1	5,7,8	0.57	0	6,8,10	0.37	0
1	DTH	f	1	1	5,6,7	0.48	0	5,7,9	0.81	0
1	DVA	r	5	1	4,6,7	0.63	0	6,7,9	1.00	0
1	DTR	v	6	1	13,15,16	0.76	0	11,20,22	0.98	0
1	DVA	5	5	1	4,6,7	0.62	0	6,7,9	0.98	0
1	DLY	3	3	1	7,8,9	0.51	0	3,8,10	0.38	0
1	DLE	Z	2	1	5,7,8	0.56	0	6,8,10	0.16	0
1	DLY	F	3	1	7,8,9	0.51	0	3,8,10	0.39	0
1	DIL	P	4	1	6,7,8	0.50	0	4,8,10	0.91	0
1	DTH	T	1	1	5,6,7	0.49	0	5,7,9	0.79	0
1	DIL	T	4	1	6,7,8	0.51	0	4,8,10	0.89	0
1	DIL	h	4	1	6,7,8	0.53	0	4,8,10	0.92	0
1	DTR	K	6	1	13,15,16	0.75	0	11,20,22	0.96	0
1	DLY	l	3	1	7,8,9	0.52	0	3,8,10	0.36	0
1	DVA	K	5	1	4,6,7	0.64	0	6,7,9	0.93	0
1	DTR	f	6	1	13,15,16	0.76	0	11,20,22	0.97	0
1	DIL	l	7	1	8,8,8	0.82	1 (12%)	9,10,10	1.15	1 (11%)
1	DIL	X	7	1	8,8,8	0.85	1 (12%)	9,10,10	1.18	2 (22%)
1	DTH	m	1	1	5,6,7	0.51	0	5,7,9	0.81	0
1	DVA	w	5	1	4,6,7	0.64	0	6,7,9	1.01	0
1	DTR	q	6	1	13,15,16	0.74	0	11,20,22	0.98	0
1	DTH	o	1	1	5,6,7	0.49	0	5,7,9	0.84	0
1	DVA	9	5	1	4,6,7	0.62	0	6,7,9	0.92	0
1	DIL	s	4	1	6,7,8	0.50	0	4,8,10	0.90	0
1	DVA	q	5	1	4,6,7	0.60	0	6,7,9	0.90	0
1	DTH	C	1	1	5,6,7	0.48	0	5,7,9	0.80	0
1	DLE	w	2	1	5,7,8	0.57	0	6,8,10	0.19	0
1	DLY	X	3	1	7,8,9	0.53	0	3,8,10	0.24	0
1	DIL	E	7	1	8,8,8	0.83	1 (12%)	9,10,10	1.12	1 (11%)
1	DLY	e	3	1	7,8,9	0.51	0	3,8,10	0.23	0
1	DIL	T	7	1	8,8,8	0.84	1 (12%)	9,10,10	1.17	1 (11%)
1	DLY	j	3	1	7,8,9	0.51	0	3,8,10	0.38	0
1	DTH	W	1	1	5,6,7	0.48	0	5,7,9	0.80	0
1	DIL	C	7	1	8,8,8	0.84	1 (12%)	9,10,10	1.16	2 (22%)
1	DVA	1	5	1	4,6,7	0.62	0	6,7,9	0.97	0
1	DIL	F	7	1	8,8,8	0.85	1 (12%)	9,10,10	1.18	1 (11%)
1	DIL	R	4	1	6,7,8	0.53	0	4,8,10	0.91	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	DTR	H	6	1	13,15,16	0.74	0	11,20,22	0.98	1 (9%)
1	DTH	J	1	1	5,6,7	0.47	0	5,7,9	0.88	0
1	DIL	e	4	1	6,7,8	0.53	0	4,8,10	0.89	0
1	DTH	u	1	1	5,6,7	0.48	0	5,7,9	0.86	0
1	DLE	9	2	1	5,7,8	0.56	0	6,8,10	0.30	0
1	DLY	r	3	1	7,8,9	0.52	0	3,8,10	0.36	0
1	DVA	e	5	1	4,6,7	0.65	0	6,7,9	0.92	0
1	DLY	N	3	1	7,8,9	0.51	0	3,8,10	0.35	0
1	DIL	r	7	1	8,8,8	0.82	1 (12%)	9,10,10	1.16	2 (22%)
1	DIL	Y	7	1	8,8,8	0.82	1 (12%)	9,10,10	1.12	1 (11%)
1	DTR	J	6	1	13,15,16	0.75	0	11,20,22	0.98	0
1	DLE	3	2	1	5,7,8	0.57	0	6,8,10	0.44	0
1	DLY	W	3	1	7,8,9	0.53	0	3,8,10	0.37	0
1	DTR	u	6	1	13,15,16	0.76	0	11,20,22	0.97	0
1	DIL	b	7	1	8,8,8	0.86	1 (12%)	9,10,10	1.18	2 (22%)
1	DIL	t	4	1	6,7,8	0.51	0	4,8,10	0.90	0
1	DLY	0	3	1	7,8,9	0.52	0	3,8,10	0.41	0
1	DTH	O	1	1	5,6,7	0.49	0	5,7,9	0.84	0
1	DIL	D	4	1	6,7,8	0.52	0	4,8,10	0.89	0
1	DIL	0	7	1	8,8,8	0.83	1 (12%)	9,10,10	1.26	2 (22%)
1	DTR	V	6	1	13,15,16	0.78	0	11,20,22	0.97	0
1	DLY	c	3	1	7,8,9	0.52	0	3,8,10	0.36	0
1	DTH	t	1	1	5,6,7	0.48	0	5,7,9	0.85	0
1	DVA	V	5	1	4,6,7	0.63	0	6,7,9	0.95	0
1	DIL	2	4	1	6,7,8	0.53	0	4,8,10	0.89	0
1	DIL	c	7	1	8,8,8	0.83	1 (12%)	9,10,10	1.14	1 (11%)
1	DVA	N	5	1	4,6,7	0.62	0	6,7,9	1.00	0
1	DLE	Y	2	1	5,7,8	0.58	0	6,8,10	0.18	0
1	DLE	P	2	1	5,7,8	0.56	0	6,8,10	0.30	0
1	DTR	Y	6	1	13,15,16	0.75	0	11,20,22	0.98	0
1	DLY	M	3	1	7,8,9	0.49	0	3,8,10	0.47	0
1	DIL	0	4	1	6,7,8	0.53	0	4,8,10	0.91	0
1	DIL	W	7	1	8,8,8	0.85	1 (12%)	9,10,10	1.16	2 (22%)
1	DLE	T	2	1	5,7,8	0.58	0	6,8,10	0.19	0
1	DLE	h	2	1	5,7,8	0.57	0	6,8,10	0.46	0
1	DTH	Q	1	1	5,6,7	0.48	0	5,7,9	0.86	0
1	DTH	v	1	1	5,6,7	0.49	0	5,7,9	0.85	0
1	DLE	q	2	1	5,7,8	0.58	0	6,8,10	0.14	0
1	DTR	b	6	1	13,15,16	0.77	0	11,20,22	0.97	0
1	DLE	L	2	1	5,7,8	0.57	0	6,8,10	0.20	0
1	DTH	6	1	1	5,6,7	0.50	0	5,7,9	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	DVA	k	5	1	4,6,7	0.62	0	6,7,9	0.93	0
1	DLY	R	3	1	7,8,9	0.52	0	3,8,10	0.30	0
1	DTR	i	6	1	13,15,16	0.75	0	11,20,22	0.97	0
1	DLE	5	2	1	5,7,8	0.57	0	6,8,10	0.20	0
1	DIL	M	4	1	6,7,8	0.52	0	4,8,10	0.84	0
1	DLE	G	2	1	5,7,8	0.58	0	6,8,10	0.18	0
1	DLE	x	2	1	5,7,8	0.58	0	6,8,10	0.19	0
1	DIL	B	7	1	8,8,8	0.89	1 (12%)	9,10,10	1.08	1 (11%)
1	DLE	Q	2	1	5,7,8	0.57	0	6,8,10	0.29	0
1	DTR	m	6	1	13,15,16	0.75	0	11,20,22	0.95	0
1	DIL	A	7	1	8,8,8	0.85	1 (12%)	9,10,10	1.13	1 (11%)
1	DTH	j	1	1	5,6,7	0.48	0	5,7,9	0.79	0
1	DTR	Q	6	1	13,15,16	0.74	0	11,20,22	0.97	1 (9%)
1	DTR	S	6	1	13,15,16	0.74	0	11,20,22	0.98	0
1	DVA	S	5	1	4,6,7	0.62	0	6,7,9	1.00	0
1	DLE	n	2	1	5,7,8	0.57	0	6,8,10	0.44	0
1	DIL	q	7	1	8,8,8	0.84	1 (12%)	9,10,10	1.24	2 (22%)
1	DTR	s	6	1	13,15,16	0.74	0	11,20,22	0.97	0
1	DIL	F	4	1	6,7,8	0.53	0	4,8,10	0.90	0
1	DTH	X	1	1	5,6,7	0.47	0	5,7,9	0.92	0
1	DVA	a	5	1	4,6,7	0.63	0	6,7,9	0.89	0
1	DTR	p	6	1	13,15,16	0.77	0	11,20,22	1.00	0
1	DTH	M	1	1	5,6,7	0.49	0	5,7,9	0.81	0
1	DTH	B	1	1	5,6,7	0.49	0	5,7,9	0.81	0
1	DIL	R	7	1	8,8,8	0.85	1 (12%)	9,10,10	1.16	2 (22%)
1	DLE	s	2	1	5,7,8	0.58	0	6,8,10	0.39	0
1	DTH	r	1	1	5,6,7	0.50	0	5,7,9	0.77	0
1	DLY	G	3	1	7,8,9	0.51	0	3,8,10	0.41	0
1	DIL	Y	4	1	6,7,8	0.52	0	4,8,10	0.89	0
1	DLE	1	2	1	5,7,8	0.57	0	6,8,10	0.22	0
1	DIL	h	7	1	8,8,8	0.84	1 (12%)	9,10,10	1.17	2 (22%)
1	DLY	I	3	1	7,8,9	0.52	0	3,8,10	0.40	0
1	DTR	4	6	1	13,15,16	0.75	0	11,20,22	0.97	0
1	DVA	L	5	1	4,6,7	0.62	0	6,7,9	0.97	0
1	DVA	7	5	1	4,6,7	0.62	0	6,7,9	0.99	0
1	DTR	o	6	1	13,15,16	0.77	0	11,20,22	0.97	0
1	DIL	7	7	1	8,8,8	0.82	1 (12%)	9,10,10	1.15	2 (22%)
1	DLE	K	2	1	5,7,8	0.58	0	6,8,10	0.32	0
1	DIL	1	7	1	8,8,8	0.82	1 (12%)	9,10,10	1.15	1 (11%)
1	DIL	v	7	1	8,8,8	0.86	1 (12%)	9,10,10	1.16	2 (22%)
1	DTR	l	6	1	13,15,16	0.75	0	11,20,22	0.98	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	DIL	G	7	1	8,8,8	0.84	1 (12%)	9,10,10	1.25	2 (22%)
1	DLY	C	3	1	7,8,9	0.52	0	3,8,10	0.36	0
