



Full wwPDB EM Validation Report ⓘ

Nov 5, 2023 – 12:01 AM EDT

PDB ID : 7LQE
EMDB ID : EMD-23483
Title : Cryo-EM of 1-protofilament of the KFE8 thinner nanotube
Authors : Wang, F.; Gnewou, O.M.; Egelman, E.H.; Conticello, V.P.
Deposited on : 2021-02-13
Resolution : 3.40 Å (reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

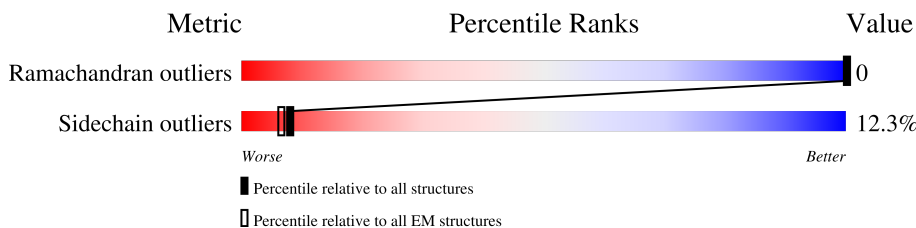
EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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 3.40 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)
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 $\leq 5\%$. 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	8	50% 75% 25%
1	1	8	50% 75% 25%
1	2	8	50% 62% 38%
1	3	8	50% 75% 25%
1	4	8	50% 75% 25%
1	5	8	50% 62% 38%
1	6	8	50% 75% 25%
1	7	8	38% 75% 25%
1	8	8	50% 62% 38%

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Mol	Chain	Length	Quality of chain
1	9	8	50%
1	A	8	25% 88% 12%
1	AA	8	38% 75% 25%
1	B	8	25% 75% 25%
1	BA	8	50% 62% 38%
1	C	8	25% 75% 25%
1	CA	8	50% 75% 25%
1	D	8	25% 75% 25%
1	DA	8	38% 75% 25%
1	E	8	25% 88% 12%
1	EA	8	50% 62% 38%
1	F	8	25% 75% 25%
1	FA	8	50% 75% 25%
1	G	8	25% 88% 12%
1	GA	8	50% 75% 25%
1	H	8	25% 88% 12%
1	HA	8	50% 62% 38%
1	I	8	25% 75% 25%
1	IA	8	50% 75% 25%
1	J	8	25% 50% 50%
1	JA	8	62% 75% 25%
1	K	8	12% 75% 25%
1	L	8	25% 62% 38%
1	M	8	12% 50% 50%
1	N	8	12% 75% 25%



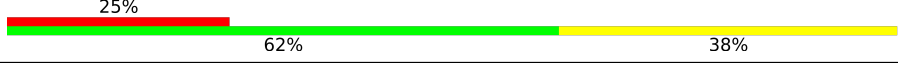
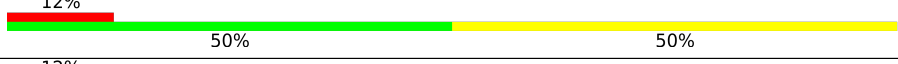

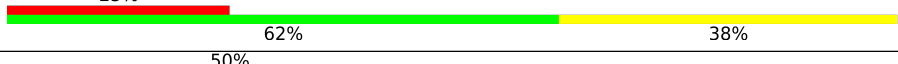
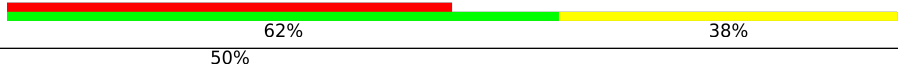


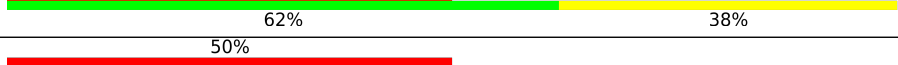



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Mol	Chain	Length	Quality of chain
1	O	8	
1	P	8	
1	Q	8	
1	R	8	
1	S	8	
1	T	8	
1	U	8	
1	V	8	
1	W	8	
1	X	8	
1	Y	8	
1	Z	8	
1	a	8	
1	b	8	
1	c	8	
1	d	8	
1	e	8	
1	f	8	
1	g	8	
1	h	8	
1	i	8	
1	j	8	
1	k	8	
1	l	8	
1	m	8	

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Mol	Chain	Length	Quality of chain
1	n	8	
1	o	8	
1	p	8	
1	q	8	
1	r	8	
1	s	8	
1	t	8	
1	u	8	
1	v	8	
1	w	8	
1	x	8	
1	y	8	
1	z	8	

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 6048 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 KFE8 peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	A	8	84	60	11	13	0	0
1	J	8	84	60	11	13	0	0
1	K	8	84	60	11	13	0	0
1	L	8	84	60	11	13	0	0
1	B	8	84	60	11	13	0	0
1	M	8	84	60	11	13	0	0
1	N	8	84	60	11	13	0	0
1	O	8	84	60	11	13	0	0
1	C	8	84	60	11	13	0	0
1	P	8	84	60	11	13	0	0
1	Q	8	84	60	11	13	0	0
1	R	8	84	60	11	13	0	0
1	D	8	84	60	11	13	0	0
1	S	8	84	60	11	13	0	0
1	T	8	84	60	11	13	0	0
1	U	8	84	60	11	13	0	0
1	E	8	84	60	11	13	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	V	8	84	60	11	13	0	0
1	W	8	84	60	11	13	0	0
1	X	8	84	60	11	13	0	0
1	F	8	84	60	11	13	0	0
1	Y	8	84	60	11	13	0	0
1	Z	8	84	60	11	13	0	0
1	j	8	84	60	11	13	0	0
1	G	8	84	60	11	13	0	0
1	k	8	84	60	11	13	0	0
1	l	8	84	60	11	13	0	0
1	m	8	84	60	11	13	0	0
1	H	8	84	60	11	13	0	0
1	n	8	84	60	11	13	0	0
1	o	8	84	60	11	13	0	0
1	p	8	84	60	11	13	0	0
1	I	8	84	60	11	13	0	0
1	q	8	84	60	11	13	0	0
1	r	8	84	60	11	13	0	0
1	s	8	84	60	11	13	0	0
1	a	8	84	60	11	13	0	0
1	t	8	84	60	11	13	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	u	8	Total 84	C 60	N 11	O 13	0	0
1	v	8	Total 84	C 60	N 11	O 13	0	0
1	b	8	Total 84	C 60	N 11	O 13	0	0
1	w	8	Total 84	C 60	N 11	O 13	0	0
1	x	8	Total 84	C 60	N 11	O 13	0	0
1	y	8	Total 84	C 60	N 11	O 13	0	0
1	c	8	Total 84	C 60	N 11	O 13	0	0
1	z	8	Total 84	C 60	N 11	O 13	0	0
1	0	8	Total 84	C 60	N 11	O 13	0	0
1	1	8	Total 84	C 60	N 11	O 13	0	0
1	d	8	Total 84	C 60	N 11	O 13	0	0
1	2	8	Total 84	C 60	N 11	O 13	0	0
1	3	8	Total 84	C 60	N 11	O 13	0	0
1	4	8	Total 84	C 60	N 11	O 13	0	0
1	e	8	Total 84	C 60	N 11	O 13	0	0
1	5	8	Total 84	C 60	N 11	O 13	0	0
1	6	8	Total 84	C 60	N 11	O 13	0	0
1	7	8	Total 84	C 60	N 11	O 13	0	0
1	f	8	Total 84	C 60	N 11	O 13	0	0
1	8	8	Total 84	C 60	N 11	O 13	0	0
1	9	8	Total 84	C 60	N 11	O 13	0	0

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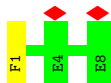
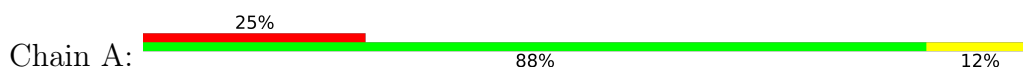
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Mol	Chain	Residues	Atoms				AltConf	Trace
1	AA	8	Total	C	N	O	0	0
			84	60	11	13		
1	g	8	Total	C	N	O	0	0
			84	60	11	13		
1	BA	8	Total	C	N	O	0	0
			84	60	11	13		
1	CA	8	Total	C	N	O	0	0
			84	60	11	13		
1	DA	8	Total	C	N	O	0	0
			84	60	11	13		
1	h	8	Total	C	N	O	0	0
			84	60	11	13		
1	EA	8	Total	C	N	O	0	0
			84	60	11	13		
1	FA	8	Total	C	N	O	0	0
			84	60	11	13		
1	GA	8	Total	C	N	O	0	0
			84	60	11	13		
1	i	8	Total	C	N	O	0	0
			84	60	11	13		
1	HA	8	Total	C	N	O	0	0
			84	60	11	13		
1	IA	8	Total	C	N	O	0	0
			84	60	11	13		
1	JA	8	Total	C	N	O	0	0
			84	60	11	13		

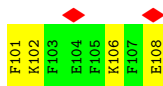
3 Residue-property plots [i](#)

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.

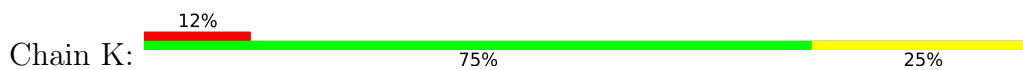
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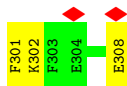
- Molecule 1: KFE8 peptide



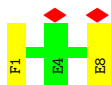
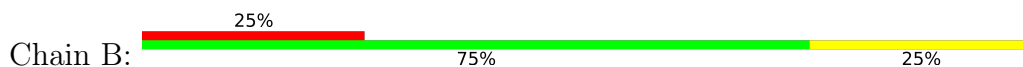
- Molecule 1: KFE8 peptide



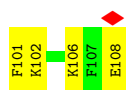
- Molecule 1: KFE8 peptide



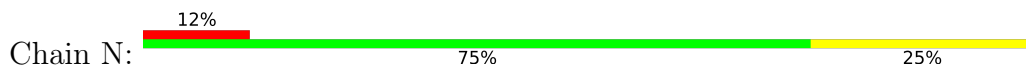
- Molecule 1: KFE8 peptide



● Molecule 1: KFE8 peptide



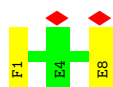
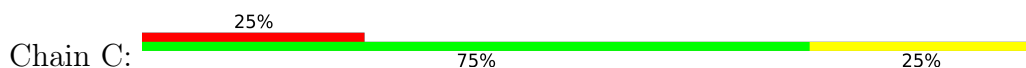
● Molecule 1: KFE8 peptide



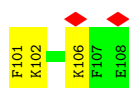
● Molecule 1: KFE8 peptide



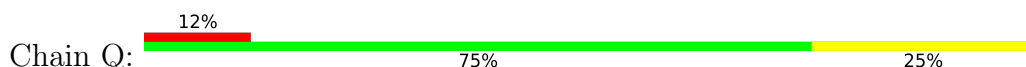
● Molecule 1: KFE8 peptide



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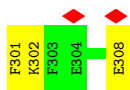


● Molecule 1: KFE8 peptide

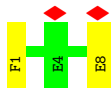
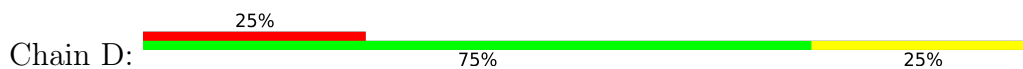


● Molecule 1: KFE8 peptide





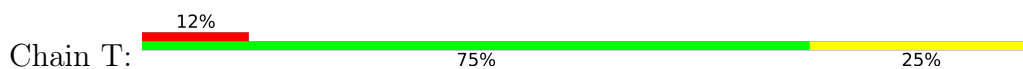
• Molecule 1: KFE8 peptide



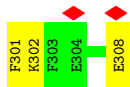
• Molecule 1: KFE8 peptide



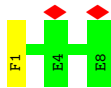
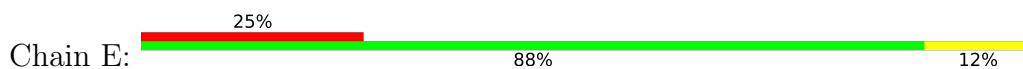
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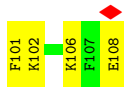
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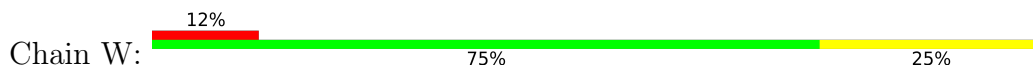
• Molecule 1: KFE8 peptide



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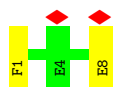
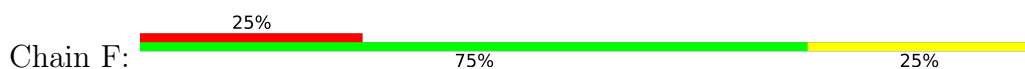
• Molecule 1: KFE8 peptide



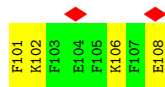
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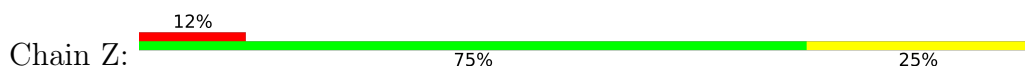
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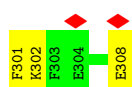
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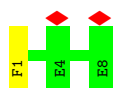
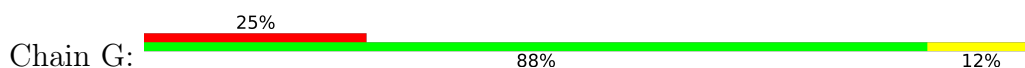
• Molecule 1: KFE8 peptide



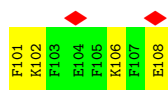
• Molecule 1: KFE8 peptide



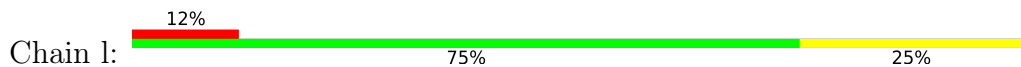
• Molecule 1: KFE8 peptide



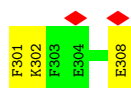
● Molecule 1: KFE8 peptide



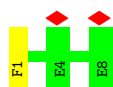
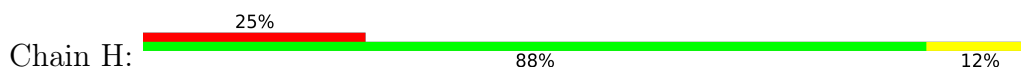
● Molecule 1: KFE8 peptide



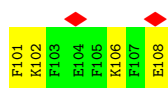
● Molecule 1: KFE8 peptide



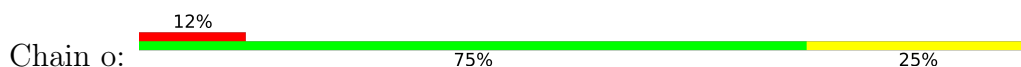
● Molecule 1: KFE8 peptide



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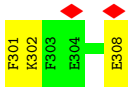


● Molecule 1: KFE8 peptide

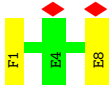
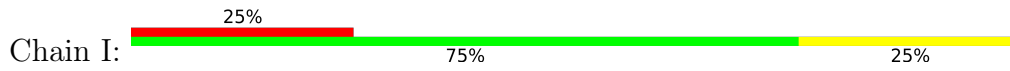


● Molecule 1: KFE8 peptide

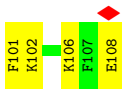




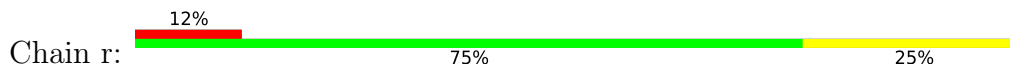
- Molecule 1: KFE8 peptide



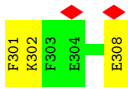
- Molecule 1: KFE8 peptide



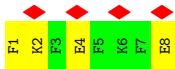
- Molecule 1: KFE8 peptide



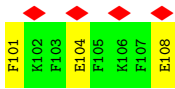
- Molecule 1: KFE8 peptide



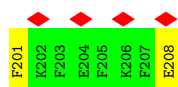
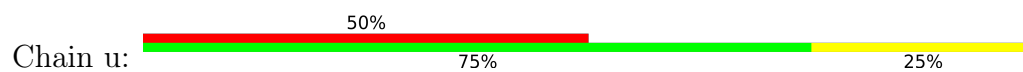
- Molecule 1: KFE8 peptide



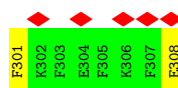
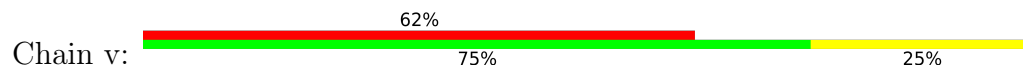
- Molecule 1: KFE8 peptide



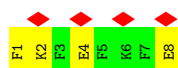
- Molecule 1: KFE8 peptide



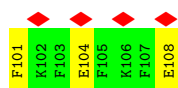
- Molecule 1: KFE8 peptide



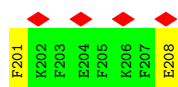
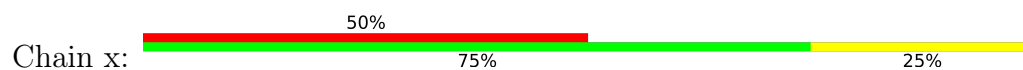
- Molecule 1: KFE8 peptide



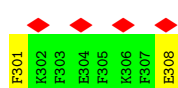
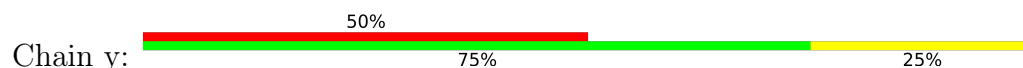
- Molecule 1: KFE8 peptide



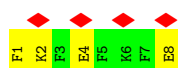
- Molecule 1: KFE8 peptide



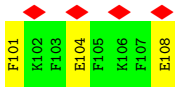
- Molecule 1: KFE8 peptide



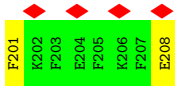
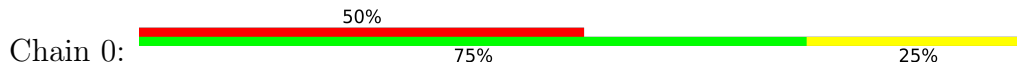
- Molecule 1: KFE8 peptide



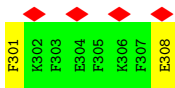
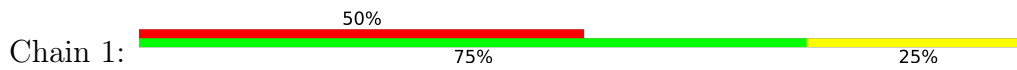
- Molecule 1: KFE8 peptide



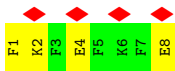
- Molecule 1: KFE8 peptide



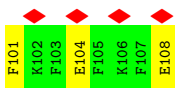
- Molecule 1: KFE8 peptide



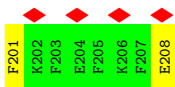
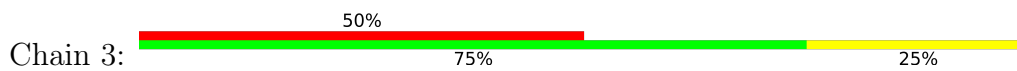
- Molecule 1: KFE8 peptide



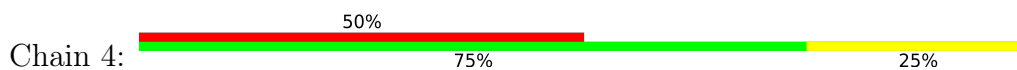
- Molecule 1: KFE8 peptide

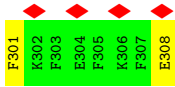


- Molecule 1: KFE8 peptide



- Molecule 1: KFE8 peptide





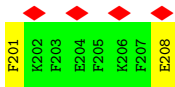
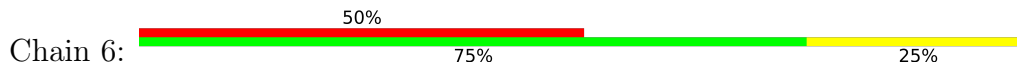
• Molecule 1: KFE8 peptide



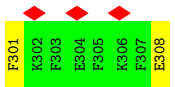
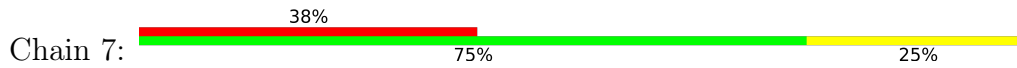
• Molecule 1: KFE8 peptide



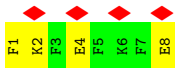
• Molecule 1: KFE8 peptide



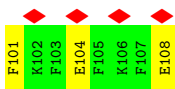
• Molecule 1: KFE8 peptide



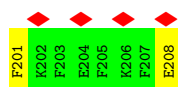
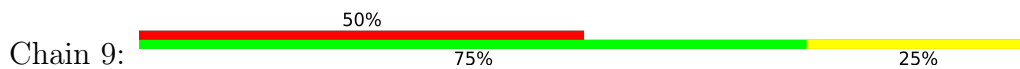
• Molecule 1: KFE8 peptide



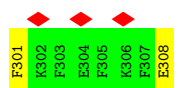
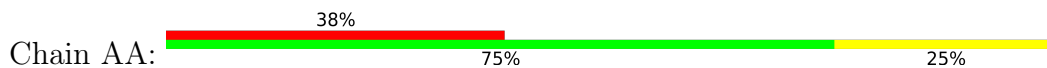
• Molecule 1: KFE8 peptide



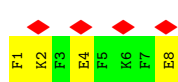
• Molecule 1: KFE8 peptide



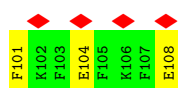
• Molecule 1: KFE8 peptide



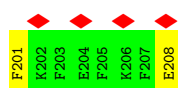
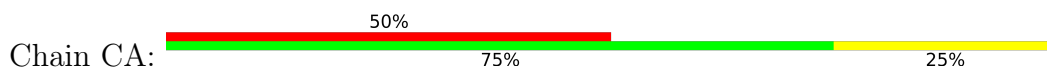
• Molecule 1: KFE8 peptide



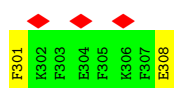
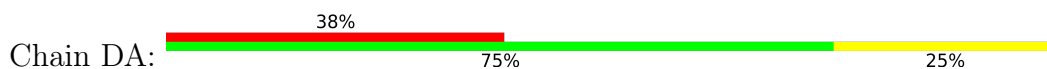
• Molecule 1: KFE8 peptide



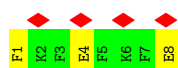
• Molecule 1: KFE8 peptide



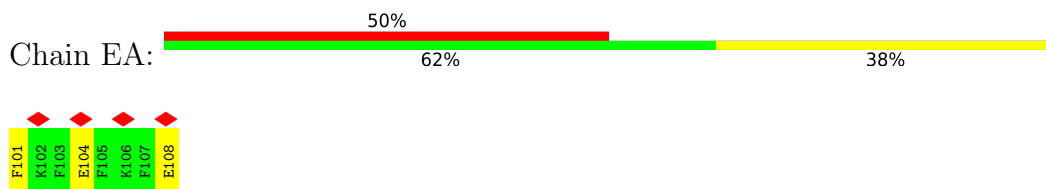
• Molecule 1: KFE8 peptide



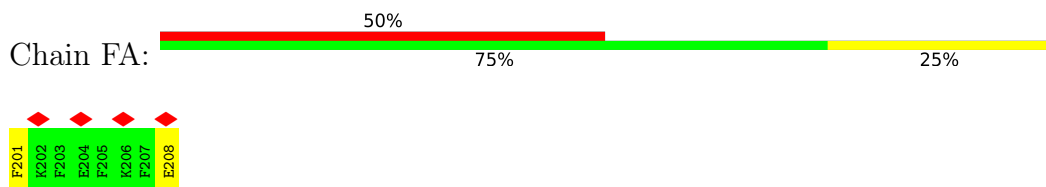
• Molecule 1: KFE8 peptide



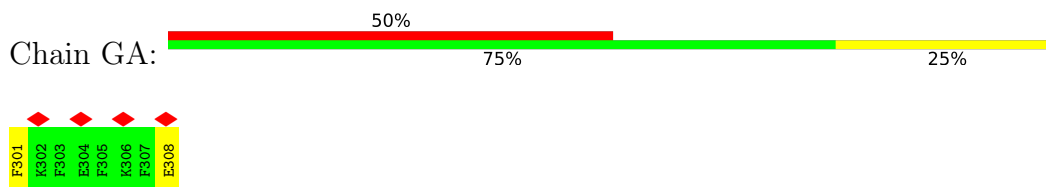
- Molecule 1: KFE8 peptide



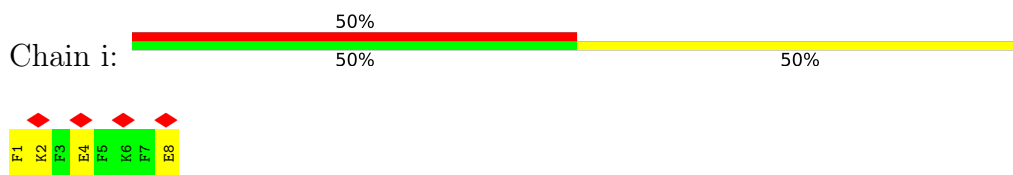
- Molecule 1: KFE8 peptide



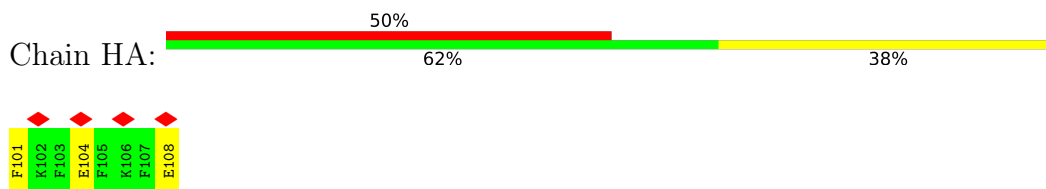
- Molecule 1: KFE8 peptide



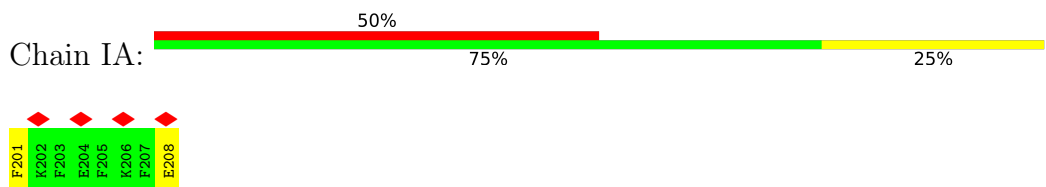
- Molecule 1: KFE8 peptide



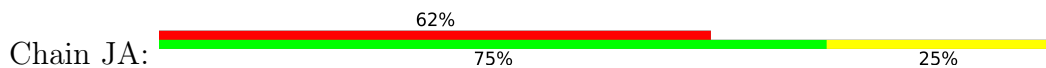
- Molecule 1: KFE8 peptide

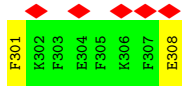


- Molecule 1: KFE8 peptide



- Molecule 1: KFE8 peptide





4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-15.8°, rise=7.93 Å, axial sym=C1	Depositor
Number of segments used	64959	Depositor
Resolution determination method	OTHER	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)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.010	Depositor
Minimum map value	-0.000	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.264	Depositor
Map size (Å)	345.6, 345.6, 345.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GMA, 5CR

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	0	0.51	0/62	0.48	0/79
1	1	0.50	0/62	0.48	0/79
1	2	0.48	0/62	0.50	0/79
1	3	0.50	0/62	0.48	0/79
1	4	0.51	0/62	0.48	0/79
1	5	0.49	0/62	0.50	0/79
1	6	0.50	0/62	0.48	0/79
1	7	0.50	0/62	0.48	0/79
1	8	0.49	0/62	0.49	0/79
1	9	0.51	0/62	0.48	0/79
1	A	0.55	0/62	0.45	0/79
1	AA	0.51	0/62	0.48	0/79
1	B	0.55	0/62	0.45	0/79
1	BA	0.49	0/62	0.49	0/79
1	C	0.55	0/62	0.45	0/79
1	CA	0.50	0/62	0.48	0/79
1	D	0.55	0/62	0.45	0/79
1	DA	0.51	0/62	0.48	0/79
1	E	0.55	0/62	0.45	0/79
1	EA	0.49	0/62	0.49	0/79
1	F	0.55	0/62	0.45	0/79
1	FA	0.50	0/62	0.48	0/79
1	G	0.55	0/62	0.45	0/79
1	GA	0.50	0/62	0.48	0/79
1	H	0.54	0/62	0.45	0/79
1	HA	0.49	0/62	0.49	0/79
1	I	0.55	0/62	0.45	0/79
1	IA	0.51	0/62	0.47	0/79
1	J	0.53	0/62	0.45	0/79
1	JA	0.50	0/62	0.48	0/79
1	K	0.60	0/62	0.42	0/79
1	L	0.55	0/62	0.37	0/79

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	M	0.54	0/62	0.45	0/79
1	N	0.60	0/62	0.42	0/79
1	O	0.56	0/62	0.37	0/79
1	P	0.53	0/62	0.45	0/79
1	Q	0.60	0/62	0.42	0/79
1	R	0.56	0/62	0.37	0/79
1	S	0.53	0/62	0.45	0/79
1	T	0.60	0/62	0.42	0/79
1	U	0.55	0/62	0.37	0/79
1	V	0.53	0/62	0.45	0/79
1	W	0.60	0/62	0.42	0/79
1	X	0.55	0/62	0.37	0/79
1	Y	0.53	0/62	0.45	0/79
1	Z	0.60	0/62	0.42	0/79
1	a	0.55	0/62	0.60	0/79
1	b	0.55	0/62	0.60	0/79
1	c	0.55	0/62	0.60	0/79
1	d	0.55	0/62	0.60	0/79
1	e	0.54	0/62	0.60	0/79
1	f	0.55	0/62	0.60	0/79
1	g	0.55	0/62	0.60	0/79
1	h	0.55	0/62	0.60	0/79
1	i	0.55	0/62	0.60	0/79
1	j	0.56	0/62	0.37	0/79
1	k	0.54	0/62	0.45	0/79
1	l	0.60	0/62	0.41	0/79
1	m	0.56	0/62	0.37	0/79
1	n	0.54	0/62	0.45	0/79
1	o	0.60	0/62	0.42	0/79
1	p	0.56	0/62	0.37	0/79
1	q	0.53	0/62	0.45	0/79
1	r	0.60	0/62	0.42	0/79
1	s	0.56	0/62	0.37	0/79
1	t	0.48	0/62	0.49	0/79
1	u	0.51	0/62	0.48	0/79
1	v	0.50	0/62	0.48	0/79
1	w	0.48	0/62	0.49	0/79
1	x	0.50	0/62	0.47	0/79
1	y	0.51	0/62	0.48	0/79
1	z	0.49	0/62	0.50	0/79
All	All	0.54	0/4464	0.47	0/5688

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](#)

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	0	6/8 (75%)	6 (100%)	0	0	100	100
1	1	6/8 (75%)	6 (100%)	0	0	100	100
1	2	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	3	6/8 (75%)	6 (100%)	0	0	100	100
1	4	6/8 (75%)	6 (100%)	0	0	100	100
1	5	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	6	6/8 (75%)	6 (100%)	0	0	100	100
1	7	6/8 (75%)	6 (100%)	0	0	100	100
1	8	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	9	6/8 (75%)	6 (100%)	0	0	100	100
1	A	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	AA	6/8 (75%)	6 (100%)	0	0	100	100
1	B	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	BA	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	C	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	CA	6/8 (75%)	6 (100%)	0	0	100	100
1	D	6/8 (75%)	5 (83%)	1 (17%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	DA	6/8 (75%)	6 (100%)	0	0	100	100
1	E	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	EA	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	F	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	FA	6/8 (75%)	6 (100%)	0	0	100	100
1	G	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	GA	6/8 (75%)	6 (100%)	0	0	100	100
1	H	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	HA	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	I	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	IA	6/8 (75%)	6 (100%)	0	0	100	100
1	J	6/8 (75%)	6 (100%)	0	0	100	100
1	JA	6/8 (75%)	6 (100%)	0	0	100	100
1	K	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	L	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	M	6/8 (75%)	6 (100%)	0	0	100	100
1	N	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	O	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	P	6/8 (75%)	6 (100%)	0	0	100	100
1	Q	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	R	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	S	6/8 (75%)	6 (100%)	0	0	100	100
1	T	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	U	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	V	6/8 (75%)	6 (100%)	0	0	100	100
1	W	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	X	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	Y	6/8 (75%)	6 (100%)	0	0	100	100
1	Z	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	a	6/8 (75%)	6 (100%)	0	0	100	100
1	b	6/8 (75%)	6 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	c	6/8 (75%)	6 (100%)	0	0	100	100
1	d	6/8 (75%)	6 (100%)	0	0	100	100
1	e	6/8 (75%)	6 (100%)	0	0	100	100
1	f	6/8 (75%)	6 (100%)	0	0	100	100
1	g	6/8 (75%)	6 (100%)	0	0	100	100
1	h	6/8 (75%)	6 (100%)	0	0	100	100
1	i	6/8 (75%)	6 (100%)	0	0	100	100
1	j	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	k	6/8 (75%)	6 (100%)	0	0	100	100
1	l	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	m	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	n	6/8 (75%)	6 (100%)	0	0	100	100
1	o	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	p	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	q	6/8 (75%)	6 (100%)	0	0	100	100
1	r	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	s	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	t	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	u	6/8 (75%)	6 (100%)	0	0	100	100
1	v	6/8 (75%)	6 (100%)	0	0	100	100
1	w	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	x	6/8 (75%)	6 (100%)	0	0	100	100
1	y	6/8 (75%)	6 (100%)	0	0	100	100
1	z	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
All	All	432/576 (75%)	396 (92%)	36 (8%)	0	100	100

There are no Ramachandran outliers to report.