1	DVA	d	5	1	4,6,7	0.60	0	6,7,9	0.89	0
1	DTH	c	1	1	5,6,7	0.51	0	5,7,9	0.78	0
1	DVA	6	5	1	4,6,7	0.60	0	6,7,9	0.91	0
1	DIL	o	4	1	6,7,8	0.52	0	4,8,10	0.88	0
1	DIL	p	7	1	8,8,8	0.84	1 (12%)	9,10,10	1.20	2 (22%)
1	DIL	e	7	1	8,8,8	0.82	1 (12%)	9,10,10	1.13	1 (11%)
1	DIL	D	7	1	8,8,8	0.86	1 (12%)	9,10,10	1.18	2 (22%)
1	DIL	N	4	1	6,7,8	0.52	0	4,8,10	0.93	0
1	DIL	c	4	1	6,7,8	0.54	0	4,8,10	0.92	0
1	DVA	s	5	1	4,6,7	0.63	0	6,7,9	0.93	0
1	DTH	2	1	1	5,6,7	0.51	0	5,7,9	0.80	0
1	DVA	p	5	1	4,6,7	0.61	0	6,7,9	0.97	0
1	DTR	3	6	1	13,15,16	0.74	0	11,20,22	0.97	0
1	DLY	8	3	1	7,8,9	0.52	0	3,8,10	0.40	0
1	DIL	U	7	1	8,8,8	0.85	1 (12%)	9,10,10	1.14	1 (11%)
1	DIL	W	4	1	6,7,8	0.50	0	4,8,10	0.91	0
1	DVA	F	5	1	4,6,7	0.59	0	6,7,9	0.98	0
1	DLY	7	3	1	7,8,9	0.52	0	3,8,10	0.35	0
1	DIL	H	7	1	8,8,8	0.84	1 (12%)	9,10,10	1.15	1 (11%)
1	DLY	B	3	1	7,8,9	0.49	0	3,8,10	0.40	0
1	DIL	V	7	1	8,8,8	0.88	1 (12%)	9,10,10	1.10	1 (11%)
1	DVA	Y	5	1	4,6,7	0.63	0	6,7,9	0.93	0
1	DIL	a	7	1	8,8,8	0.84	1 (12%)	9,10,10	1.18	1 (11%)
1	DTR	X	6	1	13,15,16	0.75	0	11,20,22	0.97	0
1	DTH	w	1	1	5,6,7	0.52	0	5,7,9	0.77	0
1	DVA	X	5	1	4,6,7	0.63	0	6,7,9	0.93	0
1	DIL	3	4	1	6,7,8	0.50	0	4,8,10	0.88	0
1	DIL	N	7	1	8,8,8	0.82	1 (12%)	9,10,10	1.14	1 (11%)
1	DLE	e	2	1	5,7,8	0.59	0	6,8,10	0.36	0
1	DTR	r	6	1	13,15,16	0.76	0	11,20,22	0.97	0
1	DIL	5	7	1	8,8,8	0.84	1 (12%)	9,10,10	1.17	2 (22%)
1	DLE	j	2	1	5,7,8	0.57	0	6,8,10	0.17	0
1	DLY	1	3	1	7,8,9	0.51	0	3,8,10	0.36	0
1	DTH	H	1	1	5,6,7	0.51	0	5,7,9	0.78	0
1	DIL	7	4	1	6,7,8	0.52	0	4,8,10	0.93	0
1	DIL	K	7	1	8,8,8	0.83	1 (12%)	9,10,10	1.14	2 (22%)
1	DVA	8	5	1	4,6,7	0.63	0	6,7,9	0.91	0
1	DIL	A	4	1	6,7,8	0.53	0	4,8,10	0.89	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	DIL	8	7	1	8,8,8	0.87	1 (12%)	9,10,10	1.11	1 (11%)
1	DTR	w	6	1	13,15,16	0.73	0	11,20,22	0.98	0
1	DTR	A	6	1	13,15,16	0.77	0	11,20,22	0.98	0
1	DIL	k	7	1	8,8,8	0.83	1 (12%)	9,10,10	1.24	2 (22%)
1	DVA	Z	5	1	4,6,7	0.60	0	6,7,9	0.97	0
1	DIL	l	4	1	6,7,8	0.53	0	4,8,10	0.92	0
1	DTH	s	1	1	5,6,7	0.48	0	5,7,9	0.84	0
1	DIL	S	7	1	8,8,8	0.83	1 (12%)	9,10,10	1.15	2 (22%)
1	DIL	i	7	1	8,8,8	0.82	1 (12%)	9,10,10	1.11	1 (11%)
1	DVA	f	5	1	4,6,7	0.62	0	6,7,9	0.96	0
1	DLY	H	3	1	7,8,9	0.50	0	3,8,10	0.37	0
1	DTR	9	6	1	13,15,16	0.76	0	11,20,22	0.99	1 (9%)
1	DLE	0	2	1	5,7,8	0.58	0	6,8,10	0.18	0
1	DLE	U	2	1	5,7,8	0.61	0	6,8,10	0.37	0
1	DIL	v	4	1	6,7,8	0.53	0	4,8,10	0.86	0
1	DTR	n	6	1	13,15,16	0.76	0	11,20,22	0.99	0
1	DTR	U	6	1	13,15,16	0.76	0	11,20,22	0.97	0
1	DVA	n	5	1	4,6,7	0.63	0	6,7,9	0.94	0
1	DLE	A	2	1	5,7,8	0.59	0	6,8,10	0.35	0
1	DVA	U	5	1	4,6,7	0.66	0	6,7,9	0.93	0
1	DLY	f	3	1	7,8,9	0.50	0	3,8,10	0.40	0
1	DLE	4	2	1	5,7,8	0.59	0	6,8,10	0.32	0
1	DLY	Y	3	1	7,8,9	0.52	0	3,8,10	0.42	0
1	DLY	E	3	1	7,8,9	0.53	0	3,8,10	0.40	0
1	DIL	9	7	1	8,8,8	0.87	1 (12%)	9,10,10	1.16	2 (22%)
1	DLE	N	2	1	5,7,8	0.57	0	6,8,10	0.19	0
1	DVA	u	5	1	4,6,7	0.61	0	6,7,9	0.91	0
1	DIL	o	7	1	8,8,8	0.84	1 (12%)	9,10,10	1.14	1 (11%)
1	DLY	u	3	1	7,8,9	0.49	0	3,8,10	0.34	0
1	DIL	d	4	1	6,7,8	0.52	0	4,8,10	0.88	0
1	DLE	S	2	1	5,7,8	0.57	0	6,8,10	0.18	0
1	DLE	6	2	1	5,7,8	0.58	0	6,8,10	0.14	0
1	DTH	4	1	1	5,6,7	0.46	0	5,7,9	0.83	0
1	DIL	q	4	1	6,7,8	0.51	0	4,8,10	0.85	0
1	DLY	g	3	1	7,8,9	0.53	0	3,8,10	0.37	0
1	DLE	R	2	1	5,7,8	0.56	0	6,8,10	0.24	0
1	DIL	J	4	1	6,7,8	0.51	0	4,8,10	0.90	0
1	DIL	n	7	1	8,8,8	0.83	1 (12%)	9,10,10	1.14	2 (22%)
1	DLE	p	2	1	5,7,8	0.57	0	6,8,10	0.21	0
1	DVA	J	5	1	4,6,7	0.63	0	6,7,9	0.94	0
1	DTR	T	6	1	13,15,16	0.74	0	11,20,22	0.98	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	DTR	h	6	1	13,15,16	0.74	0	11,20,22	0.98	0
1	DIL	s	7	1	8,8,8	0.87	1 (12%)	9,10,10	1.11	1 (11%)
1	DLE	b	2	1	5,7,8	0.55	0	6,8,10	0.25	0
1	DTH	e	1	1	5,6,7	0.50	0	5,7,9	0.83	0
1	DTH	G	1	1	5,6,7	0.51	0	5,7,9	0.78	0
1	DIL	G	4	1	6,7,8	0.54	0	4,8,10	0.90	0
1	DIL	K	4	1	6,7,8	0.52	0	4,8,10	0.88	0
1	DTH	D	1	1	5,6,7	0.49	0	5,7,9	0.92	0
1	DTR	L	6	1	13,15,16	0.77	0	11,20,22	0.96	0
1	DIL	i	4	1	6,7,8	0.52	0	4,8,10	0.90	0
1	DTR	a	6	1	13,15,16	0.76	0	11,20,22	0.98	0
1	DIL	x	4	1	6,7,8	0.52	0	4,8,10	0.88	0
1	DIL	Q	4	1	6,7,8	0.52	0	4,8,10	0.90	0
1	DIL	8	4	1	6,7,8	0.50	0	4,8,10	0.89	0
1	DTR	5	6	1	13,15,16	0.76	0	11,20,22	0.97	0
1	DLE	l	2	1	5,7,8	0.56	0	6,8,10	0.22	0
1	DVA	i	5	1	4,6,7	0.62	0	6,7,9	0.92	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	DLY	m	3	1	-	0/6/7/9	-
1	DLE	8	2	1	-	0/5/6/8	-
1	DTH	g	1	1	-	1/5/6/8	-
1	DTH	L	1	1	-	0/5/6/8	-
1	DTH	a	1	1	-	0/5/6/8	-
1	DTR	t	6	1	-	1/4/6/8	0/2/2/2
1	DTH	x	1	1	-	0/5/6/8	-
1	DVA	t	5	1	-	0/5/6/8	-
1	DLE	7	2	1	-	0/5/6/8	-
1	DIL	2	7	1	-	1/10/10/10	-
1	DTR	I	6	1	-	0/4/6/8	0/2/2/2
1	DVA	R	5	1	-	0/5/6/8	-
1	DVA	I	5	1	-	0/5/6/8	-
1	DIL	L	7	1	-	1/10/10/10	-
1	DIL	f	4	1	-	0/7/8/10	-
1	DLE	F	2	1	-	0/5/6/8	-
1	DLY	S	3	1	-	0/6/7/9	-
1	DIL	4	7	1	-	1/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	DLE	B	2	1	-	0/5/6/8	-
1	DIL	3	7	1	-	1/10/10/10	-
1	DLE	V	2	1	-	0/5/6/8	-
1	DLY	b	3	1	-	0/6/7/9	-
1	DLY	q	3	1	-	0/6/7/9	-
1	DTR	B	6	1	-	2/4/6/8	0/2/2/2
1	DVA	B	5	1	-	0/5/6/8	-
1	DLE	X	2	1	-	0/5/6/8	-
1	DLY	a	3	1	-	0/6/7/9	-
1	DLY	p	3	1	-	0/6/7/9	-
1	DVA	G	5	1	-	0/5/6/8	-
1	DLY	P	3	1	-	0/6/7/9	-
1	DTR	x	6	1	-	1/4/6/8	0/2/2/2
1	DLE	r	2	1	-	0/5/6/8	-
1	DVA	x	5	1	-	1/5/6/8	-
1	DLY	x	3	1	-	0/6/7/9	-
1	DIL	w	4	1	-	0/7/8/10	-
1	DIL	t	7	1	-	1/10/10/10	-
1	DLE	d	2	1	-	0/5/6/8	-
1	DIL	f	7	1	-	2/10/10/10	-
1	DVA	D	5	1	-	0/5/6/8	-
1	DTH	F	1	1	-	0/5/6/8	-
1	DTH	i	1	1	-	1/5/6/8	-
1	DIL	H	4	1	-	0/7/8/10	-
1	DTH	l	1	1	-	0/5/6/8	-
1	DIL	d	7	1	-	1/10/10/10	-
1	DTR	F	6	1	-	1/4/6/8	0/2/2/2
1	DIL	P	7	1	-	1/10/10/10	-
1	DIL	S	4	1	-	0/7/8/10	-
1	DIL	I	4	1	-	0/7/8/10	-
1	DLY	k	3	1	-	0/6/7/9	-
1	DTH	Y	1	1	-	1/5/6/8	-
1	DIL	w	7	1	-	1/10/10/10	-
1	DIL	u	7	1	-	2/10/10/10	-
1	DVA	l	5	1	-	0/5/6/8	-
1	DTH	9	1	1	-	0/5/6/8	-
1	DLE	i	2	1	-	0/5/6/8	-
1	DIL	u	4	1	-	0/7/8/10	-
1	DIL	E	4	1	-	0/7/8/10	-
1	DLE	f	2	1	-	0/5/6/8	-
1	DTH	b	1	1	-	0/5/6/8	-
1	DTR	G	6	1	-	1/4/6/8	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	DLE	2	2	1	-	0/5/6/8	-
1	DIL	U	4	1	-	0/7/8/10	-
1	DTR	W	6	1	-	1/4/6/8	0/2/2/2
1	DLY	4	3	1	-	1/6/7/9	-
1	DLY	v	3	1	-	0/6/7/9	-
1	DTR	2	6	1	-	0/4/6/8	0/2/2/2
1	DVA	2	5	1	-	0/5/6/8	-
1	DVA	Q	5	1	-	0/5/6/8	-
1	DTH	n	1	1	-	0/5/6/8	-
1	DLY	K	3	1	-	1/6/7/9	-
1	DIL	C	4	1	-	0/7/8/10	-
1	DLY	i	3	1	-	1/6/7/9	-
1	DLY	d	3	1	-	0/6/7/9	-
1	DLY	V	3	1	-	0/6/7/9	-
1	DTR	j	6	1	-	1/4/6/8	0/2/2/2
1	DLY	Z	3	1	-	0/6/7/9	-
1	DVA	j	5	1	-	0/5/6/8	-
1	DTR	O	6	1	-	0/4/6/8	0/2/2/2
1	DTH	Z	1	1	-	0/5/6/8	-
1	DTR	c	6	1	-	2/4/6/8	0/2/2/2
1	DVA	c	5	1	-	0/5/6/8	-
1	DTH	N	1	1	-	1/5/6/8	-
1	DLY	w	3	1	-	0/6/7/9	-
1	DVA	H	5	1	-	0/5/6/8	-
1	DLE	M	2	1	-	0/5/6/8	-
1	DLY	O	3	1	-	0/6/7/9	-
1	DLE	H	2	1	-	2/5/6/8	-
1	DLY	n	3	1	-	0/6/7/9	-
1	DTR	M	6	1	-	0/4/6/8	0/2/2/2
1	DTH	3	1	1	-	0/5/6/8	-
1	DVA	W	5	1	-	0/5/6/8	-
1	DVA	M	5	1	-	1/5/6/8	-
1	DIL	Z	7	1	-	2/10/10/10	-
1	DTH	P	1	1	-	0/5/6/8	-
1	DTH	h	1	1	-	1/5/6/8	-
1	DTH	0	1	1	-	0/5/6/8	-
1	DTR	e	6	1	-	1/4/6/8	0/2/2/2
1	DIL	4	4	1	-	0/7/8/10	-
1	DTR	6	6	1	-	0/4/6/8	0/2/2/2
1	DTH	A	1	1	-	0/5/6/8	-
1	DLY	2	3	1	-	0/6/7/9	-
1	DLE	J	2	1	-	1/5/6/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	DIL	m	4	1	-	0/7/8/10	-
1	DLY	9	3	1	-	0/6/7/9	-
1	DLE	k	2	1	-	0/5/6/8	-
1	DLE	u	2	1	-	0/5/6/8	-
1	DLE	E	2	1	-	0/5/6/8	-
1	DTR	0	6	1	-	1/4/6/8	0/2/2/2
1	DIL	I	7	1	-	1/10/10/10	-
1	DIL	J	7	1	-	1/10/10/10	-
1	DVA	O	5	1	-	0/5/6/8	-
1	DIL	6	4	1	-	3/7/8/10	-
1	DTH	E	1	1	-	1/5/6/8	-
1	DVA	o	5	1	-	0/5/6/8	-
1	DIL	O	4	1	-	0/7/8/10	-
1	DTR	Z	6	1	-	1/4/6/8	0/2/2/2
1	DTR	N	6	1	-	0/4/6/8	0/2/2/2
1	DTH	q	1	1	-	0/5/6/8	-
1	DLY	A	3	1	-	2/6/7/9	-
1	DLY	s	3	1	-	0/6/7/9	-
1	DTH	R	1	1	-	0/5/6/8	-
1	DIL	g	7	1	-	1/10/10/10	-
1	DLE	D	2	1	-	0/5/6/8	-
1	DIL	x	7	1	-	1/10/10/10	-
1	DIL	p	4	1	-	0/7/8/10	-
1	DLE	I	2	1	-	0/5/6/8	-
1	DIL	L	4	1	-	0/7/8/10	-
1	DIL	a	4	1	-	0/7/8/10	-
1	DTR	k	6	1	-	1/4/6/8	0/2/2/2
1	DTR	R	6	1	-	0/4/6/8	0/2/2/2
1	DTH	1	1	1	-	0/5/6/8	-
1	DTR	E	6	1	-	0/4/6/8	0/2/2/2
1	DVA	E	5	1	-	0/5/6/8	-
1	DLY	J	3	1	-	0/6/7/9	-
1	DVA	4	5	1	-	0/5/6/8	-
1	DVA	v	5	1	-	0/5/6/8	-
1	DIL	X	4	1	-	0/7/8/10	-
1	DVA	3	5	1	-	0/5/6/8	-
1	DLE	v	2	1	-	0/5/6/8	-
1	DVA	A	5	1	-	0/5/6/8	-
1	DTH	d	1	1	-	0/5/6/8	-
1	DLE	g	2	1	-	0/5/6/8	-
1	DVA	T	5	1	-	1/5/6/8	-
1	DLE	a	2	1	-	0/5/6/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	DTR	C	6	1	-	1/4/6/8	0/2/2/2
1	DVA	0	5	1	-	0/5/6/8	-
1	DVA	C	5	1	-	0/5/6/8	-
1	DLY	U	3	1	-	2/6/7/9	-
1	DLE	m	2	1	-	0/5/6/8	-
1	DLE	C	2	1	-	0/5/6/8	-
1	DLE	t	2	1	-	0/5/6/8	-
1	DIL	m	7	1	-	1/10/10/10	-
1	DTH	7	1	1	-	1/5/6/8	-
1	DTH	p	1	1	-	0/5/6/8	-
1	DIL	Q	7	1	-	2/10/10/10	-
1	DTH	5	1	1	-	0/5/6/8	-
1	DLY	D	3	1	-	2/6/7/9	-
1	DTR	8	6	1	-	0/4/6/8	0/2/2/2
1	DLY	6	3	1	-	0/6/7/9	-
1	DTH	K	1	1	-	0/5/6/8	-
1	DIL	l	4	1	-	0/7/8/10	-
1	DIL	B	4	1	-	0/7/8/10	-
1	DTR	7	6	1	-	0/4/6/8	0/2/2/2
1	DIL	j	7	1	-	2/10/10/10	-
1	DIL	V	4	1	-	0/7/8/10	-
1	DVA	b	5	1	-	0/5/6/8	-
1	DTR	g	6	1	-	1/4/6/8	0/2/2/2
1	DVA	g	5	1	-	0/5/6/8	-
1	DTR	P	6	1	-	1/4/6/8	0/2/2/2
1	DVA	m	5	1	-	0/5/6/8	-
1	DVA	h	5	1	-	0/5/6/8	-
1	DTH	k	1	1	-	0/5/6/8	-
1	DIL	k	4	1	-	0/7/8/10	-
1	DLY	T	3	1	-	0/6/7/9	-
1	DLY	h	3	1	-	2/6/7/9	-
1	DIL	9	4	1	-	0/7/8/10	-
1	DLY	L	3	1	-	0/6/7/9	-
1	DTR	1	6	1	-	0/4/6/8	0/2/2/2
1	DIL	M	7	1	-	2/10/10/10	-
1	DTH	8	1	1	-	0/5/6/8	-
1	DTH	U	1	1	-	0/5/6/8	-
1	DTR	D	6	1	-	1/4/6/8	0/2/2/2
1	DIL	b	4	1	-	0/7/8/10	-
1	DIL	j	4	1	-	1/7/8/10	-
1	DLY	o	3	1	-	1/6/7/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	DLY	Q	3	1	-	0/6/7/9	-
1	DLY	5	3	1	-	0/6/7/9	-
1	DIL	n	4	1	-	0/7/8/10	-
1	DIL	6	7	1	-	2/10/10/10	-
1	DTR	d	6	1	-	1/4/6/8	0/2/2/2
1	DLE	O	2	1	-	0/5/6/8	-
1	DLE	c	2	1	-	0/5/6/8	-
1	DIL	g	4	1	-	0/7/8/10	-
1	DVA	P	5	1	-	0/5/6/8	-
1	DLE	o	2	1	-	1/5/6/8	-
1	DIL	Z	4	1	-	1/7/8/10	-
1	DTH	S	1	1	-	0/5/6/8	-
1	DTH	V	1	1	-	0/5/6/8	-
1	DIL	r	4	1	-	1/7/8/10	-
1	DIL	O	7	1	-	1/10/10/10	-
1	DLY	t	3	1	-	0/6/7/9	-
1	DIL	5	4	1	-	0/7/8/10	-
1	DTH	I	1	1	-	0/5/6/8	-
1	DLE	W	2	1	-	0/5/6/8	-
1	DTH	f	1	1	-	0/5/6/8	-
1	DVA	r	5	1	-	0/5/6/8	-
1	DTR	v	6	1	-	0/4/6/8	0/2/2/2
1	DVA	5	5	1	-	0/5/6/8	-
1	DLY	3	3	1	-	0/6/7/9	-
1	DLE	Z	2	1	-	0/5/6/8	-
1	DLY	F	3	1	-	0/6/7/9	-
1	DIL	P	4	1	-	0/7/8/10	-
1	DTH	T	1	1	-	0/5/6/8	-
1	DIL	T	4	1	-	0/7/8/10	-
1	DIL	h	4	1	-	0/7/8/10	-
1	DTR	K	6	1	-	0/4/6/8	0/2/2/2
1	DLY	l	3	1	-	0/6/7/9	-
1	DVA	K	5	1	-	0/5/6/8	-
1	DTR	f	6	1	-	2/4/6/8	0/2/2/2
1	DIL	l	7	1	-	0/10/10/10	-
1	DIL	X	7	1	-	1/10/10/10	-
1	DTH	m	1	1	-	0/5/6/8	-
1	DVA	w	5	1	-	0/5/6/8	-
1	DTR	q	6	1	-	0/4/6/8	0/2/2/2
1	DTH	o	1	1	-	0/5/6/8	-
1	DVA	9	5	1	-	0/5/6/8	-
1	DIL	s	4	1	-	0/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	DVA	q	5	1	-	1/5/6/8	-
1	DTH	C	1	1	-	1/5/6/8	-
1	DLE	w	2	1	-	0/5/6/8	-
1	DLY	X	3	1	-	2/6/7/9	-
1	DIL	E	7	1	-	2/10/10/10	-
1	DLY	e	3	1	-	2/6/7/9	-