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	0	6/6 (100%)	6 (100%)	0	100	100
1	1	6/6 (100%)	6 (100%)	0	100	100
1	2	6/6 (100%)	5 (83%)	1 (17%)	2	8
1	3	6/6 (100%)	6 (100%)	0	100	100
1	4	6/6 (100%)	6 (100%)	0	100	100
1	5	6/6 (100%)	5 (83%)	1 (17%)	2	8
1	6	6/6 (100%)	6 (100%)	0	100	100
1	7	6/6 (100%)	6 (100%)	0	100	100
1	8	6/6 (100%)	5 (83%)	1 (17%)	2	8
1	9	6/6 (100%)	6 (100%)	0	100	100
1	A	6/6 (100%)	6 (100%)	0	100	100
1	AA	6/6 (100%)	6 (100%)	0	100	100
1	B	6/6 (100%)	6 (100%)	0	100	100
1	BA	6/6 (100%)	5 (83%)	1 (17%)	2	8
1	C	6/6 (100%)	6 (100%)	0	100	100
1	CA	6/6 (100%)	6 (100%)	0	100	100
1	D	6/6 (100%)	6 (100%)	0	100	100
1	DA	6/6 (100%)	6 (100%)	0	100	100
1	E	6/6 (100%)	6 (100%)	0	100	100
1	EA	6/6 (100%)	5 (83%)	1 (17%)	2	8
1	F	6/6 (100%)	6 (100%)	0	100	100
1	FA	6/6 (100%)	6 (100%)	0	100	100
1	G	6/6 (100%)	6 (100%)	0	100	100
1	GA	6/6 (100%)	6 (100%)	0	100	100
1	H	6/6 (100%)	6 (100%)	0	100	100
1	HA	6/6 (100%)	5 (83%)	1 (17%)	2	8
1	I	6/6 (100%)	6 (100%)	0	100	100
1	IA	6/6 (100%)	6 (100%)	0	100	100
1	J	6/6 (100%)	4 (67%)	2 (33%)	0	1
1	JA	6/6 (100%)	6 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	6/6 (100%)	6 (100%)	0	100	100
1	L	6/6 (100%)	5 (83%)	1 (17%)	2	8
1	M	6/6 (100%)	4 (67%)	2 (33%)	0	1
1	N	6/6 (100%)	6 (100%)	0	100	100
1	O	6/6 (100%)	5 (83%)	1 (17%)	2	8
1	P	6/6 (100%)	4 (67%)	2 (33%)	0	1
1	Q	6/6 (100%)	6 (100%)	0	100	100
1	R	6/6 (100%)	5 (83%)	1 (17%)	2	8
1	S	6/6 (100%)	4 (67%)	2 (33%)	0	1
1	T	6/6 (100%)	6 (100%)	0	100	100
1	U	6/6 (100%)	5 (83%)	1 (17%)	2	8
1	V	6/6 (100%)	4 (67%)	2 (33%)	0	1
1	W	6/6 (100%)	6 (100%)	0	100	100
1	X	6/6 (100%)	5 (83%)	1 (17%)	2	8
1	Y	6/6 (100%)	4 (67%)	2 (33%)	0	1
1	Z	6/6 (100%)	6 (100%)	0	100	100
1	a	6/6 (100%)	4 (67%)	2 (33%)	0	1
1	b	6/6 (100%)	4 (67%)	2 (33%)	0	1
1	c	6/6 (100%)	4 (67%)	2 (33%)	0	1
1	d	6/6 (100%)	4 (67%)	2 (33%)	0	1
1	e	6/6 (100%)	4 (67%)	2 (33%)	0	1
1	f	6/6 (100%)	4 (67%)	2 (33%)	0	1
1	g	6/6 (100%)	4 (67%)	2 (33%)	0	1
1	h	6/6 (100%)	5 (83%)	1 (17%)	2	8
1	i	6/6 (100%)	4 (67%)	2 (33%)	0	1
1	j	6/6 (100%)	5 (83%)	1 (17%)	2	8
1	k	6/6 (100%)	4 (67%)	2 (33%)	0	1
1	l	6/6 (100%)	6 (100%)	0	100	100
1	m	6/6 (100%)	5 (83%)	1 (17%)	2	8
1	n	6/6 (100%)	4 (67%)	2 (33%)	0	1
1	o	6/6 (100%)	6 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	p	6/6 (100%)	5 (83%)	1 (17%)	2	8
1	q	6/6 (100%)	4 (67%)	2 (33%)	0	1
1	r	6/6 (100%)	6 (100%)	0	100	100
1	s	6/6 (100%)	5 (83%)	1 (17%)	2	8
1	t	6/6 (100%)	5 (83%)	1 (17%)	2	8
1	u	6/6 (100%)	6 (100%)	0	100	100
1	v	6/6 (100%)	6 (100%)	0	100	100
1	w	6/6 (100%)	5 (83%)	1 (17%)	2	8
1	x	6/6 (100%)	6 (100%)	0	100	100
1	y	6/6 (100%)	6 (100%)	0	100	100
1	z	6/6 (100%)	5 (83%)	1 (17%)	2	8
All	All	432/432 (100%)	379 (88%)	53 (12%)	8	17

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	102	LYS
1	J	106	LYS
1	L	302	LYS
1	M	102	LYS
1	M	106	LYS
1	O	302	LYS
1	P	102	LYS
1	P	106	LYS
1	R	302	LYS
1	S	102	LYS
1	S	106	LYS
1	U	302	LYS
1	V	102	LYS
1	V	106	LYS
1	X	302	LYS
1	Y	102	LYS
1	Y	106	LYS
1	j	302	LYS
1	k	102	LYS
1	k	106	LYS
1	m	302	LYS
1	n	102	LYS

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Mol	Chain	Res	Type
1	n	106	LYS
1	p	302	LYS
1	q	102	LYS
1	q	106	LYS
1	s	302	LYS
1	a	2	LYS
1	a	4	GLU
1	t	104	GLU
1	b	2	LYS
1	b	4	GLU
1	w	104	GLU
1	c	2	LYS
1	c	4	GLU
1	z	104	GLU
1	d	2	LYS
1	d	4	GLU
1	2	104	GLU
1	e	2	LYS
1	e	4	GLU
1	5	104	GLU
1	f	2	LYS
1	f	4	GLU
1	8	104	GLU
1	g	2	LYS
1	g	4	GLU
1	BA	104	GLU
1	h	4	GLU
1	EA	104	GLU
1	i	2	LYS
1	i	4	GLU
1	HA	104	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