1	DIL	T	7	1	-	1/10/10/10	-
1	DLY	j	3	1	-	0/6/7/9	-
1	DTH	W	1	1	-	1/5/6/8	-
1	DIL	C	7	1	-	1/10/10/10	-
1	DVA	l	5	1	-	0/5/6/8	-
1	DIL	F	7	1	-	2/10/10/10	-
1	DIL	R	4	1	-	0/7/8/10	-
1	DTR	H	6	1	-	0/4/6/8	0/2/2/2
1	DTH	J	1	1	-	0/5/6/8	-
1	DIL	e	4	1	-	0/7/8/10	-
1	DTH	u	1	1	-	0/5/6/8	-
1	DLE	9	2	1	-	0/5/6/8	-
1	DLY	r	3	1	-	0/6/7/9	-
1	DVA	e	5	1	-	0/5/6/8	-
1	DLY	N	3	1	-	0/6/7/9	-
1	DIL	r	7	1	-	1/10/10/10	-
1	DIL	Y	7	1	-	2/10/10/10	-
1	DTR	J	6	1	-	1/4/6/8	0/2/2/2
1	DLE	3	2	1	-	1/5/6/8	-
1	DLY	W	3	1	-	0/6/7/9	-
1	DTR	u	6	1	-	0/4/6/8	0/2/2/2
1	DIL	b	7	1	-	1/10/10/10	-
1	DIL	t	4	1	-	0/7/8/10	-
1	DLY	0	3	1	-	0/6/7/9	-
1	DTH	O	1	1	-	0/5/6/8	-
1	DIL	D	4	1	-	0/7/8/10	-
1	DIL	0	7	1	-	3/10/10/10	-
1	DTR	V	6	1	-	2/4/6/8	0/2/2/2
1	DLY	c	3	1	-	0/6/7/9	-
1	DTH	t	1	1	-	0/5/6/8	-
1	DVA	V	5	1	-	0/5/6/8	-
1	DIL	2	4	1	-	0/7/8/10	-
1	DIL	c	7	1	-	1/10/10/10	-
1	DVA	N	5	1	-	0/5/6/8	-
1	DLE	Y	2	1	-	0/5/6/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	DLE	P	2	1	-	0/5/6/8	-
1	DTR	Y	6	1	-	0/4/6/8	0/2/2/2
1	DLY	M	3	1	-	0/6/7/9	-
1	DIL	0	4	1	-	0/7/8/10	-
1	DIL	W	7	1	-	1/10/10/10	-
1	DLE	T	2	1	-	0/5/6/8	-
1	DLE	h	2	1	-	0/5/6/8	-
1	DTH	Q	1	1	-	0/5/6/8	-
1	DTH	v	1	1	-	0/5/6/8	-
1	DLE	q	2	1	-	0/5/6/8	-
1	DTR	b	6	1	-	0/4/6/8	0/2/2/2
1	DLE	L	2	1	-	0/5/6/8	-
1	DTH	6	1	1	-	0/5/6/8	-
1	DVA	k	5	1	-	0/5/6/8	-
1	DLY	R	3	1	-	0/6/7/9	-
1	DTR	i	6	1	-	0/4/6/8	0/2/2/2
1	DLE	5	2	1	-	0/5/6/8	-
1	DIL	M	4	1	-	3/7/8/10	-
1	DLE	G	2	1	-	0/5/6/8	-
1	DLE	x	2	1	-	0/5/6/8	-
1	DIL	B	7	1	-	2/10/10/10	-
1	DLE	Q	2	1	-	0/5/6/8	-
1	DTR	m	6	1	-	0/4/6/8	0/2/2/2
1	DIL	A	7	1	-	2/10/10/10	-
1	DTH	j	1	1	-	0/5/6/8	-
1	DTR	Q	6	1	-	0/4/6/8	0/2/2/2
1	DTR	S	6	1	-	2/4/6/8	0/2/2/2
1	DVA	S	5	1	-	0/5/6/8	-
1	DLE	n	2	1	-	1/5/6/8	-
1	DIL	q	7	1	-	2/10/10/10	-
1	DTR	s	6	1	-	0/4/6/8	0/2/2/2
1	DIL	F	4	1	-	1/7/8/10	-
1	DTH	X	1	1	-	1/5/6/8	-
1	DVA	a	5	1	-	0/5/6/8	-
1	DTR	p	6	1	-	0/4/6/8	0/2/2/2
1	DTH	M	1	1	-	0/5/6/8	-
1	DTH	B	1	1	-	0/5/6/8	-
1	DIL	R	7	1	-	1/10/10/10	-
1	DLE	s	2	1	-	0/5/6/8	-
1	DTH	r	1	1	-	1/5/6/8	-
1	DLY	G	3	1	-	0/6/7/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	DIL	Y	4	1	-	0/7/8/10	-
1	DLE	1	2	1	-	2/5/6/8	-
1	DIL	h	7	1	-	1/10/10/10	-
1	DLY	I	3	1	-	0/6/7/9	-
1	DTR	4	6	1	-	0/4/6/8	0/2/2/2
1	DVA	L	5	1	-	0/5/6/8	-
1	DVA	7	5	1	-	0/5/6/8	-
1	DTR	o	6	1	-	0/4/6/8	0/2/2/2
1	DIL	7	7	1	-	1/10/10/10	-
1	DLE	K	2	1	-	1/5/6/8	-
1	DIL	1	7	1	-	0/10/10/10	-
1	DIL	v	7	1	-	1/10/10/10	-
1	DTR	l	6	1	-	0/4/6/8	0/2/2/2
1	DIL	G	7	1	-	3/10/10/10	-
1	DLY	C	3	1	-	0/6/7/9	-
1	DVA	d	5	1	-	1/5/6/8	-
1	DTH	c	1	1	-	0/5/6/8	-
1	DVA	6	5	1	-	1/5/6/8	-
1	DIL	o	4	1	-	0/7/8/10	-
1	DIL	p	7	1	-	1/10/10/10	-
1	DIL	e	7	1	-	2/10/10/10	-
1	DIL	D	7	1	-	1/10/10/10	-
1	DIL	N	4	1	-	1/7/8/10	-
1	DIL	c	4	1	-	0/7/8/10	-
1	DVA	s	5	1	-	0/5/6/8	-
1	DTH	2	1	1	-	0/5/6/8	-
1	DVA	p	5	1	-	0/5/6/8	-
1	DTR	3	6	1	-	1/4/6/8	0/2/2/2
1	DLY	8	3	1	-	0/6/7/9	-
1	DIL	U	7	1	-	2/10/10/10	-
1	DIL	W	4	1	-	0/7/8/10	-
1	DVA	F	5	1	-	0/5/6/8	-
1	DLY	7	3	1	-	0/6/7/9	-
1	DIL	H	7	1	-	0/10/10/10	-
1	DLY	B	3	1	-	0/6/7/9	-
1	DIL	V	7	1	-	2/10/10/10	-
1	DVA	Y	5	1	-	0/5/6/8	-
1	DIL	a	7	1	-	2/10/10/10	-
1	DTR	X	6	1	-	1/4/6/8	0/2/2/2
1	DTH	w	1	1	-	0/5/6/8	-
1	DVA	X	5	1	-	0/5/6/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	DIL	3	4	1	-	0/7/8/10	-
1	DIL	N	7	1	-	1/10/10/10	-
1	DLE	e	2	1	-	0/5/6/8	-
1	DTR	r	6	1	-	0/4/6/8	0/2/2/2
1	DIL	5	7	1	-	1/10/10/10	-
1	DLE	j	2	1	-	0/5/6/8	-
1	DLY	1	3	1	-	0/6/7/9	-
1	DTH	H	1	1	-	0/5/6/8	-
1	DIL	7	4	1	-	1/7/8/10	-
1	DIL	K	7	1	-	1/10/10/10	-
1	DVA	8	5	1	-	0/5/6/8	-
1	DIL	A	4	1	-	0/7/8/10	-
1	DIL	8	7	1	-	1/10/10/10	-
1	DTR	w	6	1	-	2/4/6/8	0/2/2/2
1	DTR	A	6	1	-	1/4/6/8	0/2/2/2
1	DIL	k	7	1	-	4/10/10/10	-
1	DVA	Z	5	1	-	0/5/6/8	-
1	DIL	1	4	1	-	0/7/8/10	-
1	DTH	s	1	1	-	0/5/6/8	-
1	DIL	S	7	1	-	1/10/10/10	-
1	DIL	i	7	1	-	2/10/10/10	-
1	DVA	f	5	1	-	0/5/6/8	-
1	DLY	H	3	1	-	0/6/7/9	-
1	DTR	9	6	1	-	1/4/6/8	0/2/2/2
1	DLE	0	2	1	-	0/5/6/8	-
1	DLE	U	2	1	-	0/5/6/8	-
1	DIL	v	4	1	-	0/7/8/10	-
1	DTR	n	6	1	-	1/4/6/8	0/2/2/2
1	DTR	U	6	1	-	1/4/6/8	0/2/2/2
1	DVA	n	5	1	-	0/5/6/8	-
1	DLE	A	2	1	-	0/5/6/8	-
1	DVA	U	5	1	-	0/5/6/8	-
1	DLY	f	3	1	-	0/6/7/9	-
1	DLE	4	2	1	-	1/5/6/8	-
1	DLY	Y	3	1	-	1/6/7/9	-
1	DLY	E	3	1	-	1/6/7/9	-
1	DIL	9	7	1	-	1/10/10/10	-
1	DLE	N	2	1	-	0/5/6/8	-
1	DVA	u	5	1	-	0/5/6/8	-
1	DIL	o	7	1	-	1/10/10/10	-
1	DLY	u	3	1	-	0/6/7/9	-
1	DIL	d	4	1	-	0/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	DLE	S	2	1	-	0/5/6/8	-
1	DLE	6	2	1	-	0/5/6/8	-
1	DTH	4	1	1	-	0/5/6/8	-
1	DIL	q	4	1	-	3/7/8/10	-
1	DLY	g	3	1	-	0/6/7/9	-
1	DLE	R	2	1	-	0/5/6/8	-
1	DIL	J	4	1	-	0/7/8/10	-
1	DIL	n	7	1	-	1/10/10/10	-
1	DLE	p	2	1	-	0/5/6/8	-
1	DVA	J	5	1	-	0/5/6/8	-
1	DTR	T	6	1	-	1/4/6/8	0/2/2/2
1	DTR	h	6	1	-	1/4/6/8	0/2/2/2
1	DIL	s	7	1	-	1/10/10/10	-
1	DLE	b	2	1	-	0/5/6/8	-
1	DTH	e	1	1	-	0/5/6/8	-
1	DTH	G	1	1	-	0/5/6/8	-
1	DIL	G	4	1	-	0/7/8/10	-
1	DIL	K	4	1	-	0/7/8/10	-
1	DTH	D	1	1	-	1/5/6/8	-
1	DTR	L	6	1	-	0/4/6/8	0/2/2/2
1	DIL	i	4	1	-	0/7/8/10	-
1	DTR	a	6	1	-	0/4/6/8	0/2/2/2
1	DIL	x	4	1	-	0/7/8/10	-
1	DIL	Q	4	1	-	0/7/8/10	-
1	DIL	8	4	1	-	0/7/8/10	-
1	DTR	5	6	1	-	0/4/6/8	0/2/2/2
1	DLE	l	2	1	-	2/5/6/8	-
1	DVA	i	5	1	-	0/5/6/8	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	7	DIL	OXT-C	-2.28	1.23	1.30
1	D	7	DIL	OXT-C	-2.28	1.23	1.30
1	h	7	DIL	OXT-C	-2.28	1.23	1.30
1	q	7	DIL	OXT-C	-2.27	1.23	1.30
1	j	7	DIL	OXT-C	-2.27	1.23	1.30

The worst 5 of 91 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	7	DIL	OXT-C-O	-2.92	117.45	124.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	7	DIL	OXT-C-O	-2.90	117.49	124.08
1	k	7	DIL	OXT-C-O	-2.88	117.55	124.08
1	6	7	DIL	OXT-C-O	-2.87	117.57	124.08
1	q	7	DIL	OXT-C-O	-2.87	117.57	124.08

There are no chirality outliers.

5 of 181 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	E	1	DTH	O-C-CA-CB
1	N	1	DTH	O-C-CA-CB
1	Y	1	DTH	O-C-CA-CB
1	7	1	DTH	O-C-CA-CB
1	i	1	DTH	O-C-CA-CB

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](#)

There are no ligands in this entry.

## 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.

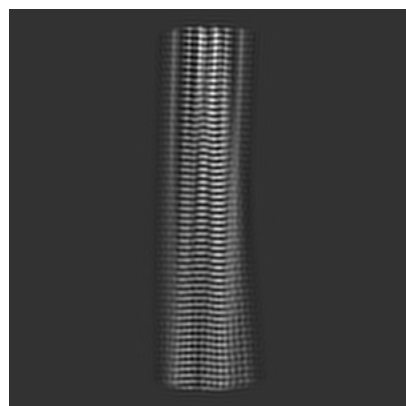
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44181. These allow visual inspection of the internal detail of the map and identification of artifacts.

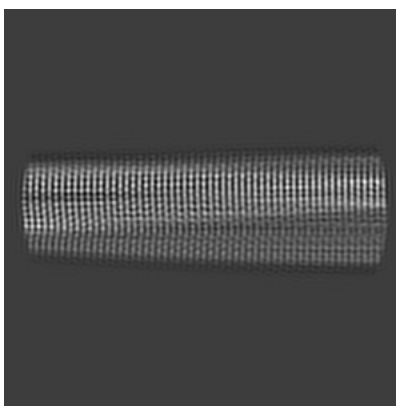
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

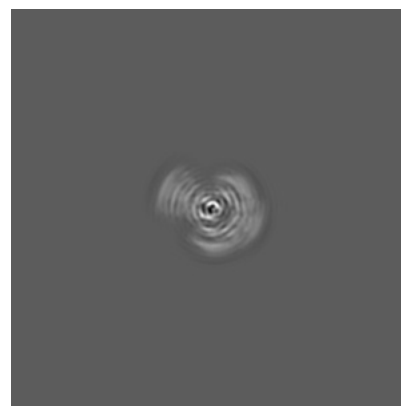
#### 6.1.1 Primary map



X

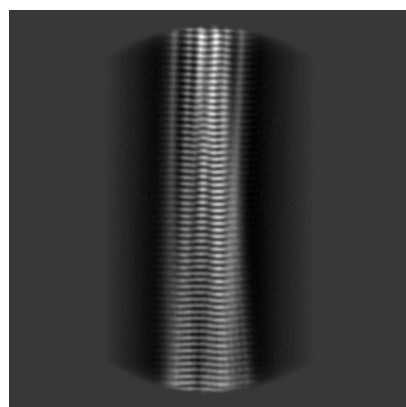


Y

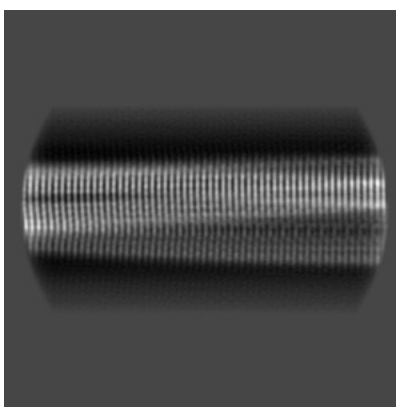


Z

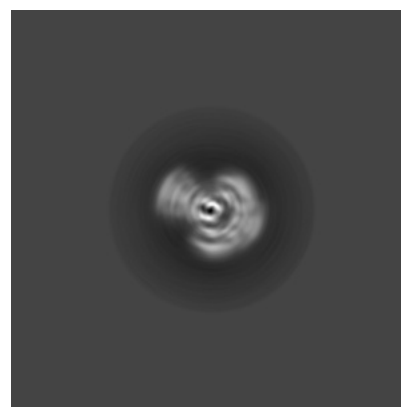
#### 6.1.2 Raw map



X



Y

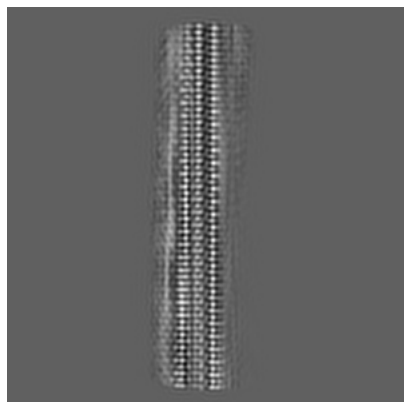


Z

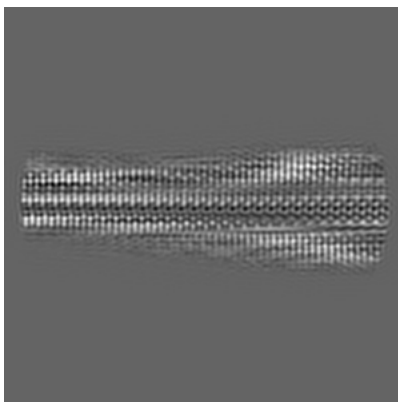
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

### 6.2.1 Primary map



X Index: 160

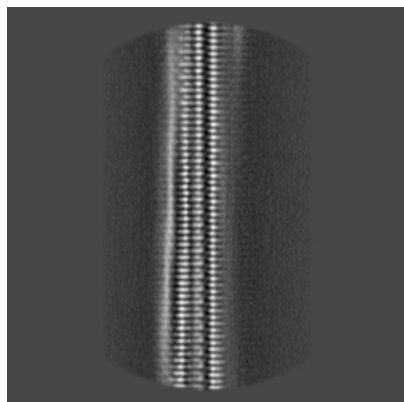


Y Index: 160

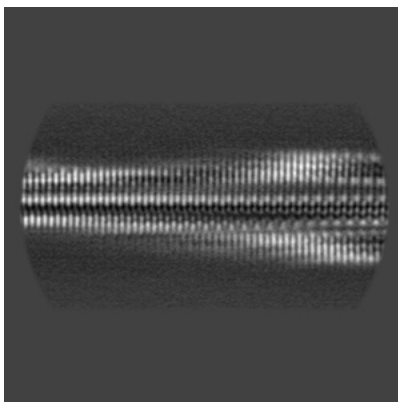


Z Index: 160

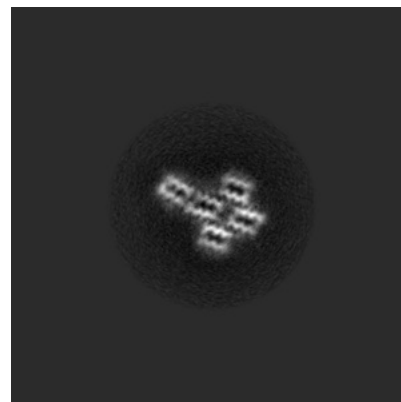
### 6.2.2 Raw map



X Index: 160



Y Index: 160

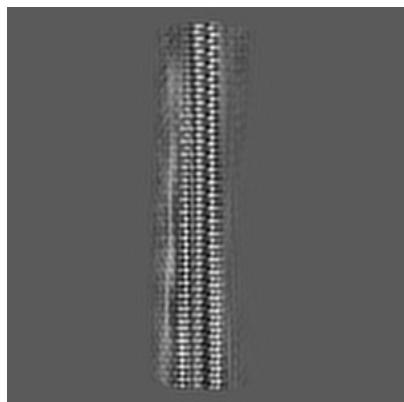


Z Index: 160

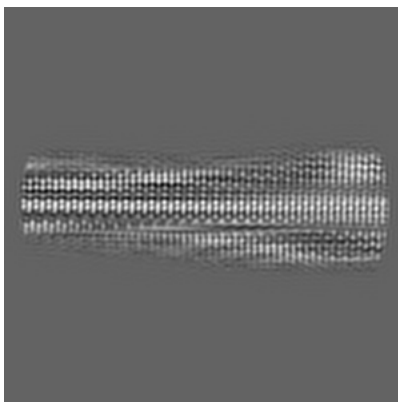
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

### 6.3.1 Primary map



X Index: 158

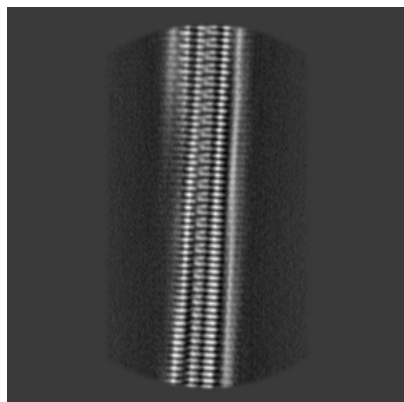


Y Index: 164

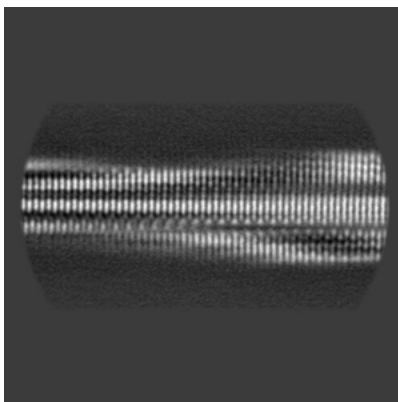


Z Index: 26

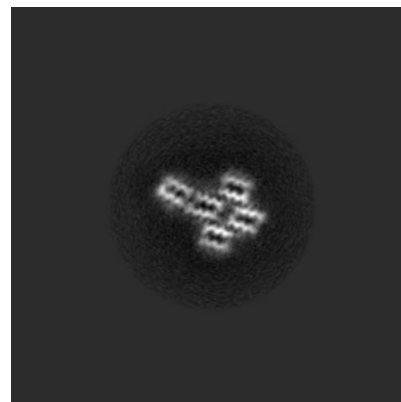
### 6.3.2 Raw map



X Index: 180



Y Index: 164

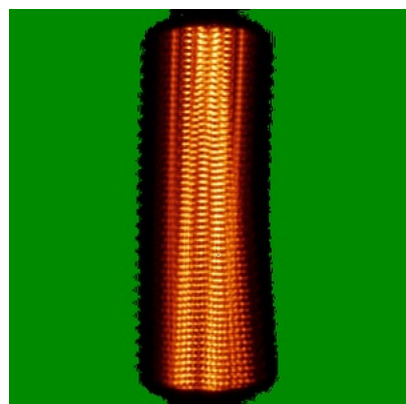


Z Index: 170

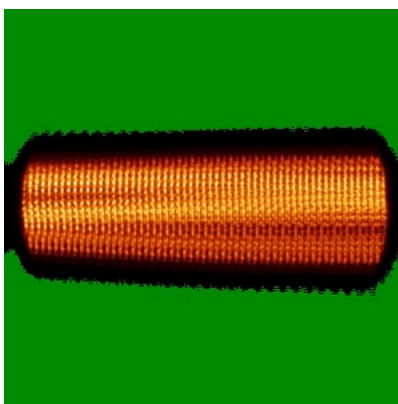
The images above show the largest variance slices of the map in three orthogonal directions.