144 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	5CR	j	301	1	13,14,15	1.23	2 (15%)	16,17,19	1.29	3 (18%)
1	GMA	6	208	1	9,9,9	1.18	1 (11%)	10,11,11	1.13	0
1	GMA	EA	108	1	9,9,9	1.15	1 (11%)	10,11,11	1.19	0
1	GMA	f	8	1	9,9,9	1.19	1 (11%)	10,11,11	1.15	0
1	GMA	e	8	1	9,9,9	1.20	1 (11%)	10,11,11	1.15	0
1	5CR	6	201	1	13,14,15	1.22	1 (7%)	16,17,19	1.15	1 (6%)
1	GMA	K	208	1	9,9,9	1.17	1 (11%)	10,11,11	1.26	1 (10%)
1	5CR	C	1	1	13,14,15	1.22	2 (15%)	16,17,19	1.70	3 (18%)
1	GMA	h	8	1	9,9,9	1.18	1 (11%)	10,11,11	1.14	0
1	GMA	A	8	1	9,9,9	1.14	0	10,11,11	1.25	0
1	GMA	X	308	1	9,9,9	1.16	1 (11%)	10,11,11	1.24	0
1	GMA	n	108	1	9,9,9	1.13	1 (11%)	10,11,11	1.22	1 (10%)
1	GMA	2	108	1	9,9,9	1.14	1 (11%)	10,11,11	1.18	0
1	GMA	o	208	1	9,9,9	1.18	1 (11%)	10,11,11	1.27	2 (20%)
1	GMA	q	108	1	9,9,9	1.14	1 (11%)	10,11,11	1.23	1 (10%)
1	5CR	9	201	1	13,14,15	1.22	1 (7%)	16,17,19	1.14	1 (6%)
1	5CR	L	301	1	13,14,15	1.22	2 (15%)	16,17,19	1.28	3 (18%)
1	5CR	t	101	1	13,14,15	1.22	1 (7%)	16,17,19	1.25	2 (12%)
1	5CR	M	101	1	13,14,15	1.22	1 (7%)	16,17,19	1.52	2 (12%)
1	5CR	S	101	1	13,14,15	1.23	1 (7%)	16,17,19	1.51	2 (12%)
1	5CR	o	201	1	13,14,15	1.23	1 (7%)	16,17,19	1.33	2 (12%)
1	5CR	H	1	1	13,14,15	1.22	1 (7%)	16,17,19	1.69	3 (18%)
1	GMA	T	208	1	9,9,9	1.17	1 (11%)	10,11,11	1.26	1 (10%)
1	GMA	O	308	1	9,9,9	1.16	1 (11%)	10,11,11	1.23	0
1	GMA	y	308	1	9,9,9	1.14	1 (11%)	10,11,11	1.32	0
1	GMA	p	308	1	9,9,9	1.16	1 (11%)	10,11,11	1.24	0
1	5CR	m	301	1	13,14,15	1.24	2 (15%)	16,17,19	1.28	3 (18%)
1	5CR	I	1	1	13,14,15	1.22	2 (15%)	16,17,19	1.71	3 (18%)
1	GMA	b	8	1	9,9,9	1.19	1 (11%)	10,11,11	1.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5CR	f	1	1	13,14,15	1.28	2 (15%)	16,17,19	1.74	4 (25%)
1	GMA	G	8	1	9,9,9	1.14	0	10,11,11	1.26	0
1	GMA	l	208	1	9,9,9	1.18	1 (11%)	10,11,11	1.28	2 (20%)
1	GMA	x	208	1	9,9,9	1.18	1 (11%)	10,11,11	1.12	0
1	5CR	r	201	1	13,14,15	1.24	1 (7%)	16,17,19	1.34	2 (12%)
1	5CR	U	301	1	13,14,15	1.22	2 (15%)	16,17,19	1.28	3 (18%)
1	GMA	1	308	1	9,9,9	1.14	1 (11%)	10,11,11	1.32	0
1	5CR	d	1	1	13,14,15	1.28	2 (15%)	16,17,19	1.74	4 (25%)
1	GMA	8	108	1	9,9,9	1.15	1 (11%)	10,11,11	1.19	0
1	GMA	5	108	1	9,9,9	1.15	1 (11%)	10,11,11	1.18	0
1	5CR	0	201	1	13,14,15	1.22	1 (7%)	16,17,19	1.15	1 (6%)
1	GMA	Z	208	1	9,9,9	1.17	1 (11%)	10,11,11	1.27	2 (20%)
1	GMA	DA	308	1	9,9,9	1.14	1 (11%)	10,11,11	1.32	0
1	GMA	S	108	1	9,9,9	1.14	1 (11%)	10,11,11	1.23	1 (10%)
1	5CR	a	1	1	13,14,15	1.28	2 (15%)	16,17,19	1.73	4 (25%)
1	GMA	W	208	1	9,9,9	1.17	1 (11%)	10,11,11	1.26	1 (10%)
1	5CR	3	201	1	13,14,15	1.22	1 (7%)	16,17,19	1.14	1 (6%)
1	GMA	m	308	1	9,9,9	1.16	1 (11%)	10,11,11	1.25	0
1	5CR	N	201	1	13,14,15	1.24	1 (7%)	16,17,19	1.34	2 (12%)
1	5CR	E	1	1	13,14,15	1.22	2 (15%)	16,17,19	1.70	3 (18%)
1	5CR	s	301	1	13,14,15	1.23	2 (15%)	16,17,19	1.28	3 (18%)
1	GMA	a	8	1	9,9,9	1.18	1 (11%)	10,11,11	1.14	0
1	5CR	1	301	1	13,14,15	1.22	1 (7%)	16,17,19	1.02	1 (6%)
1	5CR	J	101	1	13,14,15	1.23	1 (7%)	16,17,19	1.50	2 (12%)
1	GMA	3	208	1	9,9,9	1.18	1 (11%)	10,11,11	1.12	0
1	GMA	E	8	1	9,9,9	1.15	0	10,11,11	1.26	0
1	5CR	R	301	1	13,14,15	1.24	2 (15%)	16,17,19	1.27	3 (18%)
1	GMA	j	308	1	9,9,9	1.16	1 (11%)	10,11,11	1.24	0
1	GMA	w	108	1	9,9,9	1.15	1 (11%)	10,11,11	1.20	0
1	5CR	x	201	1	13,14,15	1.22	1 (7%)	16,17,19	1.14	1 (6%)
1	GMA	v	308	1	9,9,9	1.14	1 (11%)	10,11,11	1.32	0
1	5CR	u	201	1	13,14,15	1.22	1 (7%)	16,17,19	1.15	1 (6%)
1	5CR	G	1	1	13,14,15	1.22	2 (15%)	16,17,19	1.70	3 (18%)
1	GMA	7	308	1	9,9,9	1.14	1 (11%)	10,11,11	1.31	0
1	5CR	7	301	1	13,14,15	1.22	1 (7%)	16,17,19	1.02	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	GMA	C	8	1	9,9,9	1.15	1 (11%)	10,11,11	1.26	0
1	GMA	GA	308	1	9,9,9	1.14	1 (11%)	10,11,11	1.32	0
1	GMA	JA	308	1	9,9,9	1.15	1 (11%)	10,11,11	1.32	0
1	5CR	O	301	1	13,14,15	1.22	2 (15%)	16,17,19	1.29	3 (18%)
1	GMA	CA	208	1	9,9,9	1.17	1 (11%)	10,11,11	1.13	0
1	GMA	d	8	1	9,9,9	1.19	1 (11%)	10,11,11	1.14	0
1	5CR	EA	101	1	13,14,15	1.22	1 (7%)	16,17,19	1.25	2 (12%)
1	GMA	L	308	1	9,9,9	1.17	1 (11%)	10,11,11	1.24	0
1	5CR	GA	301	1	13,14,15	1.23	1 (7%)	16,17,19	1.02	1 (6%)
1	GMA	4	308	1	9,9,9	1.14	1 (11%)	10,11,11	1.31	0
1	5CR	AA	301	1	13,14,15	1.22	1 (7%)	16,17,19	1.02	1 (6%)
1	5CR	Q	201	1	13,14,15	1.24	2 (15%)	16,17,19	1.34	2 (12%)
1	5CR	V	101	1	13,14,15	1.23	1 (7%)	16,17,19	1.51	2 (12%)
1	5CR	BA	101	1	13,14,15	1.22	1 (7%)	16,17,19	1.25	2 (12%)
1	5CR	IA	201	1	13,14,15	1.21	1 (7%)	16,17,19	1.14	1 (6%)
1	GMA	D	8	1	9,9,9	1.16	1 (11%)	10,11,11	1.26	0
1	GMA	P	108	1	9,9,9	1.14	0	10,11,11	1.22	0
1	GMA	FA	208	1	9,9,9	1.18	1 (11%)	10,11,11	1.14	0
1	GMA	N	208	1	9,9,9	1.18	1 (11%)	10,11,11	1.27	1 (10%)
1	GMA	r	208	1	9,9,9	1.18	1 (11%)	10,11,11	1.27	2 (20%)
1	5CR	W	201	1	13,14,15	1.24	1 (7%)	16,17,19	1.34	2 (12%)
1	5CR	8	101	1	13,14,15	1.21	1 (7%)	16,17,19	1.25	2 (12%)
1	5CR	K	201	1	13,14,15	1.24	1 (7%)	16,17,19	1.33	2 (12%)
1	5CR	p	301	1	13,14,15	1.22	2 (15%)	16,17,19	1.28	3 (18%)
1	GMA	B	8	1	9,9,9	1.15	1 (11%)	10,11,11	1.27	1 (10%)
1	GMA	BA	108	1	9,9,9	1.15	1 (11%)	10,11,11	1.19	0
1	GMA	HA	108	1	9,9,9	1.14	1 (11%)	10,11,11	1.18	0
1	5CR	HA	101	1	13,14,15	1.21	1 (7%)	16,17,19	1.25	2 (12%)
1	GMA	R	308	1	9,9,9	1.16	1 (11%)	10,11,11	1.24	0
1	5CR	w	101	1	13,14,15	1.21	1 (7%)	16,17,19	1.25	2 (12%)
1	5CR	DA	301	1	13,14,15	1.23	1 (7%)	16,17,19	1.02	1 (6%)
1	GMA	H	8	1	9,9,9	1.15	0	10,11,11	1.26	0
1	GMA	c	8	1	9,9,9	1.19	1 (11%)	10,11,11	1.15	0
1	GMA	k	108	1	9,9,9	1.13	1 (11%)	10,11,11	1.22	1 (10%)
1	5CR	FA	201	1	13,14,15	1.22	1 (7%)	16,17,19	1.14	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5CR	JA	301	1	13,14,15	1.23	1 (7%)	16,17,19	1.02	1 (6%)
1	5CR	X	301	1	13,14,15	1.24	2 (15%)	16,17,19	1.28	3 (18%)
1	GMA	g	8	1	9,9,9	1.19	1 (11%)	10,11,11	1.15	0
1	GMA	U	308	1	9,9,9	1.17	1 (11%)	10,11,11	1.24	0
1	5CR	b	1	1	13,14,15	1.28	2 (15%)	16,17,19	1.74	4 (25%)
1	5CR	2	101	1	13,14,15	1.22	1 (7%)	16,17,19	1.25	2 (12%)
1	5CR	q	101	1	13,14,15	1.23	1 (7%)	16,17,19	1.51	2 (12%)
1	GMA	t	108	1	9,9,9	1.15	1 (11%)	10,11,11	1.19	0
1	GMA	0	208	1	9,9,9	1.18	1 (11%)	10,11,11	1.13	0
1	GMA	IA	208	1	9,9,9	1.19	1 (11%)	10,11,11	1.13	0
1	GMA	F	8	1	9,9,9	1.14	1 (11%)	10,11,11	1.26	0
1	GMA	V	108	1	9,9,9	1.14	1 (11%)	10,11,11	1.22	0
1	5CR	4	301	1	13,14,15	1.23	1 (7%)	16,17,19	1.02	1 (6%)
1	5CR	T	201	1	13,14,15	1.24	1 (7%)	16,17,19	1.34	2 (12%)
1	5CR	A	1	1	13,14,15	1.22	1 (7%)	16,17,19	1.70	3 (18%)
1	5CR	P	101	1	13,14,15	1.23	1 (7%)	16,17,19	1.51	2 (12%)
1	5CR	l	201	1	13,14,15	1.24	1 (7%)	16,17,19	1.33	2 (12%)
1	5CR	z	101	1	13,14,15	1.22	1 (7%)	16,17,19	1.26	2 (12%)
1	GMA	z	108	1	9,9,9	1.15	1 (11%)	10,11,11	1.19	0
1	GMA	u	208	1	9,9,9	1.19	1 (11%)	10,11,11	1.13	0
1	5CR	v	301	1	13,14,15	1.23	1 (7%)	16,17,19	1.02	1 (6%)
1	GMA	i	8	1	9,9,9	1.19	1 (11%)	10,11,11	1.15	0
1	5CR	e	1	1	13,14,15	1.28	2 (15%)	16,17,19	1.73	4 (25%)
1	5CR	5	101	1	13,14,15	1.22	1 (7%)	16,17,19	1.25	2 (12%)
1	GMA	I	8	1	9,9,9	1.16	1 (11%)	10,11,11	1.26	0
1	5CR	i	1	1	13,14,15	1.28	2 (15%)	16,17,19	1.73	4 (25%)
1	5CR	Z	201	1	13,14,15	1.24	2 (15%)	16,17,19	1.33	2 (12%)
1	5CR	D	1	1	13,14,15	1.22	1 (7%)	16,17,19	1.69	3 (18%)
1	5CR	Y	101	1	13,14,15	1.23	1 (7%)	16,17,19	1.51	2 (12%)
1	GMA	Y	108	1	9,9,9	1.14	1 (11%)	10,11,11	1.23	1 (10%)
1	5CR	h	1	1	13,14,15	1.28	1 (7%)	16,17,19	1.74	4 (25%)
1	GMA	AA	308	1	9,9,9	1.13	1 (11%)	10,11,11	1.31	0
1	5CR	y	301	1	13,14,15	1.22	1 (7%)	16,17,19	1.02	1 (6%)
1	5CR	F	1	1	13,14,15	1.22	1 (7%)	16,17,19	1.70	3 (18%)
1	GMA	Q	208	1	9,9,9	1.19	1 (11%)	10,11,11	1.28	2 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	GMA	s	308	1	9,9,9	1.17	1 (11%)	10,11,11	1.25	0
1	5CR	g	1	1	13,14,15	1.27	1 (7%)	16,17,19	1.74	4 (25%)
1	GMA	M	108	1	9,9,9	1.14	1 (11%)	10,11,11	1.22	0
1	5CR	B	1	1	13,14,15	1.23	2 (15%)	16,17,19	1.70	3 (18%)
1	GMA	9	208	1	9,9,9	1.18	1 (11%)	10,11,11	1.13	0
1	5CR	c	1	1	13,14,15	1.28	2 (15%)	16,17,19	1.73	4 (25%)
1	GMA	J	108	1	9,9,9	1.14	1 (11%)	10,11,11	1.23	1 (10%)
1	5CR	CA	201	1	13,14,15	1.22	1 (7%)	16,17,19	1.15	1 (6%)
1	5CR	k	101	1	13,14,15	1.23	1 (7%)	16,17,19	1.51	2 (12%)
1	5CR	n	101	1	13,14,15	1.24	1 (7%)	16,17,19	1.51	2 (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
1	5CR	j	301	1	-	3/9/10/12	0/1/1/1
1	GMA	6	208	1	-	4/9/9/9	-
1	GMA	EA	108	1	-	0/9/9/9	-
1	GMA	f	8	1	-	8/9/9/9	-
1	GMA	e	8	1	-	8/9/9/9	-
1	5CR	6	201	1	-	2/9/10/12	0/1/1/1
1	GMA	K	208	1	-	1/9/9/9	-
1	5CR	C	1	1	-	0/9/10/12	0/1/1/1
1	GMA	h	8	1	-	8/9/9/9	-
1	GMA	A	8	1	-	1/9/9/9	-
1	GMA	X	308	1	-	1/9/9/9	-
1	GMA	n	108	1	-	3/9/9/9	-
1	GMA	2	108	1	-	0/9/9/9	-
1	GMA	o	208	1	-	1/9/9/9	-
1	GMA	q	108	1	-	3/9/9/9	-
1	5CR	9	201	1	-	2/9/10/12	0/1/1/1
1	5CR	L	301	1	-	3/9/10/12	0/1/1/1
1	5CR	t	101	1	-	1/9/10/12	0/1/1/1
1	5CR	M	101	1	-	2/9/10/12	0/1/1/1
1	5CR	S	101	1	-	2/9/10/12	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5CR	o	201	1	-	4/9/10/12	0/1/1/1
1	5CR	H	1	1	-	0/9/10/12	0/1/1/1
1	GMA	T	208	1	-	1/9/9/9	-
1	GMA	O	308	1	-	1/9/9/9	-
1	GMA	y	308	1	-	0/9/9/9	-
1	GMA	p	308	1	-	1/9/9/9	-
1	5CR	m	301	1	-	3/9/10/12	0/1/1/1
1	5CR	I	1	1	-	0/9/10/12	0/1/1/1
1	GMA	b	8	1	-	8/9/9/9	-
1	5CR	f	1	1	-	6/9/10/12	0/1/1/1
1	GMA	G	8	1	-	1/9/9/9	-
1	GMA	l	208	1	-	1/9/9/9	-
1	GMA	x	208	1	-	4/9/9/9	-
1	5CR	r	201	1	-	4/9/10/12	0/1/1/1
1	5CR	U	301	1	-	3/9/10/12	0/1/1/1
1	GMA	1	308	1	-	0/9/9/9	-
1	5CR	d	1	1	-	6/9/10/12	0/1/1/1
1	GMA	8	108	1	-	0/9/9/9	-
1	GMA	5	108	1	-	0/9/9/9	-
1	5CR	0	201	1	-	2/9/10/12	0/1/1/1
1	GMA	Z	208	1	-	1/9/9/9	-
1	GMA	DA	308	1	-	0/9/9/9	-
1	GMA	S	108	1	-	3/9/9/9	-
1	5CR	a	1	1	-	6/9/10/12	0/1/1/1
1	GMA	W	208	1	-	1/9/9/9	-
1	5CR	3	201	1	-	2/9/10/12	0/1/1/1
1	GMA	m	308	1	-	1/9/9/9	-
1	5CR	N	201	1	-	4/9/10/12	0/1/1/1
1	5CR	E	1	1	-	0/9/10/12	0/1/1/1
1	5CR	s	301	1	-	3/9/10/12	0/1/1/1
1	GMA	a	8	1	-	8/9/9/9	-
1	5CR	1	301	1	-	4/9/10/12	0/1/1/1
1	5CR	J	101	1	-	2/9/10/12	0/1/1/1
1	GMA	3	208	1	-	4/9/9/9	-
1	GMA	E	8	1	-	1/9/9/9	-
1	5CR	R	301	1	-	3/9/10/12	0/1/1/1
1	GMA	j	308	1	-	1/9/9/9	-
1	GMA	w	108	1	-	0/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5CR	x	201	1	-	2/9/10/12	0/1/1/1
1	GMA	v	308	1	-	0/9/9/9	-
1	5CR	u	201	1	-	2/9/10/12	0/1/1/1
1	5CR	G	1	1	-	0/9/10/12	0/1/1/1
1	GMA	7	308	1	-	0/9/9/9	-
1	5CR	7	301	1	-	4/9/10/12	0/1/1/1
1	GMA	C	8	1	-	1/9/9/9	-
1	GMA	GA	308	1	-	0/9/9/9	-
1	GMA	JA	308	1	-	0/9/9/9	-
1	5CR	O	301	1	-	3/9/10/12	0/1/1/1
1	GMA	CA	208	1	-	4/9/9/9	-
1	GMA	d	8	1	-	8/9/9/9	-
1	5CR	EA	101	1	-	1/9/10/12	0/1/1/1
1	GMA	L	308	1	-	1/9/9/9	-
1	5CR	GA	301	1	-	4/9/10/12	0/1/1/1
1	GMA	4	308	1	-	0/9/9/9	-
1	5CR	AA	301	1	-	4/9/10/12	0/1/1/1
1	5CR	Q	201	1	-	4/9/10/12	0/1/1/1
1	5CR	V	101	1	-	2/9/10/12	0/1/1/1
1	5CR	BA	101	1	-	1/9/10/12	0/1/1/1
1	5CR	IA	201	1	-	2/9/10/12	0/1/1/1
1	GMA	D	8	1	-	1/9/9/9	-
1	GMA	P	108	1	-	3/9/9/9	-
1	GMA	FA	208	1	-	4/9/9/9	-
1	GMA	N	208	1	-	1/9/9/9	-
1	GMA	r	208	1	-	1/9/9/9	-
1	5CR	W	201	1	-	4/9/10/12	0/1/1/1
1	5CR	8	101	1	-	1/9/10/12	0/1/1/1
1	5CR	K	201	1	-	4/9/10/12	0/1/1/1
1	5CR	p	301	1	-	3/9/10/12	0/1/1/1
1	GMA	B	8	1	-	1/9/9/9	-
1	GMA	BA	108	1	-	0/9/9/9	-
1	GMA	HA	108	1	-	0/9/9/9	-
1	5CR	HA	101	1	-	1/9/10/12	0/1/1/1
1	GMA	R	308	1	-	1/9/9/9	-
1	5CR	w	101	1	-	1/9/10/12	0/1/1/1
1	5CR	DA	301	1	-	4/9/10/12	0/1/1/1
1	GMA	H	8	1	-	1/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	GMA	c	8	1	-	8/9/9/9	-
1	GMA	k	108	1	-	3/9/9/9	-
1	5CR	FA	201	1	-	2/9/10/12	0/1/1/1
1	5CR	JA	301	1	-	4/9/10/12	0/1/1/1
1	5CR	X	301	1	-	3/9/10/12	0/1/1/1
1	GMA	g	8	1	-	8/9/9/9	-
1	GMA	U	308	1	-	1/9/9/9	-
1	5CR	b	1	1	-	6/9/10/12	0/1/1/1
1	5CR	2	101	1	-	1/9/10/12	0/1/1/1
1	5CR	q	101	1	-	2/9/10/12	0/1/1/1
1	GMA	t	108	1	-	0/9/9/9	-
1	GMA	0	208	1	-	4/9/9/9	-
1	GMA	IA	208	1	-	4/9/9/9	-
1	GMA	F	8	1	-	1/9/9/9	-
1	GMA	V	108	1	-	3/9/9/9	-
1	5CR	4	301	1	-	4/9/10/12	0/1/1/1
1	5CR	T	201	1	-	4/9/10/12	0/1/1/1
1	5CR	A	1	1	-	0/9/10/12	0/1/1/1
1	5CR	P	101	1	-	2/9/10/12	0/1/1/1
1	5CR	l	201	1	-	4/9/10/12	0/1/1/1
1	5CR	z	101	1	-	1/9/10/12	0/1/1/1
1	GMA	z	108	1	-	0/9/9/9	-
1	GMA	u	208	1	-	4/9/9/9	-
1	5CR	v	301	1	-	4/9/10/12	0/1/1/1
1	GMA	i	8	1	-	8/9/9/9	-
1	5CR	e	1	1	-	6/9/10/12	0/1/1/1
1	5CR	5	101	1	-	1/9/10/12	0/1/1/1
1	GMA	I	8	1	-	1/9/9/9	-
1	5CR	i	1	1	-	6/9/10/12	0/1/1/1
1	5CR	Z	201	1	-	4/9/10/12	0/1/1/1
1	5CR	D	1	1	-	0/9/10/12	0/1/1/1
1	5CR	Y	101	1	-	2/9/10/12	0/1/1/1
1	GMA	Y	108	1	-	3/9/9/9	-
1	5CR	h	1	1	-	6/9/10/12	0/1/1/1
1	GMA	AA	308	1	-	0/9/9/9	-
1	5CR	y	301	1	-	4/9/10/12	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5CR	F	1	1	-	0/9/10/12	0/1/1/1
1	GMA	Q	208	1	-	1/9/9/9	-
1	GMA	s	308	1	-	1/9/9/9	-
1	5CR	g	1	1	-	6/9/10/12	0/1/1/1
1	GMA	M	108	1	-	3/9/9/9	-
1	5CR	B	1	1	-	0/9/10/12	0/1/1/1
1	GMA	9	208	1	-	4/9/9/9	-
1	5CR	c	1	1	-	6/9/10/12	0/1/1/1
1	GMA	J	108	1	-	3/9/9/9	-
1	5CR	CA	201	1	-	2/9/10/12	0/1/1/1
1	5CR	k	101	1	-	2/9/10/12	0/1/1/1
1	5CR	n	101	1	-	2/9/10/12	0/1/1/1