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

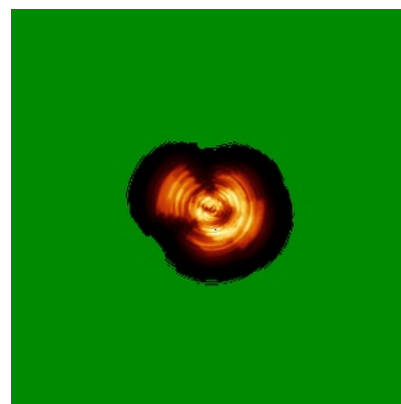
### 6.4.1 Primary map



X

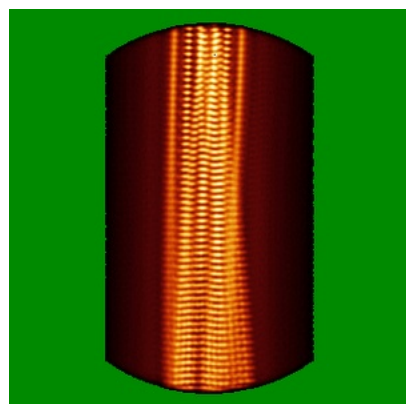


Y

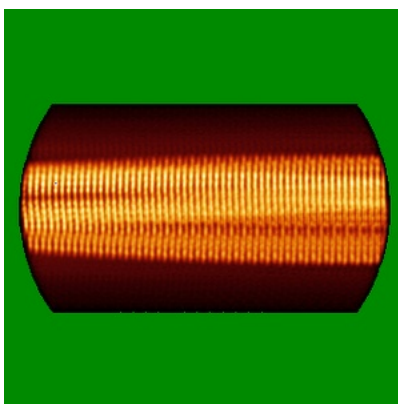


Z

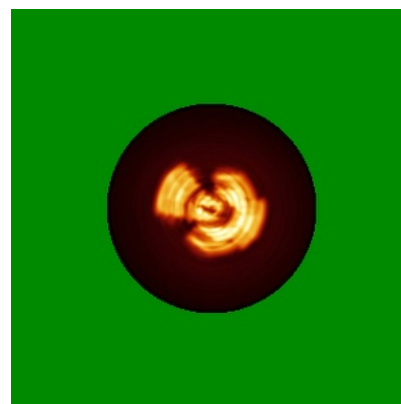
### 6.4.2 Raw map



X



Y

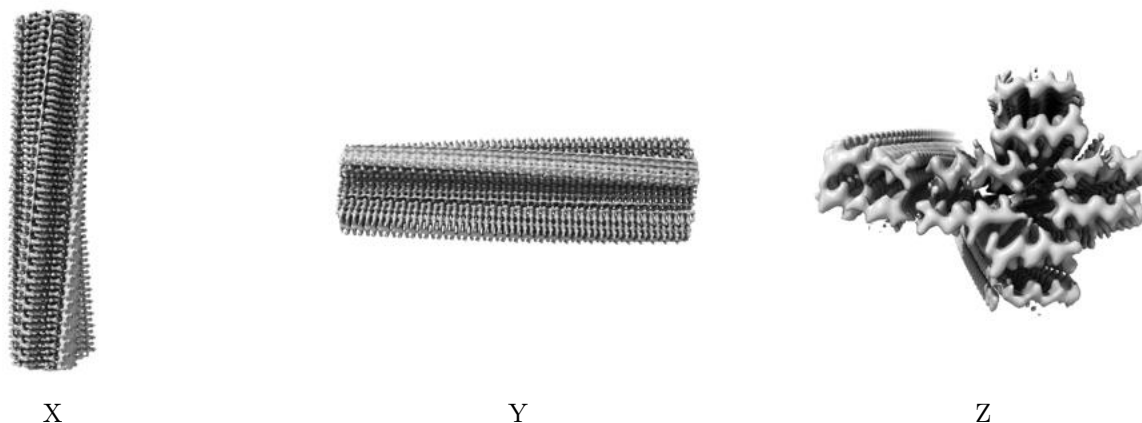


Z

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

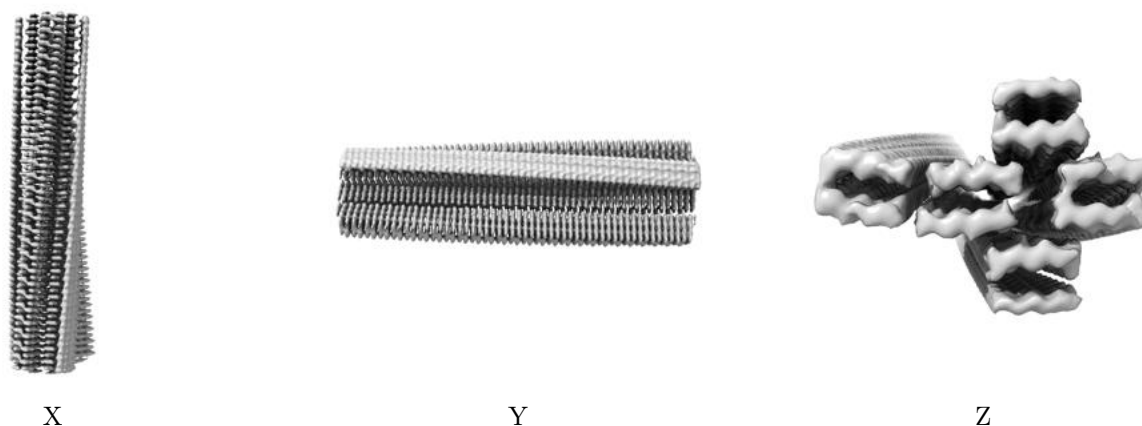
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 5.21. 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.

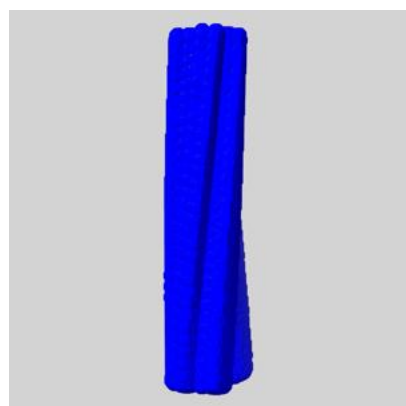
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

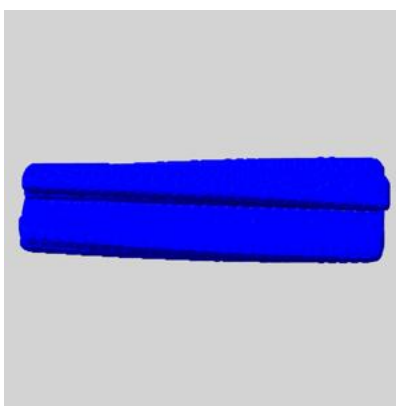
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

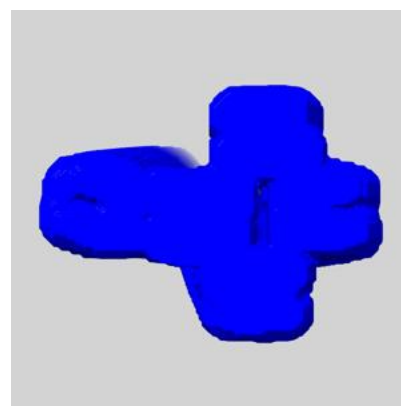
### 6.6.1 emd\_44181\_msk\_1.map [i](#)