All (162) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	e	1	5CR	CAL-N	3.49	1.46	1.34
1	a	1	5CR	CAL-N	3.48	1.46	1.34
1	i	1	5CR	CAL-N	3.47	1.46	1.34
1	f	1	5CR	CAL-N	3.47	1.46	1.34
1	h	1	5CR	CAL-N	3.47	1.46	1.34
1	d	1	5CR	CAL-N	3.47	1.46	1.34
1	b	1	5CR	CAL-N	3.46	1.46	1.34
1	c	1	5CR	CAL-N	3.46	1.46	1.34
1	g	1	5CR	CAL-N	3.45	1.46	1.34
1	Y	101	5CR	CAL-N	3.23	1.45	1.34
1	P	101	5CR	CAL-N	3.23	1.45	1.34
1	S	101	5CR	CAL-N	3.22	1.45	1.34
1	n	101	5CR	CAL-N	3.22	1.45	1.34
1	M	101	5CR	CAL-N	3.22	1.45	1.34
1	V	101	5CR	CAL-N	3.21	1.45	1.34
1	q	101	5CR	CAL-N	3.21	1.45	1.34
1	J	101	5CR	CAL-N	3.21	1.45	1.34
1	FA	201	5CR	CAL-N	3.21	1.45	1.34
1	6	201	5CR	CAL-N	3.21	1.45	1.34
1	k	101	5CR	CAL-N	3.21	1.45	1.34
1	7	301	5CR	CAL-N	3.20	1.45	1.34
1	4	301	5CR	CAL-N	3.19	1.45	1.34
1	GA	301	5CR	CAL-N	3.19	1.45	1.34
1	EA	101	5CR	CAL-N	3.19	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	JA	301	5CR	CAL-N	3.19	1.45	1.34
1	3	201	5CR	CAL-N	3.19	1.45	1.34
1	IA	201	5CR	CAL-N	3.19	1.45	1.34
1	2	101	5CR	CAL-N	3.19	1.45	1.34
1	CA	201	5CR	CAL-N	3.19	1.45	1.34
1	9	201	5CR	CAL-N	3.19	1.45	1.34
1	AA	301	5CR	CAL-N	3.19	1.45	1.34
1	DA	301	5CR	CAL-N	3.19	1.45	1.34
1	v	301	5CR	CAL-N	3.19	1.45	1.34
1	z	101	5CR	CAL-N	3.18	1.45	1.34
1	u	201	5CR	CAL-N	3.18	1.45	1.34
1	0	201	5CR	CAL-N	3.18	1.45	1.34
1	BA	101	5CR	CAL-N	3.18	1.45	1.34
1	1	301	5CR	CAL-N	3.18	1.45	1.34
1	y	301	5CR	CAL-N	3.18	1.45	1.34
1	HA	101	5CR	CAL-N	3.18	1.45	1.34
1	x	201	5CR	CAL-N	3.18	1.45	1.34
1	t	101	5CR	CAL-N	3.17	1.45	1.34
1	5	101	5CR	CAL-N	3.16	1.45	1.34
1	8	101	5CR	CAL-N	3.16	1.45	1.34
1	w	101	5CR	CAL-N	3.15	1.45	1.34
1	r	201	5CR	CAL-N	3.14	1.45	1.34
1	Q	201	5CR	CAL-N	3.14	1.45	1.34
1	N	201	5CR	CAL-N	3.14	1.45	1.34
1	T	201	5CR	CAL-N	3.13	1.45	1.34
1	K	201	5CR	CAL-N	3.13	1.45	1.34
1	l	201	5CR	CAL-N	3.12	1.45	1.34
1	W	201	5CR	CAL-N	3.12	1.45	1.34
1	o	201	5CR	CAL-N	3.12	1.45	1.34
1	Z	201	5CR	CAL-N	3.11	1.45	1.34
1	F	1	5CR	CAL-N	3.10	1.45	1.34
1	D	1	5CR	CAL-N	3.09	1.45	1.34
1	C	1	5CR	CAL-N	3.09	1.45	1.34
1	E	1	5CR	CAL-N	3.08	1.45	1.34
1	B	1	5CR	CAL-N	3.08	1.44	1.34
1	G	1	5CR	CAL-N	3.08	1.44	1.34
1	A	1	5CR	CAL-N	3.07	1.44	1.34
1	I	1	5CR	CAL-N	3.07	1.44	1.34
1	H	1	5CR	CAL-N	3.07	1.44	1.34
1	R	301	5CR	CAL-N	3.07	1.44	1.34
1	X	301	5CR	CAL-N	3.07	1.44	1.34
1	L	301	5CR	CAL-N	3.06	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	m	301	5CR	CAL-N	3.06	1.44	1.34
1	U	301	5CR	CAL-N	3.06	1.44	1.34
1	s	301	5CR	CAL-N	3.06	1.44	1.34
1	O	301	5CR	CAL-N	3.04	1.44	1.34
1	j	301	5CR	CAL-N	3.04	1.44	1.34
1	p	301	5CR	CAL-N	3.04	1.44	1.34
1	o	208	GMA	CD-N2	2.18	1.38	1.32
1	Q	208	GMA	CD-N2	2.17	1.38	1.32
1	l	208	GMA	CD-N2	2.16	1.38	1.32
1	N	208	GMA	CD-N2	2.15	1.38	1.32
1	W	208	GMA	CD-N2	2.15	1.38	1.32
1	Z	208	GMA	CD-N2	2.15	1.38	1.32
1	r	208	GMA	CD-N2	2.14	1.38	1.32
1	K	208	GMA	CD-N2	2.14	1.38	1.32
1	e	8	GMA	CD-N2	2.14	1.38	1.32
1	s	308	GMA	CD-N2	2.13	1.38	1.32
1	T	208	GMA	CD-N2	2.13	1.38	1.32
1	U	308	GMA	CD-N2	2.13	1.38	1.32
1	R	308	GMA	CD-N2	2.13	1.38	1.32
1	j	308	GMA	CD-N2	2.13	1.38	1.32
1	h	8	GMA	CD-N2	2.13	1.38	1.32
1	JA	308	GMA	CD-N2	2.12	1.38	1.32
1	X	308	GMA	CD-N2	2.12	1.38	1.32
1	l	308	GMA	CD-N2	2.12	1.38	1.32
1	u	208	GMA	CD-N2	2.12	1.38	1.32
1	O	308	GMA	CD-N2	2.12	1.38	1.32
1	g	8	GMA	CD-N2	2.12	1.38	1.32
1	i	8	GMA	CD-N2	2.12	1.38	1.32
1	c	8	GMA	CD-N2	2.11	1.38	1.32
1	DA	308	GMA	CD-N2	2.11	1.38	1.32
1	FA	208	GMA	CD-N2	2.11	1.38	1.32
1	d	8	GMA	CD-N2	2.11	1.38	1.32
1	f	8	GMA	CD-N2	2.11	1.38	1.32
1	p	308	GMA	CD-N2	2.11	1.38	1.32
1	b	8	GMA	CD-N2	2.11	1.38	1.32
1	L	308	GMA	CD-N2	2.10	1.38	1.32
1	v	308	GMA	CD-N2	2.10	1.38	1.32
1	0	208	GMA	CD-N2	2.10	1.38	1.32
1	CA	208	GMA	CD-N2	2.10	1.38	1.32
1	GA	308	GMA	CD-N2	2.10	1.38	1.32
1	4	308	GMA	CD-N2	2.10	1.38	1.32
1	IA	208	GMA	CD-N2	2.10	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	m	308	GMA	CD-N2	2.09	1.38	1.32
1	a	8	GMA	CD-N2	2.09	1.38	1.32
1	6	208	GMA	CD-N2	2.09	1.38	1.32
1	9	208	GMA	CD-N2	2.09	1.38	1.32
1	7	308	GMA	CD-N2	2.08	1.38	1.32
1	y	308	GMA	CD-N2	2.08	1.38	1.32
1	X	301	5CR	OAB-CAL	-2.08	1.18	1.23
1	s	301	5CR	OAB-CAL	-2.08	1.18	1.23
1	AA	308	GMA	CD-N2	2.08	1.38	1.32
1	m	301	5CR	OAB-CAL	-2.08	1.18	1.23
1	3	208	GMA	CD-N2	2.07	1.38	1.32
1	x	208	GMA	CD-N2	2.07	1.38	1.32
1	j	301	5CR	OAB-CAL	-2.07	1.18	1.23
1	I	8	GMA	CD-N2	2.06	1.38	1.32
1	R	301	5CR	OAB-CAL	-2.06	1.18	1.23
1	w	108	GMA	CD-N2	2.05	1.38	1.32
1	U	301	5CR	OAB-CAL	-2.05	1.18	1.23
1	B	8	GMA	CD-N2	2.05	1.38	1.32
1	L	301	5CR	OAB-CAL	-2.05	1.18	1.23
1	5	108	GMA	CD-N2	2.05	1.38	1.32
1	8	108	GMA	CD-N2	2.04	1.38	1.32
1	c	1	5CR	OAB-CAL	-2.04	1.18	1.23
1	O	301	5CR	OAB-CAL	-2.04	1.18	1.23
1	D	8	GMA	CD-N2	2.03	1.38	1.32
1	q	108	GMA	CD-N2	2.03	1.38	1.32
1	z	108	GMA	CD-N2	2.03	1.38	1.32
1	J	108	GMA	CD-N2	2.03	1.38	1.32
1	BA	108	GMA	CD-N2	2.03	1.38	1.32
1	S	108	GMA	CD-N2	2.03	1.38	1.32
1	p	301	5CR	OAB-CAL	-2.03	1.18	1.23
1	a	1	5CR	OAB-CAL	-2.03	1.18	1.23
1	C	8	GMA	CD-N2	2.03	1.38	1.32
1	2	108	GMA	CD-N2	2.03	1.38	1.32
1	t	108	GMA	CD-N2	2.03	1.38	1.32
1	EA	108	GMA	CD-N2	2.03	1.38	1.32
1	F	8	GMA	CD-N2	2.02	1.38	1.32
1	i	1	5CR	OAB-CAL	-2.02	1.18	1.23
1	HA	108	GMA	CD-N2	2.02	1.38	1.32
1	b	1	5CR	OAB-CAL	-2.02	1.18	1.23
1	Y	108	GMA	CD-N2	2.02	1.38	1.32
1	e	1	5CR	OAB-CAL	-2.02	1.18	1.23
1	f	1	5CR	OAB-CAL	-2.02	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	V	108	GMA	CD-N2	2.02	1.38	1.32
1	n	108	GMA	CD-N2	2.01	1.38	1.32
1	d	1	5CR	OAB-CAL	-2.01	1.18	1.23
1	M	108	GMA	CD-N2	2.01	1.38	1.32
1	k	108	GMA	CD-N2	2.01	1.38	1.32
1	E	1	5CR	OAB-CAL	-2.01	1.18	1.23
1	G	1	5CR	OAB-CAL	-2.00	1.18	1.23
1	B	1	5CR	OAB-CAL	-2.00	1.18	1.23
1	C	1	5CR	OAB-CAL	-2.00	1.18	1.23
1	Z	201	5CR	OAB-CAL	-2.00	1.18	1.23
1	Q	201	5CR	OAB-CAL	-2.00	1.18	1.23
1	I	1	5CR	OAB-CAL	-2.00	1.18	1.23

All (183) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	g	1	5CR	CAA-CAL-N	5.15	124.82	116.10
1	h	1	5CR	CAA-CAL-N	5.13	124.78	116.10
1	f	1	5CR	CAA-CAL-N	5.12	124.77	116.10
1	b	1	5CR	CAA-CAL-N	5.12	124.77	116.10
1	d	1	5CR	CAA-CAL-N	5.12	124.77	116.10
1	a	1	5CR	CAA-CAL-N	5.12	124.76	116.10
1	i	1	5CR	CAA-CAL-N	5.12	124.76	116.10
1	e	1	5CR	CAA-CAL-N	5.11	124.75	116.10
1	c	1	5CR	CAA-CAL-N	5.10	124.73	116.10
1	B	1	5CR	CG-CB-CA	-4.77	106.81	113.63
1	E	1	5CR	CG-CB-CA	-4.76	106.82	113.63
1	I	1	5CR	CG-CB-CA	-4.76	106.82	113.63
1	C	1	5CR	CG-CB-CA	-4.75	106.84	113.63
1	A	1	5CR	CG-CB-CA	-4.74	106.84	113.63
1	G	1	5CR	CG-CB-CA	-4.74	106.84	113.63
1	F	1	5CR	CG-CB-CA	-4.74	106.84	113.63
1	D	1	5CR	CG-CB-CA	-4.72	106.87	113.63
1	H	1	5CR	CG-CB-CA	-4.70	106.90	113.63
1	M	101	5CR	CG-CB-CA	-4.53	107.15	113.63
1	Y	101	5CR	CG-CB-CA	-4.52	107.16	113.63
1	k	101	5CR	CG-CB-CA	-4.51	107.17	113.63
1	V	101	5CR	CG-CB-CA	-4.51	107.17	113.63
1	q	101	5CR	CG-CB-CA	-4.50	107.19	113.63
1	n	101	5CR	CG-CB-CA	-4.50	107.19	113.63
1	P	101	5CR	CG-CB-CA	-4.49	107.21	113.63
1	S	101	5CR	CG-CB-CA	-4.49	107.21	113.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	101	5CR	CG-CB-CA	-4.46	107.25	113.63
1	u	201	5CR	CG-CB-CA	-2.95	109.41	113.63
1	l	201	5CR	CAA-CAL-N	2.94	121.08	116.10
1	0	201	5CR	CG-CB-CA	-2.93	109.44	113.63
1	Q	201	5CR	CAA-CAL-N	2.93	121.06	116.10
1	W	201	5CR	CAA-CAL-N	2.93	121.06	116.10
1	6	201	5CR	CG-CB-CA	-2.93	109.44	113.63
1	N	201	5CR	CAA-CAL-N	2.93	121.06	116.10
1	IA	201	5CR	CG-CB-CA	-2.93	109.44	113.63
1	r	201	5CR	CAA-CAL-N	2.93	121.06	116.10
1	CA	201	5CR	CG-CB-CA	-2.93	109.44	113.63
1	K	201	5CR	CAA-CAL-N	2.92	121.04	116.10
1	T	201	5CR	CAA-CAL-N	2.92	121.03	116.10
1	o	201	5CR	CAA-CAL-N	2.92	121.03	116.10
1	x	201	5CR	CG-CB-CA	-2.92	109.46	113.63
1	3	201	5CR	CG-CB-CA	-2.91	109.47	113.63
1	9	201	5CR	CG-CB-CA	-2.91	109.47	113.63
1	Z	201	5CR	CAA-CAL-N	2.90	121.01	116.10
1	FA	201	5CR	CG-CB-CA	-2.90	109.48	113.63
1	G	1	5CR	CA-N-CAL	-2.73	118.11	123.15
1	B	1	5CR	CA-N-CAL	-2.72	118.12	123.15
1	I	1	5CR	CA-N-CAL	-2.72	118.12	123.15
1	F	1	5CR	CA-N-CAL	-2.72	118.13	123.15
1	C	1	5CR	CA-N-CAL	-2.71	118.15	123.15
1	H	1	5CR	CA-N-CAL	-2.71	118.16	123.15
1	EA	101	5CR	CA-N-CAL	-2.71	118.16	123.15
1	A	1	5CR	CA-N-CAL	-2.71	118.16	123.15
1	E	1	5CR	CA-N-CAL	-2.70	118.16	123.15
1	D	1	5CR	CA-N-CAL	-2.70	118.17	123.15
1	w	101	5CR	CA-N-CAL	-2.69	118.19	123.15
1	2	101	5CR	CA-N-CAL	-2.69	118.19	123.15
1	8	101	5CR	CA-N-CAL	-2.69	118.19	123.15
1	z	101	5CR	CA-N-CAL	-2.68	118.20	123.15
1	t	101	5CR	CA-N-CAL	-2.68	118.20	123.15
1	5	101	5CR	CA-N-CAL	-2.68	118.20	123.15
1	HA	101	5CR	CA-N-CAL	-2.68	118.21	123.15
1	BA	101	5CR	CA-N-CAL	-2.66	118.24	123.15
1	F	1	5CR	CAA-CAL-N	2.64	120.57	116.10
1	I	1	5CR	CAA-CAL-N	2.63	120.55	116.10
1	B	1	5CR	CAA-CAL-N	2.62	120.54	116.10
1	A	1	5CR	CAA-CAL-N	2.62	120.54	116.10
1	D	1	5CR	CAA-CAL-N	2.62	120.54	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	1	5CR	CAA-CAL-N	2.61	120.53	116.10
1	E	1	5CR	CAA-CAL-N	2.61	120.52	116.10
1	C	1	5CR	CAA-CAL-N	2.61	120.52	116.10
1	G	1	5CR	CAA-CAL-N	2.60	120.50	116.10
1	z	101	5CR	CAA-CAL-N	2.51	120.35	116.10
1	5	101	5CR	CAA-CAL-N	2.51	120.35	116.10
1	HA	101	5CR	CAA-CAL-N	2.51	120.34	116.10
1	w	101	5CR	CAA-CAL-N	2.50	120.34	116.10
1	BA	101	5CR	CAA-CAL-N	2.50	120.33	116.10
1	2	101	5CR	CAA-CAL-N	2.50	120.33	116.10
1	8	101	5CR	CAA-CAL-N	2.49	120.32	116.10
1	t	101	5CR	CAA-CAL-N	2.49	120.32	116.10
1	EA	101	5CR	CAA-CAL-N	2.48	120.30	116.10
1	a	1	5CR	OAB-CAL-N	-2.41	117.53	121.95
1	g	1	5CR	OAB-CAL-CAA	-2.39	117.61	122.06
1	d	1	5CR	OAB-CAL-N	-2.39	117.56	121.95
1	f	1	5CR	OAB-CAL-N	-2.39	117.56	121.95
1	b	1	5CR	OAB-CAL-CAA	-2.38	117.63	122.06
1	g	1	5CR	OAB-CAL-N	-2.38	117.57	121.95
1	e	1	5CR	OAB-CAL-N	-2.38	117.57	121.95
1	h	1	5CR	OAB-CAL-N	-2.38	117.57	121.95
1	c	1	5CR	OAB-CAL-CAA	-2.38	117.64	122.06
1	i	1	5CR	OAB-CAL-N	-2.38	117.58	121.95
1	W	201	5CR	CG-CB-CA	-2.38	110.23	113.63
1	Q	201	5CR	CG-CB-CA	-2.38	110.23	113.63
1	T	201	5CR	CG-CB-CA	-2.38	110.23	113.63
1	h	1	5CR	OAB-CAL-CAA	-2.38	117.64	122.06
1	K	201	5CR	CG-CB-CA	-2.37	110.24	113.63
1	i	1	5CR	OAB-CAL-CAA	-2.37	117.66	122.06
1	b	1	5CR	OAB-CAL-N	-2.37	117.60	121.95
1	Z	201	5CR	CG-CB-CA	-2.36	110.25	113.63
1	f	1	5CR	OAB-CAL-CAA	-2.36	117.67	122.06
1	d	1	5CR	OAB-CAL-CAA	-2.36	117.67	122.06
1	N	201	5CR	CG-CB-CA	-2.36	110.25	113.63
1	r	201	5CR	CG-CB-CA	-2.36	110.26	113.63
1	e	1	5CR	OAB-CAL-CAA	-2.35	117.68	122.06
1	c	1	5CR	OAB-CAL-N	-2.35	117.63	121.95
1	o	201	5CR	CG-CB-CA	-2.34	110.28	113.63
1	a	1	5CR	OAB-CAL-CAA	-2.34	117.71	122.06
1	l	201	5CR	CG-CB-CA	-2.33	110.30	113.63
1	j	301	5CR	CA-N-CAL	-2.27	118.96	123.15
1	U	301	5CR	CA-N-CAL	-2.27	118.97	123.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	301	5CR	CA-N-CAL	-2.25	118.99	123.15
1	m	301	5CR	CA-N-CAL	-2.25	119.00	123.15
1	s	301	5CR	CA-N-CAL	-2.25	119.00	123.15
1	R	301	5CR	CA-N-CAL	-2.24	119.01	123.15
1	p	301	5CR	CA-N-CAL	-2.24	119.01	123.15
1	O	301	5CR	CAA-CAL-N	2.24	119.90	116.10
1	X	301	5CR	CA-N-CAL	-2.24	119.02	123.15
1	p	301	5CR	CAA-CAL-N	2.24	119.89	116.10
1	O	301	5CR	CA-N-CAL	-2.23	119.03	123.15
1	j	301	5CR	CAA-CAL-N	2.23	119.88	116.10
1	L	301	5CR	CAA-CAL-N	2.23	119.88	116.10
1	R	301	5CR	CAA-CAL-N	2.22	119.87	116.10
1	JA	301	5CR	CAA-CAL-N	2.22	119.86	116.10
1	m	301	5CR	CAA-CAL-N	2.22	119.86	116.10
1	DA	301	5CR	CAA-CAL-N	2.22	119.86	116.10
1	y	301	5CR	CAA-CAL-N	2.22	119.86	116.10
1	AA	301	5CR	CAA-CAL-N	2.22	119.85	116.10
1	U	301	5CR	CAA-CAL-N	2.21	119.85	116.10
1	s	301	5CR	CAA-CAL-N	2.21	119.84	116.10
1	4	301	5CR	CAA-CAL-N	2.21	119.84	116.10
1	1	301	5CR	CAA-CAL-N	2.21	119.84	116.10
1	v	301	5CR	CAA-CAL-N	2.21	119.84	116.10
1	j	301	5CR	O-C-CA	-2.21	119.00	124.78
1	7	301	5CR	CAA-CAL-N	2.20	119.83	116.10
1	X	301	5CR	CAA-CAL-N	2.20	119.83	116.10
1	U	301	5CR	O-C-CA	-2.20	119.01	124.78
1	GA	301	5CR	CAA-CAL-N	2.20	119.82	116.10
1	m	301	5CR	O-C-CA	-2.20	119.03	124.78
1	R	301	5CR	O-C-CA	-2.19	119.03	124.78
1	X	301	5CR	O-C-CA	-2.19	119.04	124.78
1	s	301	5CR	O-C-CA	-2.18	119.05	124.78
1	L	301	5CR	O-C-CA	-2.18	119.07	124.78
1	p	301	5CR	O-C-CA	-2.18	119.08	124.78
1	O	301	5CR	O-C-CA	-2.17	119.09	124.78
1	P	101	5CR	CAA-CAL-N	2.13	119.70	116.10
1	c	1	5CR	CA-N-CAL	2.12	127.06	123.15
1	b	1	5CR	CA-N-CAL	2.12	127.06	123.15
1	f	1	5CR	CA-N-CAL	2.11	127.04	123.15
1	J	101	5CR	CAA-CAL-N	2.11	119.67	116.10
1	d	1	5CR	CA-N-CAL	2.11	127.04	123.15
1	e	1	5CR	CA-N-CAL	2.11	127.03	123.15
1	g	1	5CR	CA-N-CAL	2.10	127.03	123.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	i	1	5CR	CA-N-CAL	2.10	127.03	123.15
1	M	101	5CR	CAA-CAL-N	2.10	119.66	116.10
1	S	101	5CR	CAA-CAL-N	2.10	119.65	116.10
1	a	1	5CR	CA-N-CAL	2.10	127.02	123.15
1	V	101	5CR	CAA-CAL-N	2.10	119.65	116.10
1	Y	101	5CR	CAA-CAL-N	2.09	119.63	116.10
1	h	1	5CR	CA-N-CAL	2.09	127.00	123.15
1	k	101	5CR	CAA-CAL-N	2.08	119.62	116.10
1	n	101	5CR	CAA-CAL-N	2.07	119.61	116.10
1	o	208	GMA	O1-CD-CA	2.07	123.33	120.30
1	q	101	5CR	CAA-CAL-N	2.07	119.60	116.10
1	Q	208	GMA	O1-CD-CA	2.06	123.31	120.30
1	l	208	GMA	O1-CD-CA	2.06	123.31	120.30
1	Q	208	GMA	O1-CD-N2	-2.04	119.45	123.00
1	N	208	GMA	O1-CD-CA	2.04	123.29	120.30
1	Z	208	GMA	O1-CD-CA	2.04	123.29	120.30
1	W	208	GMA	O1-CD-CA	2.03	123.28	120.30
1	r	208	GMA	O1-CD-CA	2.03	123.28	120.30
1	Y	108	GMA	O1-CD-CA	2.03	123.28	120.30
1	o	208	GMA	O1-CD-N2	-2.03	119.48	123.00
1	l	208	GMA	O1-CD-N2	-2.01	119.50	123.00
1	J	108	GMA	O1-CD-CA	2.01	123.25	120.30
1	B	8	GMA	O1-CD-CA	2.01	123.25	120.30
1	r	208	GMA	O1-CD-N2	-2.01	119.51	123.00
1	T	208	GMA	O1-CD-CA	2.01	123.24	120.30
1	K	208	GMA	O1-CD-CA	2.00	123.24	120.30
1	S	108	GMA	O1-CD-CA	2.00	123.24	120.30
1	k	108	GMA	O1-CD-CA	2.00	123.23	120.30
1	q	108	GMA	O1-CD-CA	2.00	123.23	120.30
1	Z	208	GMA	O1-CD-N2	-2.00	119.52	123.00
1	n	108	GMA	O1-CD-CA	2.00	123.23	120.30

There are no chirality outliers.

All (360) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	J	101	5CR	C-CA-N-CAL
1	J	101	5CR	N-CA-CB-CG
1	K	201	5CR	N-CA-CB-CG
1	L	301	5CR	N-CA-CB-CG
1	L	301	5CR	C-CA-CB-CG
1	M	101	5CR	C-CA-N-CAL

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Mol	Chain	Res	Type	Atoms
1	M	101	5CR	N-CA-CB-CG
1	N	201	5CR	N-CA-CB-CG
1	O	301	5CR	N-CA-CB-CG
1	O	301	5CR	C-CA-CB-CG
1	P	101	5CR	C-CA-N-CAL
1	P	101	5CR	N-CA-CB-CG
1	Q	201	5CR	N-CA-CB-CG
1	R	301	5CR	N-CA-CB-CG
1	R	301	5CR	C-CA-CB-CG
1	S	101	5CR	C-CA-N-CAL
1	S	101	5CR	N-CA-CB-CG
1	T	201	5CR	N-CA-CB-CG
1	U	301	5CR	N-CA-CB-CG
1	U	301	5CR	C-CA-CB-CG
1	V	101	5CR	C-CA-N-CAL
1	V	101	5CR	N-CA-CB-CG
1	W	201	5CR	N-CA-CB-CG
1	X	301	5CR	N-CA-CB-CG
1	X	301	5CR	C-CA-CB-CG
1	Y	101	5CR	C-CA-N-CAL
1	Y	101	5CR	N-CA-CB-CG
1	Z	201	5CR	N-CA-CB-CG
1	j	301	5CR	N-CA-CB-CG
1	j	301	5CR	C-CA-CB-CG
1	k	101	5CR	C-CA-N-CAL
1	k	101	5CR	N-CA-CB-CG
1	l	201	5CR	N-CA-CB-CG
1	m	301	5CR	N-CA-CB-CG
1	m	301	5CR	C-CA-CB-CG
1	n	101	5CR	C-CA-N-CAL
1	n	101	5CR	N-CA-CB-CG
1	o	201	5CR	N-CA-CB-CG
1	p	301	5CR	N-CA-CB-CG
1	p	301	5CR	C-CA-CB-CG
1	q	101	5CR	C-CA-N-CAL
1	q	101	5CR	N-CA-CB-CG
1	r	201	5CR	N-CA-CB-CG
1	s	301	5CR	N-CA-CB-CG
1	s	301	5CR	C-CA-CB-CG
1	a	1	5CR	C-CA-CB-CG
1	u	201	5CR	C-CA-N-CAL
1	b	1	5CR	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
1	x	201	5CR	C-CA-N-CAL
1	c	1	5CR	C-CA-CB-CG
1	0	201	5CR	C-CA-N-CAL
1	d	1	5CR	C-CA-CB-CG
1	3	201	5CR	C-CA-N-CAL
1	e	1	5CR	C-CA-CB-CG
1	6	201	5CR	C-CA-N-CAL
1	f	1	5CR	C-CA-CB-CG
1	9	201	5CR	C-CA-N-CAL
1	g	1	5CR	C-CA-CB-CG
1	CA	201	5CR	C-CA-N-CAL
1	h	1	5CR	C-CA-CB-CG
1	FA	201	5CR	C-CA-N-CAL
1	i	1	5CR	C-CA-CB-CG
1	IA	201	5CR	C-CA-N-CAL
1	A	8	GMA	N-CA-CD-N2
1	B	8	GMA	N-CA-CD-N2
1	C	8	GMA	N-CA-CD-N2
1	D	8	GMA	N-CA-CD-N2
1	E	8	GMA	N-CA-CD-N2
1	F	8	GMA	N-CA-CD-N2
1	G	8	GMA	N-CA-CD-N2
1	H	8	GMA	N-CA-CD-N2
1	I	8	GMA	N-CA-CD-N2
1	a	8	GMA	N-CA-CB-CG
1	a	8	GMA	CD-CA-CB-CG
1	u	208	GMA	N-CA-CB-CG
1	u	208	GMA	CD-CA-CB-CG
1	b	8	GMA	N-CA-CB-CG
1	b	8	GMA	CD-CA-CB-CG
1	x	208	GMA	N-CA-CB-CG
1	x	208	GMA	CD-CA-CB-CG
1	c	8	GMA	N-CA-CB-CG
1	c	8	GMA	CD-CA-CB-CG
1	0	208	GMA	N-CA-CB-CG
1	0	208	GMA	CD-CA-CB-CG
1	d	8	GMA	N-CA-CB-CG
1	d	8	GMA	CD-CA-CB-CG
1	3	208	GMA	N-CA-CB-CG
1	3	208	GMA	CD-CA-CB-CG
1	e	8	GMA	N-CA-CB-CG
1	e	8	GMA	CD-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
1	6	208	GMA	N-CA-CB-CG
1	6	208	GMA	CD-CA-CB-CG
1	f	8	GMA	N-CA-CB-CG
1	f	8	GMA	CD-CA-CB-CG
1	9	208	GMA	N-CA-CB-CG
1	9	208	GMA	CD-CA-CB-CG
1	g	8	GMA	N-CA-CB-CG
1	g	8	GMA	CD-CA-CB-CG
1	CA	208	GMA	N-CA-CB-CG
1	CA	208	GMA	CD-CA-CB-CG
1	h	8	GMA	N-CA-CB-CG
1	h	8	GMA	CD-CA-CB-CG
1	FA	208	GMA	N-CA-CB-CG
1	FA	208	GMA	CD-CA-CB-CG
1	i	8	GMA	N-CA-CB-CG
1	i	8	GMA	CD-CA-CB-CG
1	IA	208	GMA	N-CA-CB-CG
1	IA	208	GMA	CD-CA-CB-CG
1	K	201	5CR	CAA-CAL-N-CA
1	K	201	5CR	OAB-CAL-N-CA
1	N	201	5CR	CAA-CAL-N-CA
1	N	201	5CR	OAB-CAL-N-CA
1	Q	201	5CR	CAA-CAL-N-CA
1	Q	201	5CR	OAB-CAL-N-CA
1	T	201	5CR	CAA-CAL-N-CA
1	T	201	5CR	OAB-CAL-N-CA
1	W	201	5CR	CAA-CAL-N-CA
1	W	201	5CR	OAB-CAL-N-CA
1	Z	201	5CR	CAA-CAL-N-CA
1	Z	201	5CR	OAB-CAL-N-CA
1	l	201	5CR	CAA-CAL-N-CA
1	l	201	5CR	OAB-CAL-N-CA
1	o	201	5CR	CAA-CAL-N-CA
1	o	201	5CR	OAB-CAL-N-CA
1	r	201	5CR	CAA-CAL-N-CA
1	r	201	5CR	OAB-CAL-N-CA
1	a	1	5CR	CAA-CAL-N-CA
1	a	1	5CR	OAB-CAL-N-CA
1	b	1	5CR	CAA-CAL-N-CA
1	b	1	5CR	OAB-CAL-N-CA
1	c	1	5CR	CAA-CAL-N-CA
1	c	1	5CR	OAB-CAL-N-CA

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Mol	Chain	Res	Type	Atoms
1	d	1	5CR	CAA-CAL-N-CA
1	d	1	5CR	OAB-CAL-N-CA
1	e	1	5CR	CAA-CAL-N-CA
1	e	1	5CR	OAB-CAL-N-CA
1	f	1	5CR	CAA-CAL-N-CA
1	f	1	5CR	OAB-CAL-N-CA
1	g	1	5CR	CAA-CAL-N-CA
1	g	1	5CR	OAB-CAL-N-CA
1	h	1	5CR	CAA-CAL-N-CA
1	h	1	5CR	OAB-CAL-N-CA
1	i	1	5CR	CAA-CAL-N-CA
1	i	1	5CR	OAB-CAL-N-CA
1	K	208	GMA	CA-CB-CG-C
1	L	308	GMA	CA-CB-CG-C
1	N	208	GMA	CA-CB-CG-C
1	O	308	GMA	CA-CB-CG-C
1	Q	208	GMA	CA-CB-CG-C
1	R	308	GMA	CA-CB-CG-C
1	T	208	GMA	CA-CB-CG-C
1	U	308	GMA	CA-CB-CG-C
1	W	208	GMA	CA-CB-CG-C
1	X	308	GMA	CA-CB-CG-C
1	Z	208	GMA	CA-CB-CG-C
1	j	308	GMA	CA-CB-CG-C
1	l	208	GMA	CA-CB-CG-C
1	m	308	GMA	CA-CB-CG-C
1	o	208	GMA	CA-CB-CG-C
1	p	308	GMA	CA-CB-CG-C
1	r	208	GMA	CA-CB-CG-C
1	s	308	GMA	CA-CB-CG-C
1	a	8	GMA	N-CA-CD-O1
1	b	8	GMA	N-CA-CD-O1
1	c	8	GMA	N-CA-CD-O1
1	d	8	GMA	N-CA-CD-O1
1	e	8	GMA	N-CA-CD-O1
1	f	8	GMA	N-CA-CD-O1
1	g	8	GMA	N-CA-CD-O1
1	h	8	GMA	N-CA-CD-O1
1	i	8	GMA	N-CA-CD-O1
1	y	301	5CR	CA-CB-CG-CD2
1	4	301	5CR	CA-CB-CG-CD2
1	7	301	5CR	CA-CB-CG-CD2

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Mol	Chain	Res	Type	Atoms
1	AA	301	5CR	CA-CB-CG-CD2
1	DA	301	5CR	CA-CB-CG-CD2
1	JA	301	5CR	CA-CB-CG-CD2
1	v	301	5CR	CA-CB-CG-CD1
1	v	301	5CR	CA-CB-CG-CD2
1	y	301	5CR	CA-CB-CG-CD1
1	1	301	5CR	CA-CB-CG-CD1
1	4	301	5CR	CA-CB-CG-CD1
1	7	301	5CR	CA-CB-CG-CD1
1	AA	301	5CR	CA-CB-CG-CD1
1	DA	301	5CR	CA-CB-CG-CD1
1	GA	301	5CR	CA-CB-CG-CD1
1	GA	301	5CR	CA-CB-CG-CD2
1	JA	301	5CR	CA-CB-CG-CD1
1	1	301	5CR	CA-CB-CG-CD2
1	L	301	5CR	C-CA-N-CAL
1	O	301	5CR	C-CA-N-CAL
1	R	301	5CR	C-CA-N-CAL
1	U	301	5CR	C-CA-N-CAL
1	X	301	5CR	C-CA-N-CAL
1	j	301	5CR	C-CA-N-CAL
1	m	301	5CR	C-CA-N-CAL
1	p	301	5CR	C-CA-N-CAL
1	s	301	5CR	C-CA-N-CAL
1	a	1	5CR	CB-CA-N-CAL
1	v	301	5CR	CB-CA-N-CAL
1	b	1	5CR	CB-CA-N-CAL
1	y	301	5CR	CB-CA-N-CAL
1	c	1	5CR	CB-CA-N-CAL
1	1	301	5CR	CB-CA-N-CAL
1	d	1	5CR	CB-CA-N-CAL
1	4	301	5CR	CB-CA-N-CAL
1	e	1	5CR	CB-CA-N-CAL
1	7	301	5CR	CB-CA-N-CAL
1	f	1	5CR	CB-CA-N-CAL
1	AA	301	5CR	CB-CA-N-CAL
1	g	1	5CR	CB-CA-N-CAL
1	DA	301	5CR	CB-CA-N-CAL
1	h	1	5CR	CB-CA-N-CAL
1	GA	301	5CR	CB-CA-N-CAL
1	i	1	5CR	CB-CA-N-CAL
1	JA	301	5CR	CB-CA-N-CAL

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Mol	Chain	Res	Type	Atoms
1	J	108	GMA	N-CA-CB-CG
1	M	108	GMA	N-CA-CB-CG
1	P	108	GMA	N-CA-CB-CG
1	S	108	GMA	N-CA-CB-CG
1	V	108	GMA	N-CA-CB-CG
1	Y	108	GMA	N-CA-CB-CG
1	k	108	GMA	N-CA-CB-CG
1	n	108	GMA	N-CA-CB-CG
1	q	108	GMA	N-CA-CB-CG
1	a	8	GMA	CB-CA-CD-O1
1	a	8	GMA	CB-CA-CD-N2
1	b	8	GMA	CB-CA-CD-O1
1	b	8	GMA	CB-CA-CD-N2
1	c	8	GMA	CB-CA-CD-O1
1	c	8	GMA	CB-CA-CD-N2
1	d	8	GMA	CB-CA-CD-O1
1	d	8	GMA	CB-CA-CD-N2
1	e	8	GMA	CB-CA-CD-O1
1	e	8	GMA	CB-CA-CD-N2
1	f	8	GMA	CB-CA-CD-O1
1	f	8	GMA	CB-CA-CD-N2
1	g	8	GMA	CB-CA-CD-O1
1	g	8	GMA	CB-CA-CD-N2
1	h	8	GMA	CB-CA-CD-O1
1	h	8	GMA	CB-CA-CD-N2
1	i	8	GMA	CB-CA-CD-O1
1	i	8	GMA	CB-CA-CD-N2
1	a	8	GMA	CA-CB-CG-C
1	b	8	GMA	CA-CB-CG-C
1	c	8	GMA	CA-CB-CG-C
1	d	8	GMA	CA-CB-CG-C
1	e	8	GMA	CA-CB-CG-C
1	f	8	GMA	CA-CB-CG-C
1	g	8	GMA	CA-CB-CG-C
1	h	8	GMA	CA-CB-CG-C
1	i	8	GMA	CA-CB-CG-C
1	J	108	GMA	CD-CA-CB-CG
1	M	108	GMA	CD-CA-CB-CG
1	P	108	GMA	CD-CA-CB-CG
1	S	108	GMA	CD-CA-CB-CG
1	V	108	GMA	CD-CA-CB-CG
1	Y	108	GMA	CD-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
1	k	108	GMA	CD-CA-CB-CG
1	n	108	GMA	CD-CA-CB-CG
1	q	108	GMA	CD-CA-CB-CG
1	a	8	GMA	O-C-CG-CB
1	b	8	GMA	O-C-CG-CB
1	d	8	GMA	O-C-CG-CB
1	f	8	GMA	O-C-CG-CB
1	g	8	GMA	O-C-CG-CB
1	i	8	GMA	O-C-CG-CB
1	c	8	GMA	O-C-CG-CB
1	e	8	GMA	O-C-CG-CB
1	h	8	GMA	O-C-CG-CB
1	a	8	GMA	OXT-C-CG-CB
1	b	8	GMA	OXT-C-CG-CB
1	c	8	GMA	OXT-C-CG-CB
1	d	8	GMA	OXT-C-CG-CB
1	e	8	GMA	OXT-C-CG-CB
1	f	8	GMA	OXT-C-CG-CB
1	g	8	GMA	OXT-C-CG-CB
1	h	8	GMA	OXT-C-CG-CB
1	i	8	GMA	OXT-C-CG-CB
1	a	1	5CR	N-CA-CB-CG
1	b	1	5CR	N-CA-CB-CG
1	c	1	5CR	N-CA-CB-CG
1	d	1	5CR	N-CA-CB-CG
1	e	1	5CR	N-CA-CB-CG
1	f	1	5CR	N-CA-CB-CG
1	g	1	5CR	N-CA-CB-CG
1	h	1	5CR	N-CA-CB-CG
1	i	1	5CR	N-CA-CB-CG
1	J	108	GMA	CA-CB-CG-C
1	M	108	GMA	CA-CB-CG-C
1	P	108	GMA	CA-CB-CG-C
1	S	108	GMA	CA-CB-CG-C
1	V	108	GMA	CA-CB-CG-C
1	Y	108	GMA	CA-CB-CG-C
1	k	108	GMA	CA-CB-CG-C
1	n	108	GMA	CA-CB-CG-C
1	q	108	GMA	CA-CB-CG-C
1	a	1	5CR	C-CA-N-CAL
1	t	101	5CR	C-CA-N-CAL
1	v	301	5CR	C-CA-N-CAL