X



Y

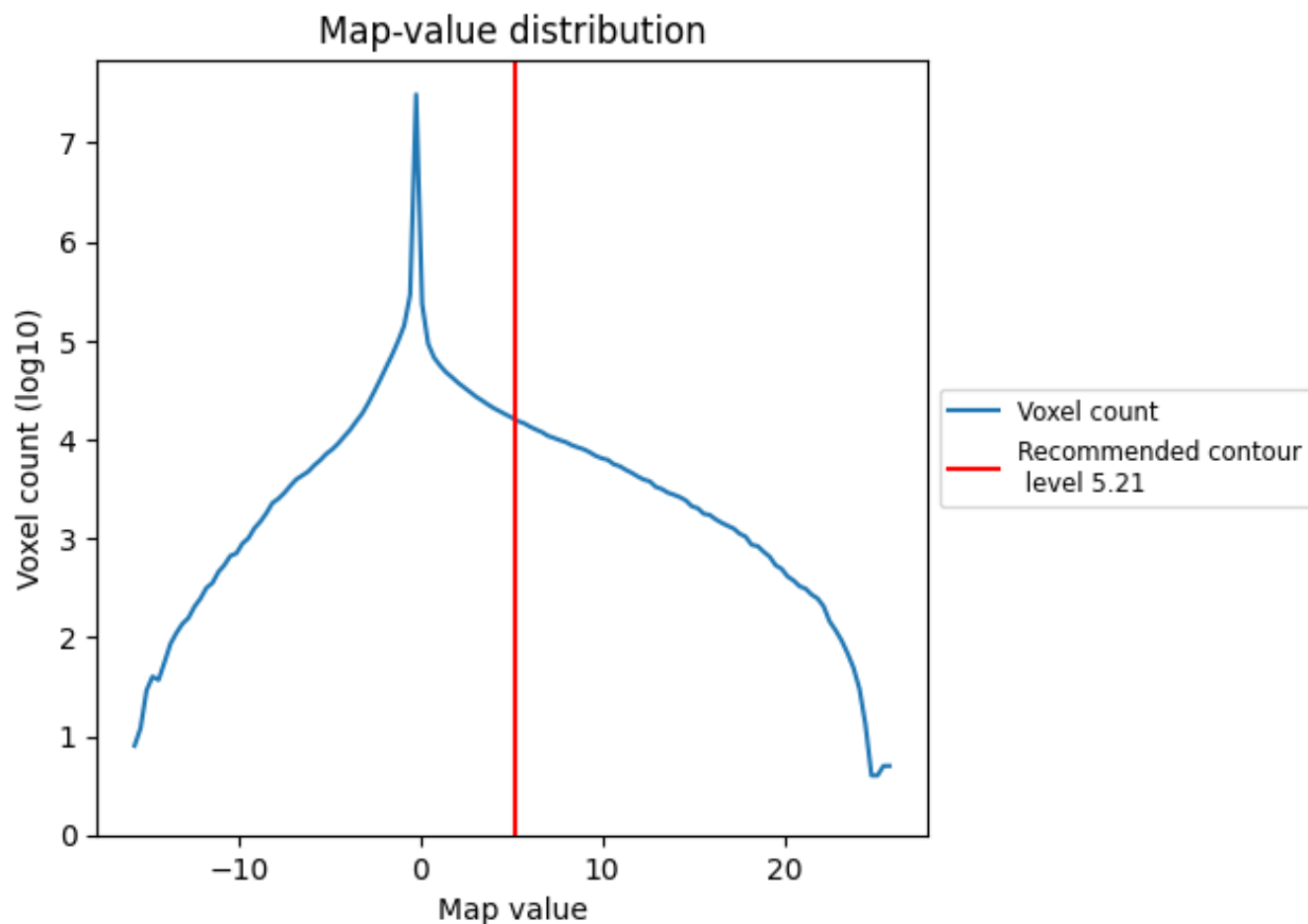


Z

## 7 Map analysis [i](#)

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

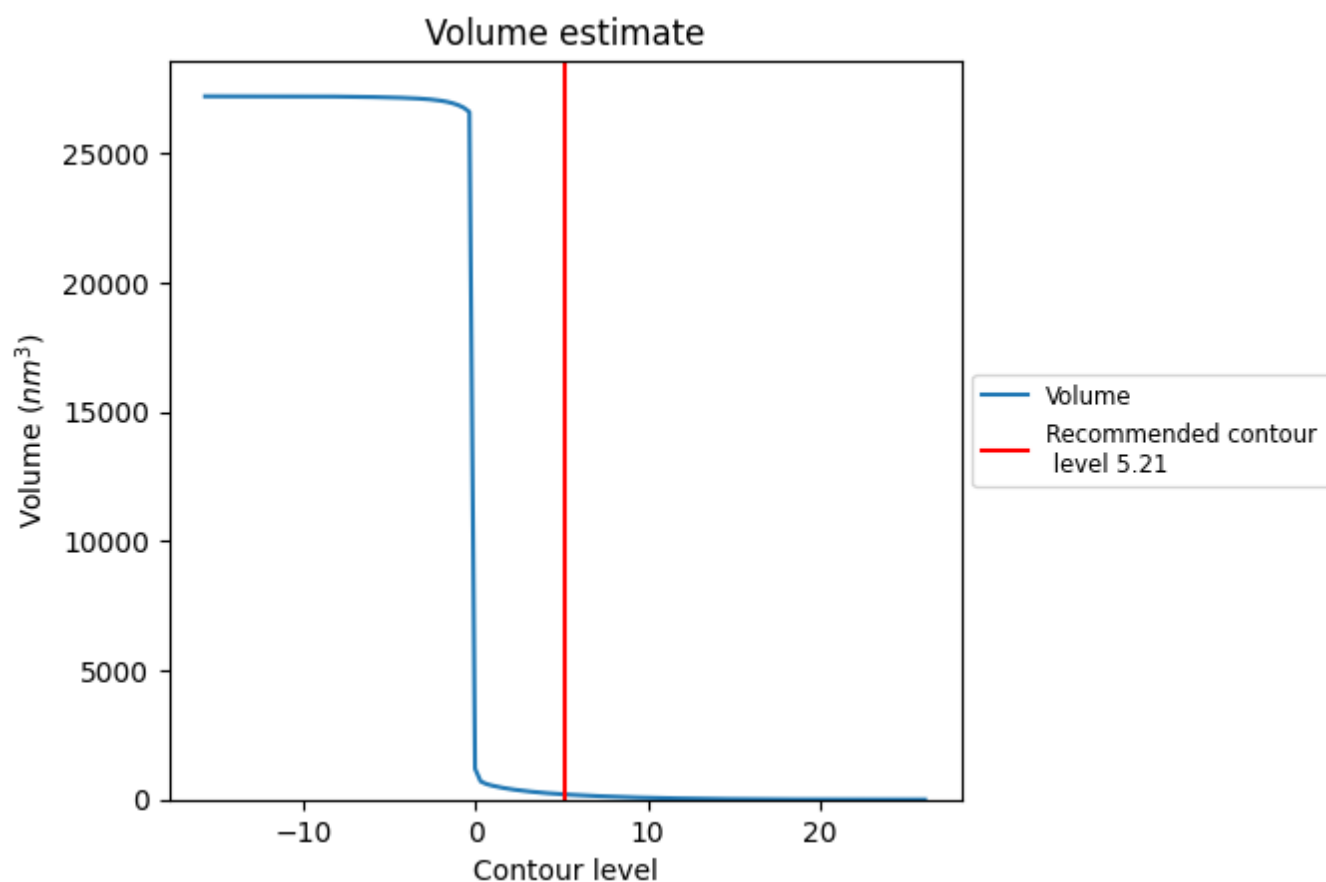
### 7.1 Map-value distribution [i](#)



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.



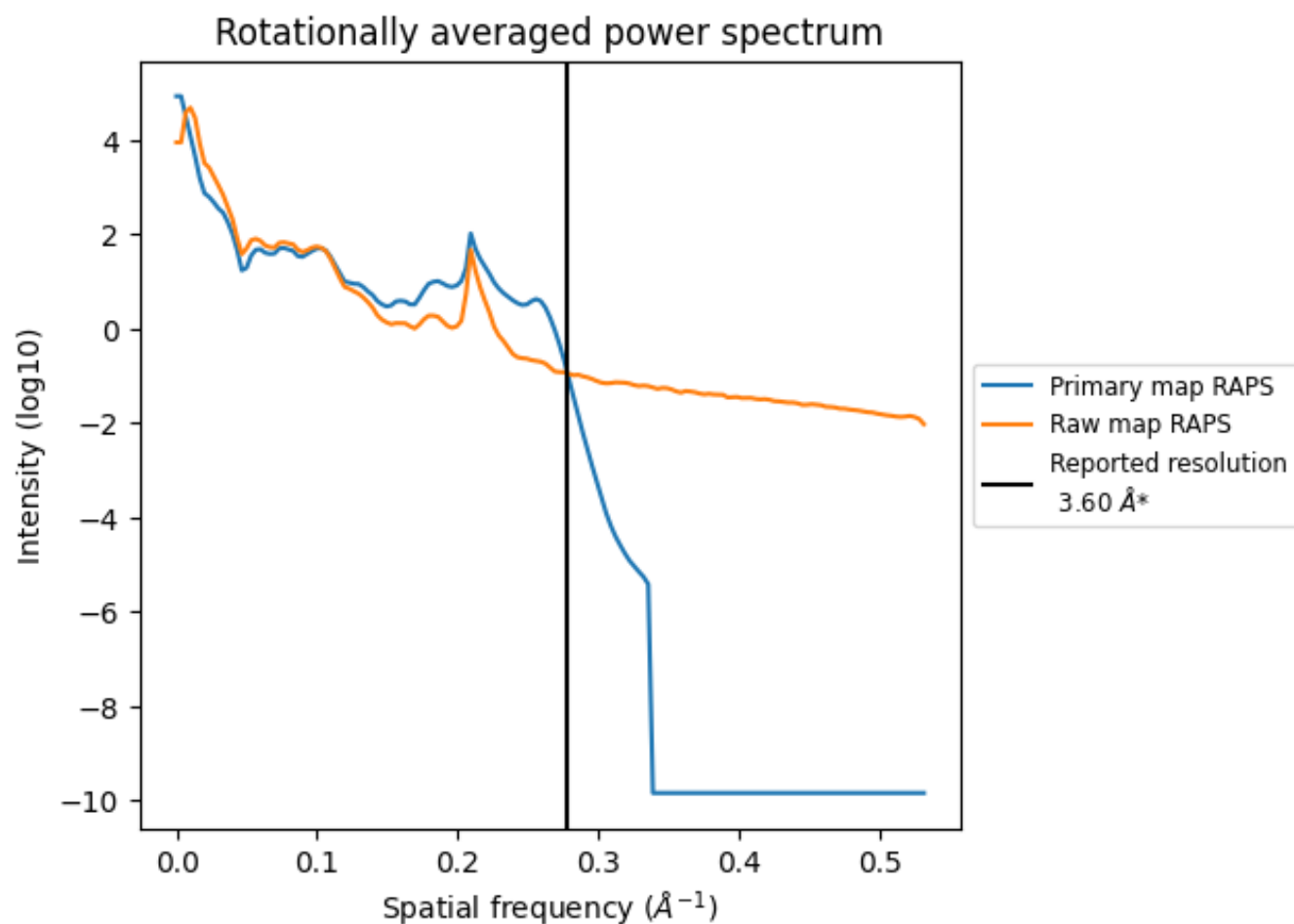
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 199  $\text{nm}^3$ ; this corresponds to an approximate mass of 180 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

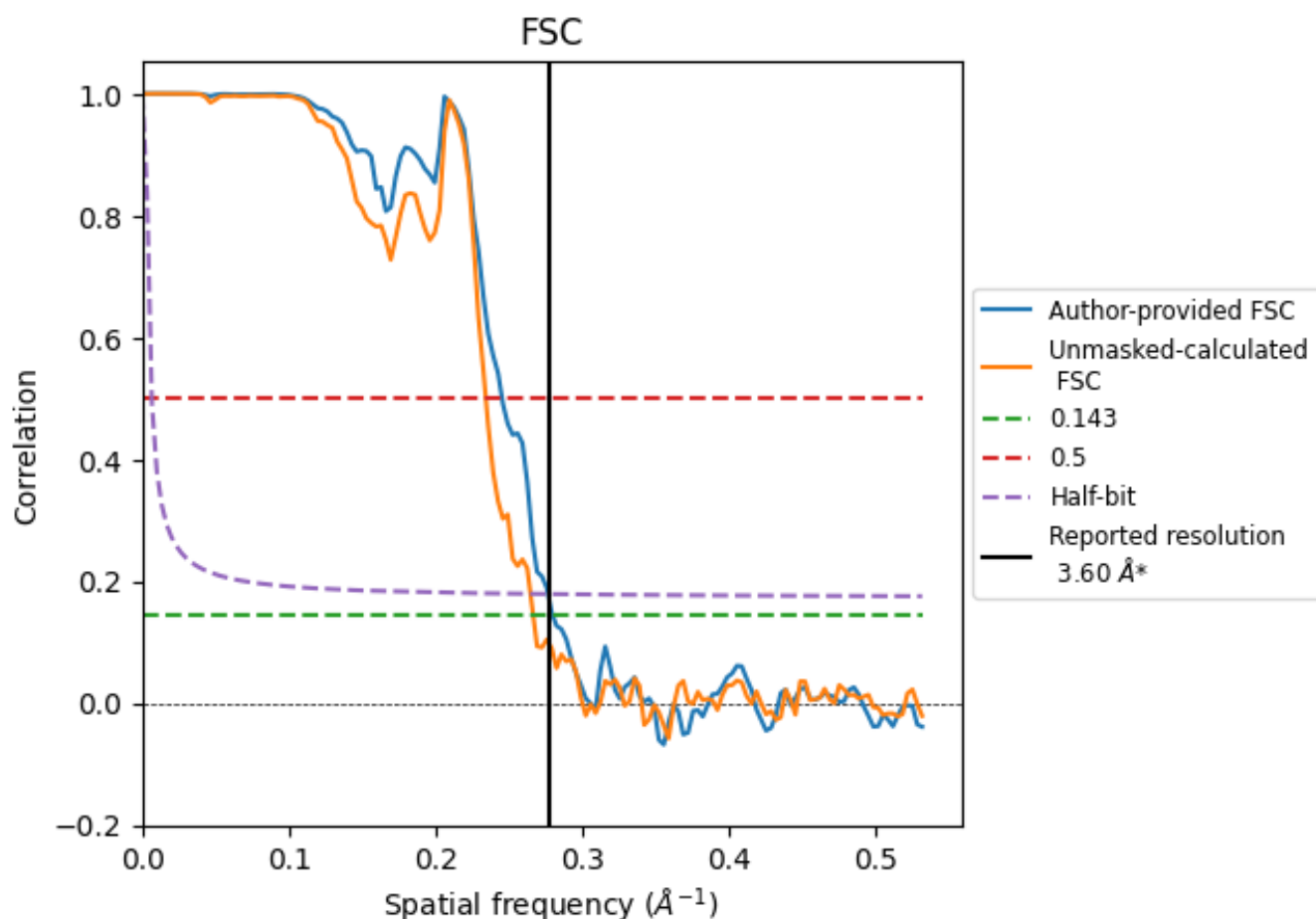


\*Reported resolution corresponds to spatial frequency of 0.278 Å<sup>-1</sup>

## 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  $0.278 \text{ \AA}^{-1}$

## 8.2 Resolution estimates

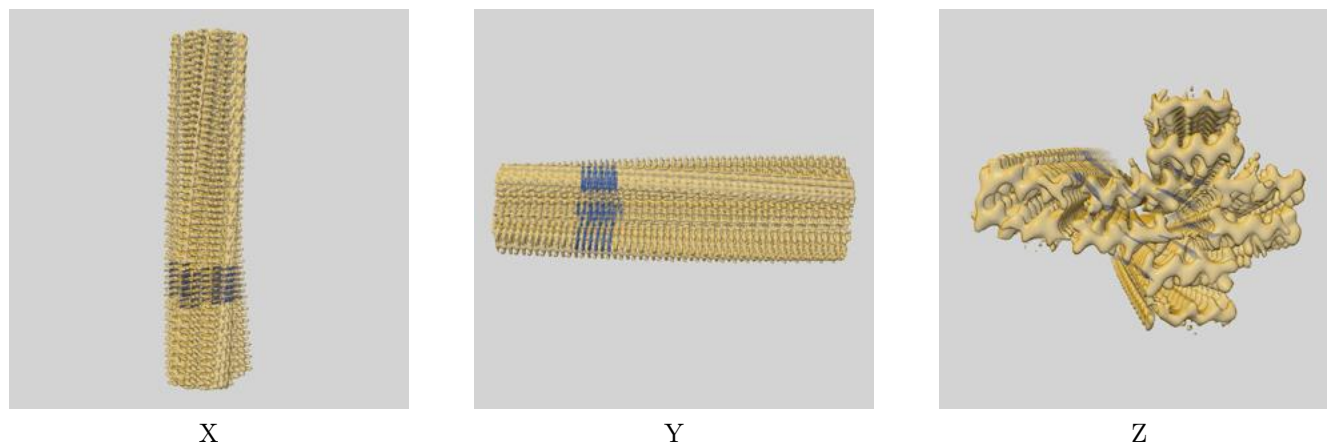
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.57	4.07	3.61
Unmasked-calculated*	3.75	4.27	3.78