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Mol	Chain	Res	Type	Atoms
1	b	1	5CR	C-CA-N-CAL
1	w	101	5CR	C-CA-N-CAL
1	y	301	5CR	C-CA-N-CAL
1	c	1	5CR	C-CA-N-CAL
1	z	101	5CR	C-CA-N-CAL
1	1	301	5CR	C-CA-N-CAL
1	d	1	5CR	C-CA-N-CAL
1	2	101	5CR	C-CA-N-CAL
1	4	301	5CR	C-CA-N-CAL
1	e	1	5CR	C-CA-N-CAL
1	5	101	5CR	C-CA-N-CAL
1	7	301	5CR	C-CA-N-CAL
1	f	1	5CR	C-CA-N-CAL
1	8	101	5CR	C-CA-N-CAL
1	AA	301	5CR	C-CA-N-CAL
1	g	1	5CR	C-CA-N-CAL
1	BA	101	5CR	C-CA-N-CAL
1	DA	301	5CR	C-CA-N-CAL
1	h	1	5CR	C-CA-N-CAL
1	EA	101	5CR	C-CA-N-CAL
1	GA	301	5CR	C-CA-N-CAL
1	i	1	5CR	C-CA-N-CAL
1	HA	101	5CR	C-CA-N-CAL
1	JA	301	5CR	C-CA-N-CAL
1	3	208	GMA	OXT-C-CG-CB
1	u	208	GMA	OXT-C-CG-CB
1	x	208	GMA	OXT-C-CG-CB
1	0	208	GMA	OXT-C-CG-CB
1	6	208	GMA	OXT-C-CG-CB
1	K	201	5CR	C-CA-CB-CG
1	N	201	5CR	C-CA-CB-CG
1	Q	201	5CR	C-CA-CB-CG
1	T	201	5CR	C-CA-CB-CG
1	W	201	5CR	C-CA-CB-CG
1	Z	201	5CR	C-CA-CB-CG
1	l	201	5CR	C-CA-CB-CG
1	o	201	5CR	C-CA-CB-CG
1	r	201	5CR	C-CA-CB-CG
1	9	208	GMA	OXT-C-CG-CB
1	FA	208	GMA	OXT-C-CG-CB
1	IA	208	GMA	OXT-C-CG-CB
1	0	208	GMA	O-C-CG-CB

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Mol	Chain	Res	Type	Atoms
1	3	208	GMA	O-C-CG-CB
1	9	208	GMA	O-C-CG-CB
1	CA	208	GMA	O-C-CG-CB
1	CA	208	GMA	OXT-C-CG-CB
1	FA	208	GMA	O-C-CG-CB
1	IA	208	GMA	O-C-CG-CB
1	u	201	5CR	CB-CA-N-CAL
1	x	201	5CR	CB-CA-N-CAL
1	0	201	5CR	CB-CA-N-CAL
1	3	201	5CR	CB-CA-N-CAL
1	6	201	5CR	CB-CA-N-CAL
1	9	201	5CR	CB-CA-N-CAL
1	CA	201	5CR	CB-CA-N-CAL
1	FA	201	5CR	CB-CA-N-CAL
1	IA	201	5CR	CB-CA-N-CAL
1	u	208	GMA	O-C-CG-CB
1	x	208	GMA	O-C-CG-CB
1	6	208	GMA	O-C-CG-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides 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.

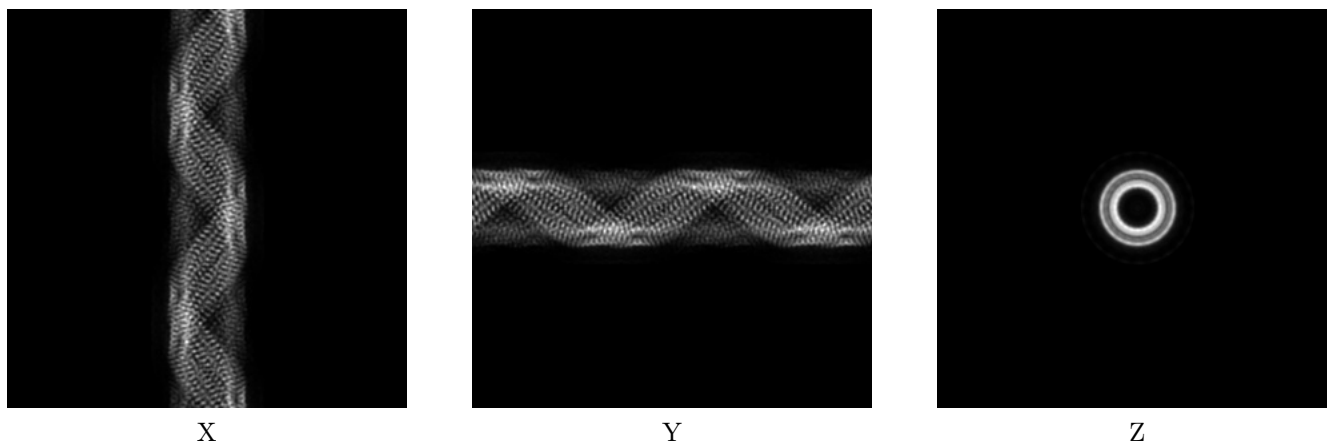
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23483. 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](#)

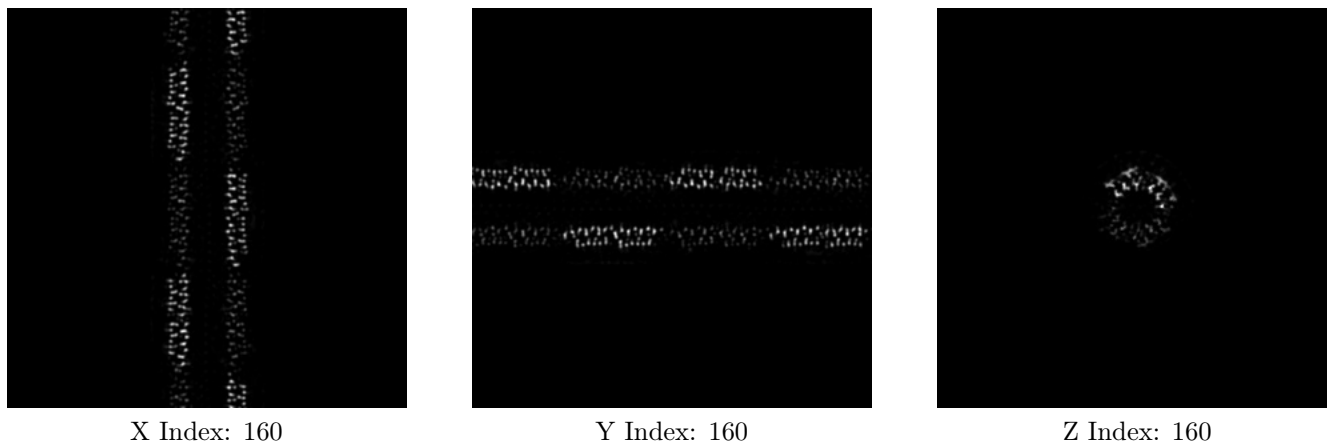
6.1.1 Primary map



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

6.2 Central slices [i](#)

6.2.1 Primary map



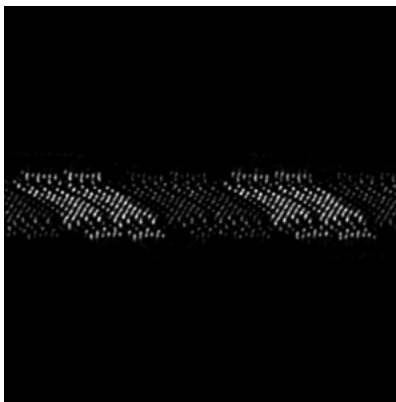
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

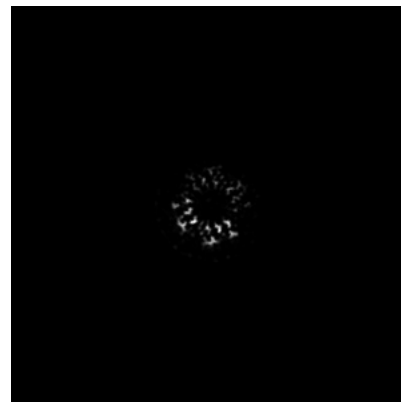
6.3.1 Primary map



X Index: 177



Y Index: 143

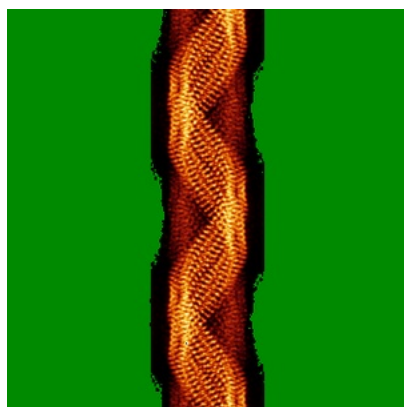


Z Index: 83

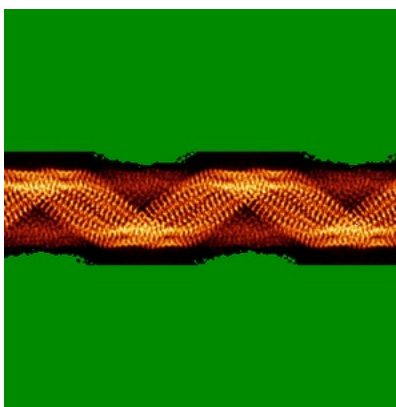
The images above show the largest variance slices of the map in three orthogonal directions.

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

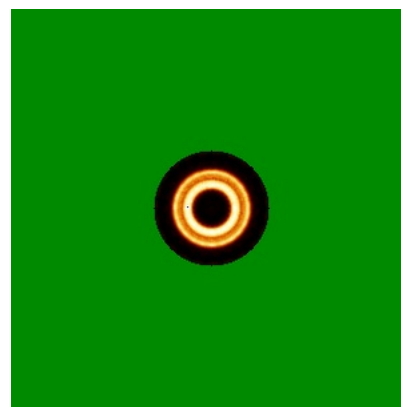
6.4.1 Primary map



X



Y

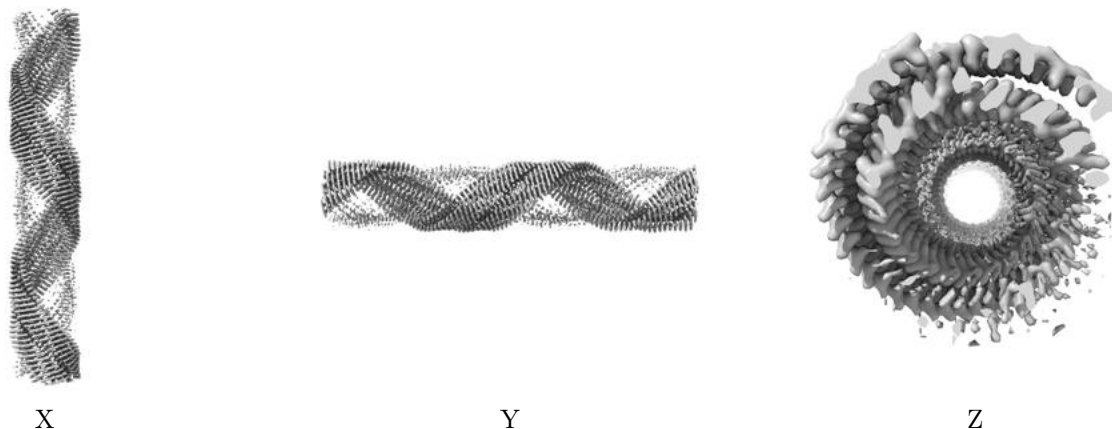


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.264. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

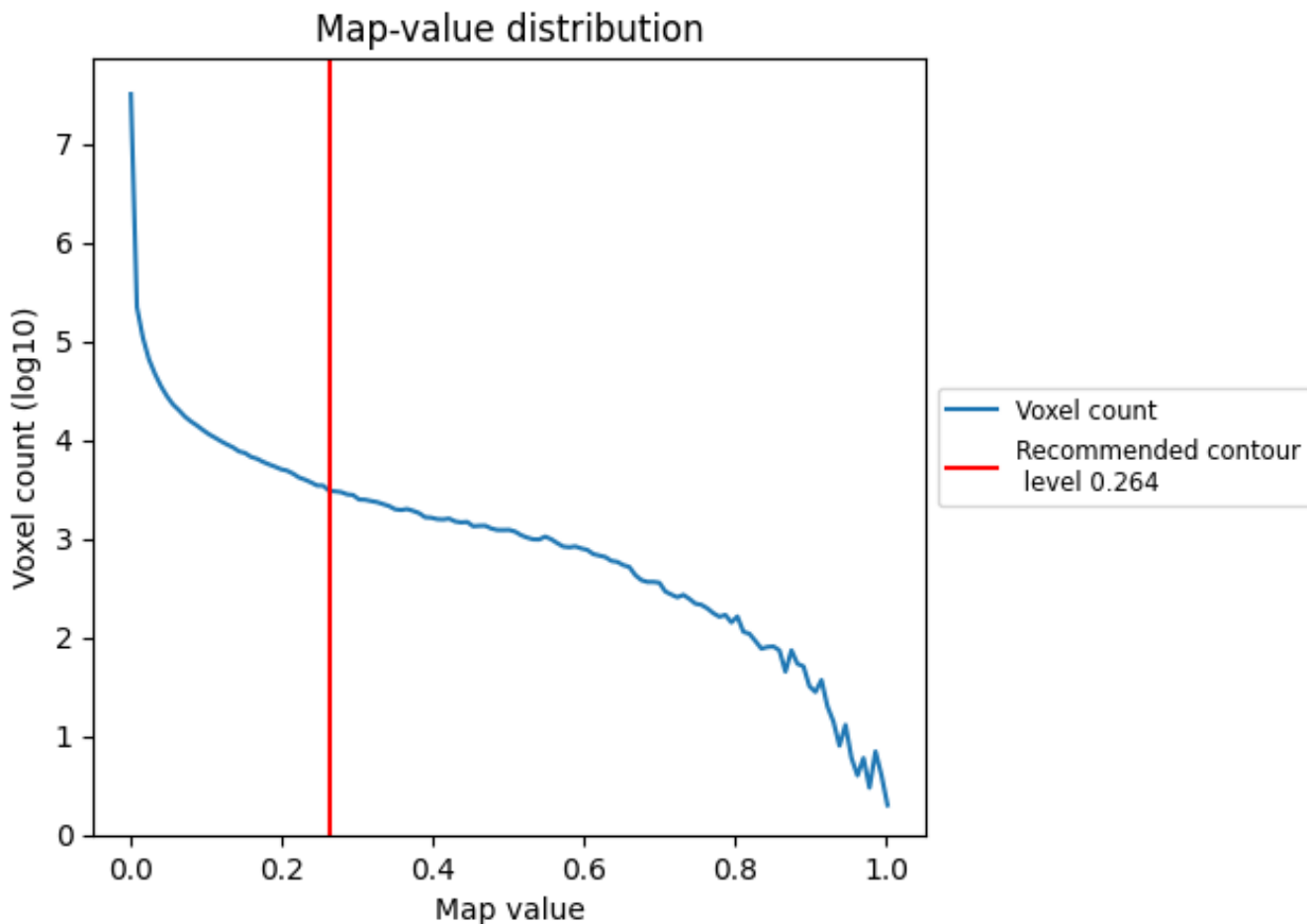
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