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

## 9 Map-model fit [i](#)

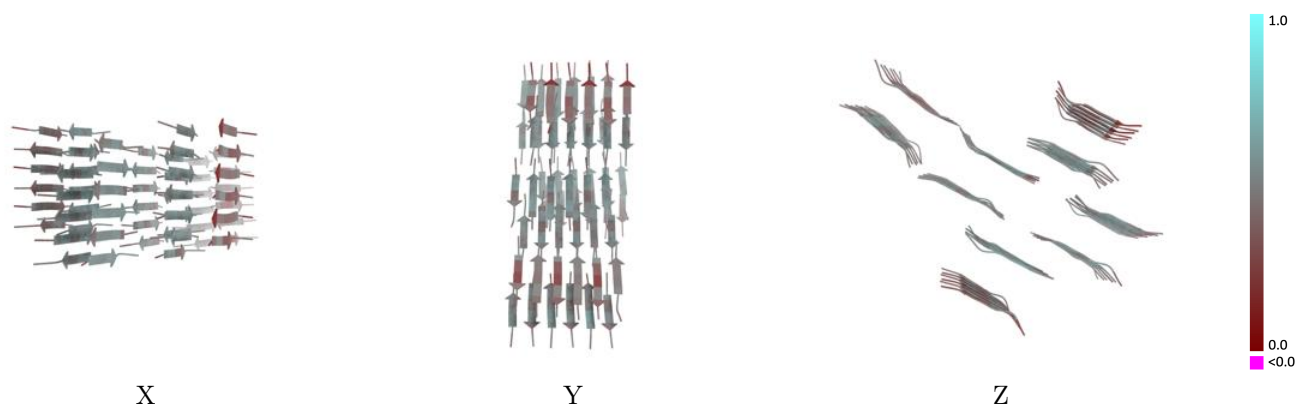
This section contains information regarding the fit between EMDB map EMD-44181 and PDB model 9B4I. Per-residue inclusion information can be found in section [3](#) on page [9](#).

### 9.1 Map-model overlay [i](#)



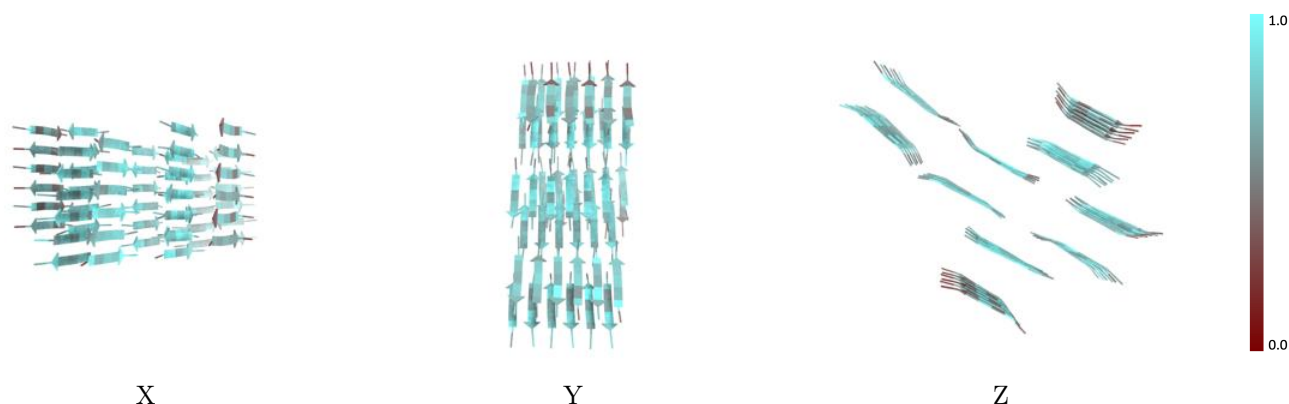
The images above show the 3D surface view of the map at the recommended contour level 5.21 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



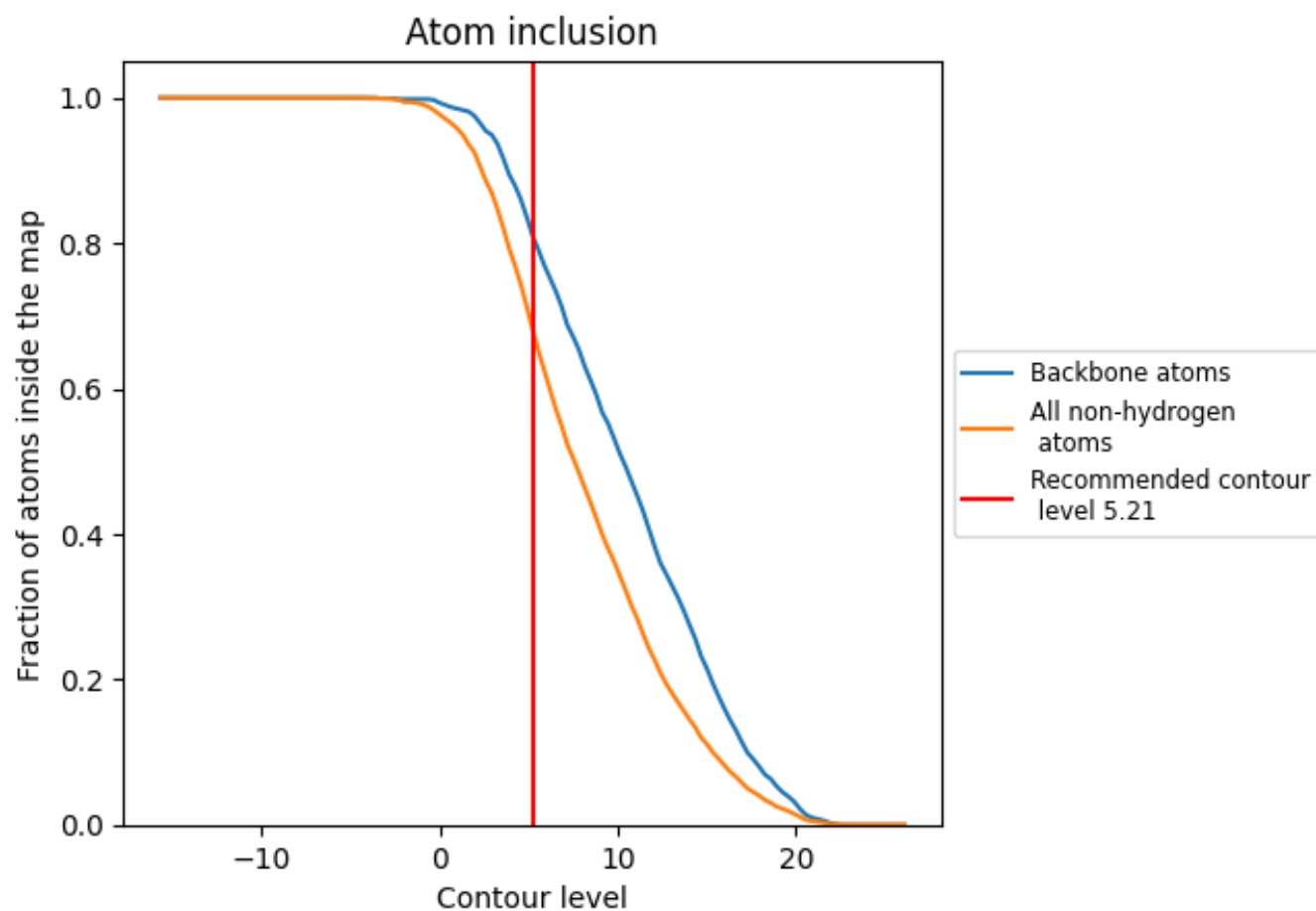
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (5.21).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 68% 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 (5.21) and Q-score for the entire model and for each chain.





















































Chain	Atom inclusion	Q-score
All	 0.6810	 0.4610
0	 0.6720	 0.4630
1	 0.7050	 0.4640
2	 0.7380	 0.5170
3	 0.6720	 0.4700
4	 0.7050	 0.4910
5	 0.7050	 0.4910
6	 0.5080	 0.3940
7	 0.4920	 0.3000
8	 0.7540	 0.4710
9	 0.7540	 0.5170
A	 0.7380	 0.4980
B	 0.7540	 0.5070
C	 0.7540	 0.4870
D	 0.7210	 0.4770
E	 0.6890	 0.3970
F	 0.6390	 0.4520
G	 0.7050	 0.4710
H	 0.7050	 0.4660
I	 0.7700	 0.5270
J	 0.6390	 0.4730
K	 0.7380	 0.4970
L	 0.6890	 0.4960
M	 0.5250	 0.3920
N	 0.5080	 0.3110
O	 0.7540	 0.4750
P	 0.8200	 0.5190
Q	 0.7540	 0.5170
R	 0.7540	 0.5200
S	 0.5410	 0.4070
T	 0.5080	 0.3800
U	 0.7210	 0.4680
V	 0.7380	 0.5080
W	 0.7210	 0.4800
X	 0.7050	 0.4790



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Chain	Atom inclusion	Q-score
Y	 0.6890	 0.3950
Z	 0.6070	 0.4400
a	 0.7870	 0.5070
b	 0.7540	 0.5200
c	 0.5410	 0.3970
d	 0.5410	 0.3720
e	 0.7540	 0.4740
f	 0.7050	 0.5050
g	 0.7540	 0.4920
h	 0.7210	 0.4810
i	 0.7050	 0.4030
j	 0.6720	 0.4480
k	 0.7050	 0.4760
l	 0.7050	 0.4630
m	 0.7700	 0.5220
n	 0.6390	 0.4630
o	 0.7210	 0.5040
p	 0.6720	 0.4840
q	 0.5410	 0.3880
r	 0.5250	 0.3250
s	 0.7380	 0.4770
t	 0.7700	 0.4980
u	 0.7540	 0.5190
v	 0.7380	 0.5140
w	 0.5410	 0.4130
x	 0.5080	 0.3790