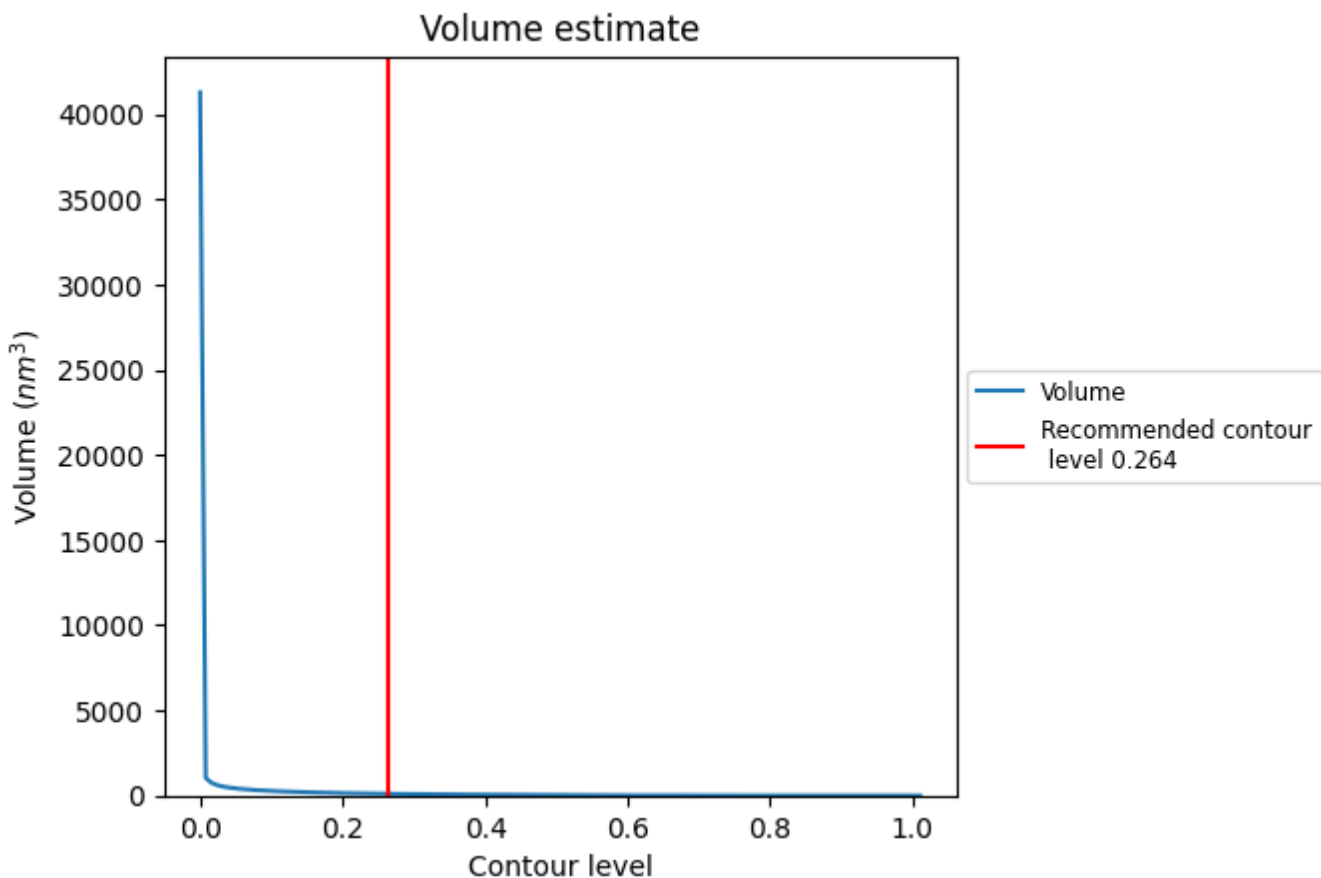
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

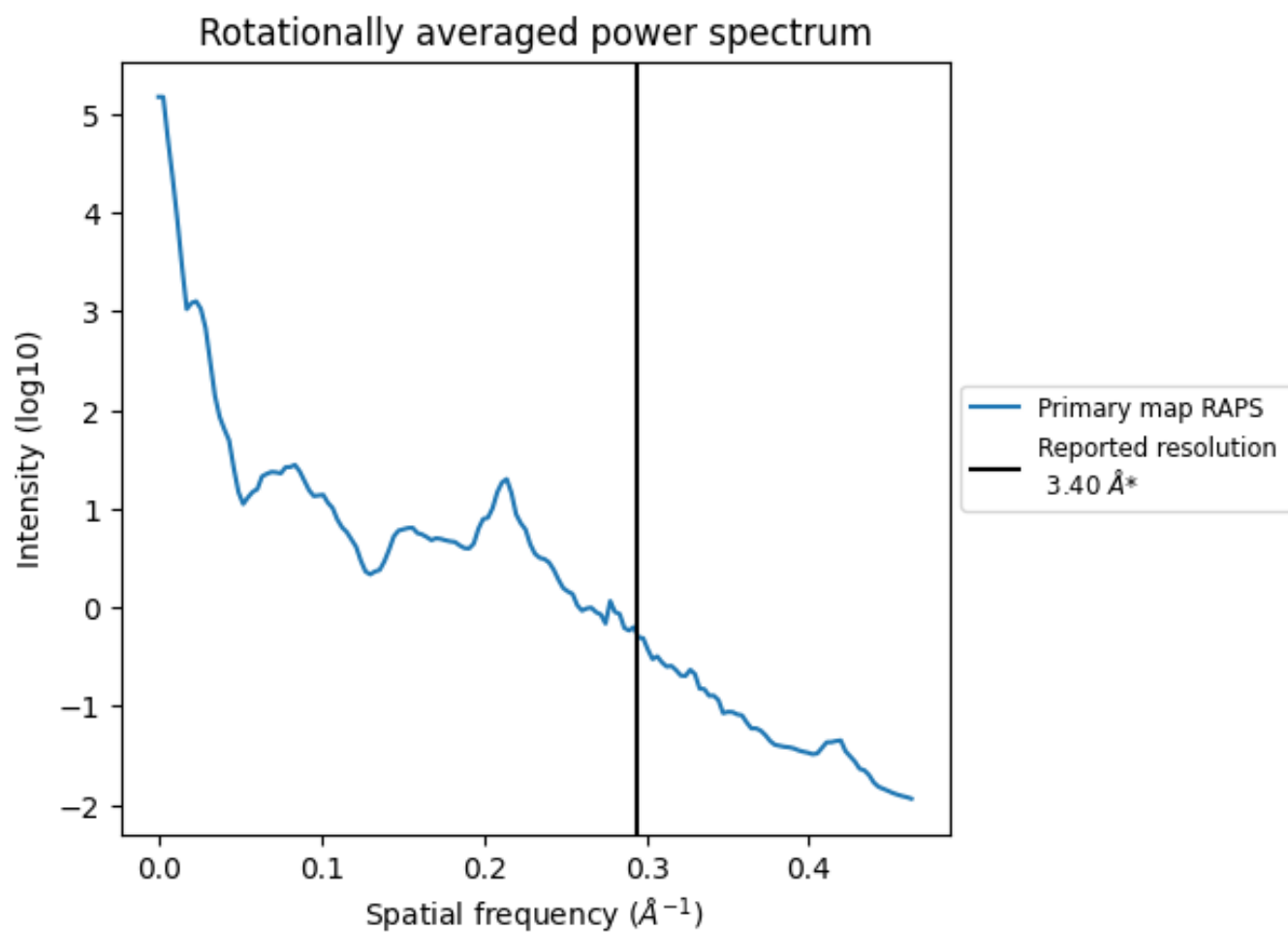
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 103 nm^3 ; this corresponds to an approximate mass of 93 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



*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

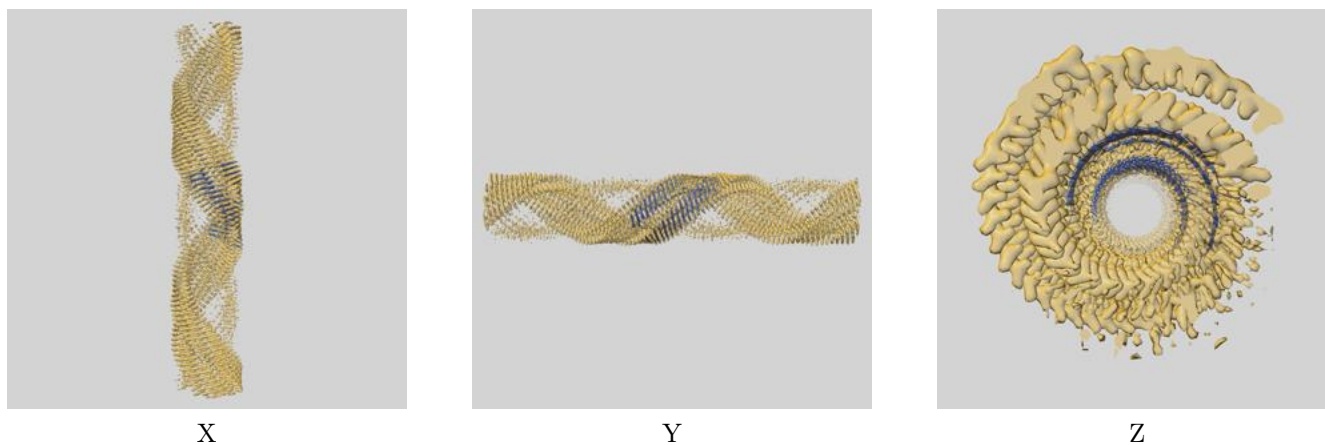
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

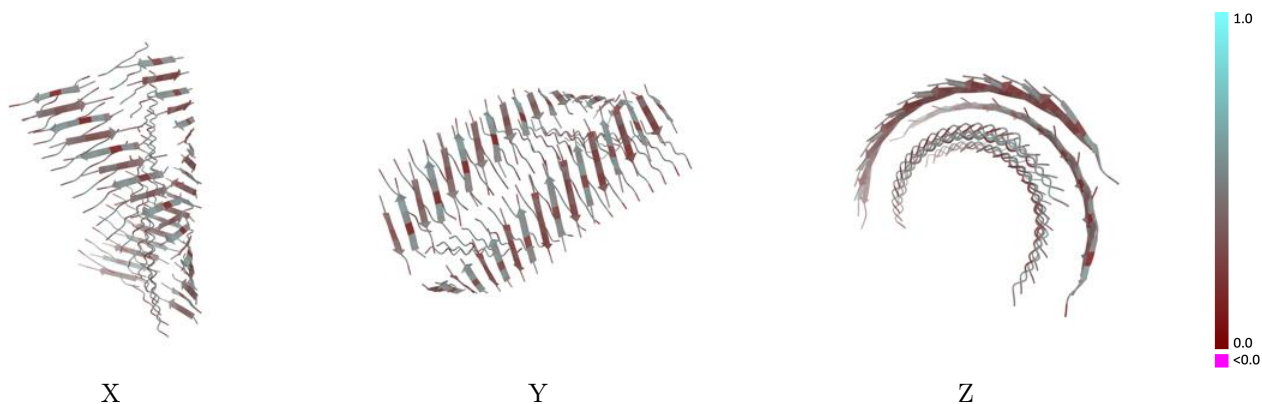
This section contains information regarding the fit between EMDB map EMD-23483 and PDB model 7LQE. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



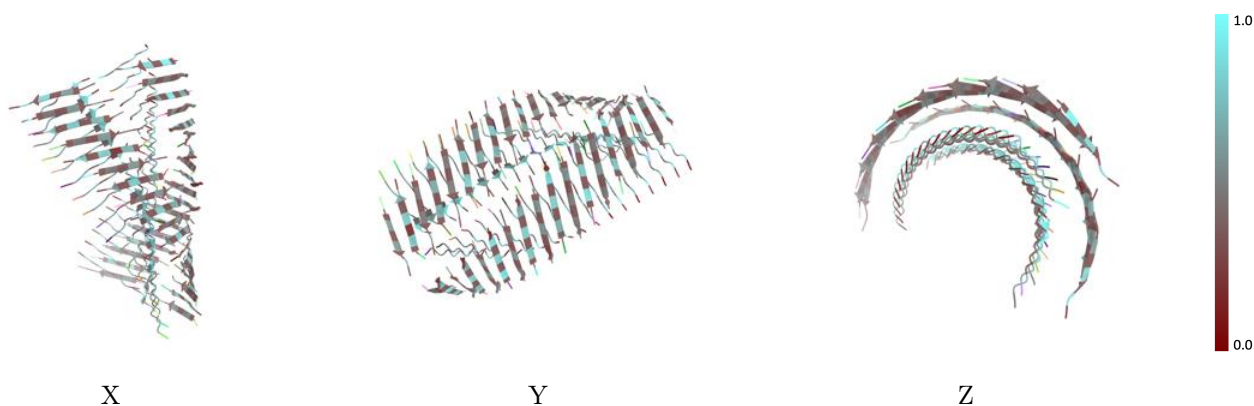
The images above show the 3D surface view of the map at the recommended contour level 0.264 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



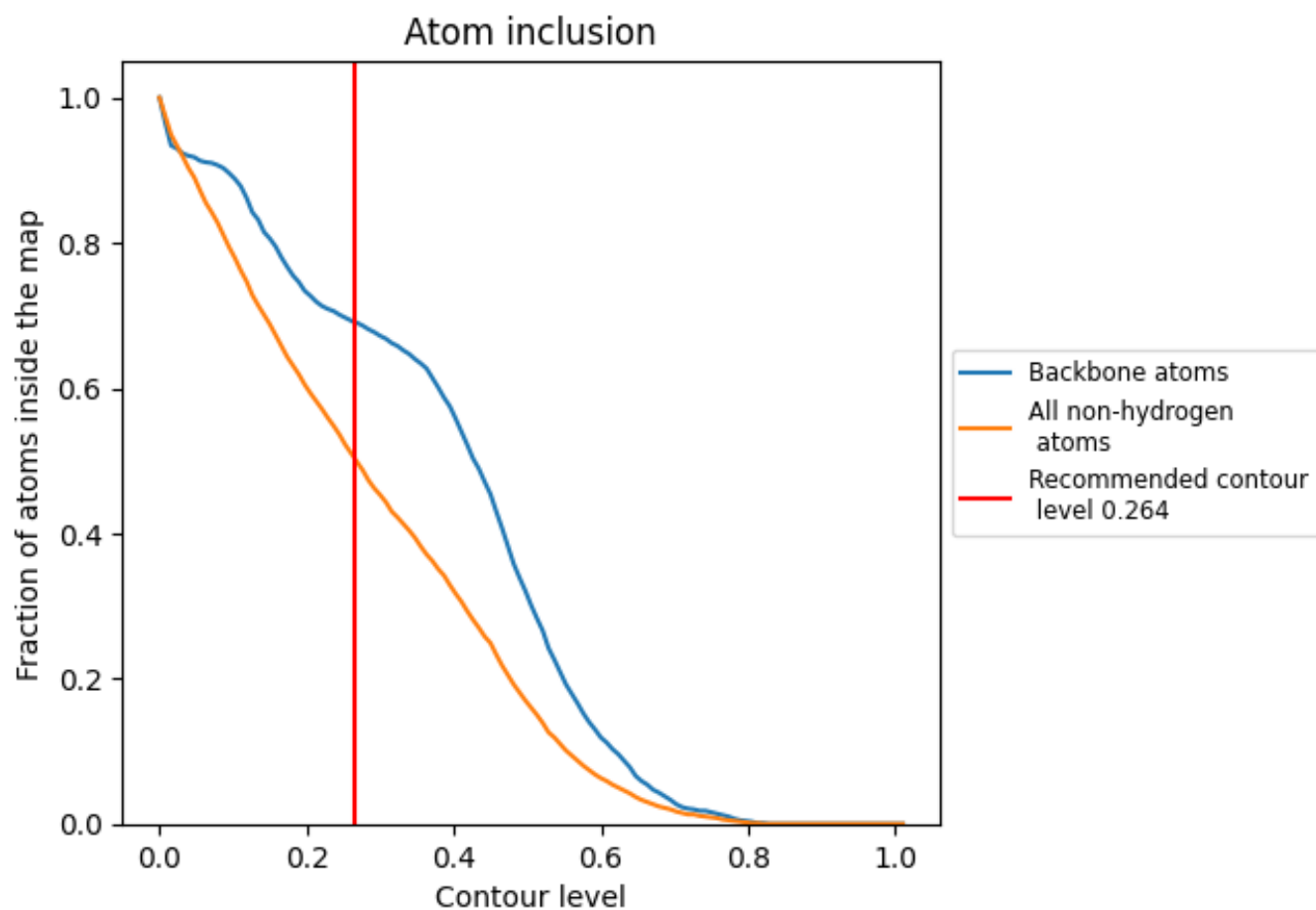
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.264).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 50% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.264) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5050	 0.4250
0	 0.5120	 0.4370
1	 0.4410	 0.3390
2	 0.4290	 0.4070
3	 0.5360	 0.4470
4	 0.4410	 0.3420
5	 0.4170	 0.3870
6	 0.5360	 0.4570
7	 0.4520	 0.3410
8	 0.4290	 0.3860
9	 0.5240	 0.4510
A	 0.5120	 0.4420
AA	 0.4520	 0.3400
B	 0.5360	 0.4280
BA	 0.4290	 0.3960
C	 0.5120	 0.4330
CA	 0.5120	 0.4520
D	 0.5240	 0.4270
DA	 0.4520	 0.3520
E	 0.5000	 0.4330
EA	 0.4170	 0.3910
F	 0.5360	 0.4310
FA	 0.5480	 0.4570
G	 0.5480	 0.4370
GA	 0.4170	 0.3380
H	 0.5360	 0.4250
HA	 0.4760	 0.3980
I	 0.5000	 0.4240
IA	 0.5120	 0.4450
J	 0.5590	 0.4260
JA	 0.4050	 0.3180
K	 0.5480	 0.4850
L	 0.5590	 0.4410
M	 0.5590	 0.4090
N	 0.5360	 0.4850



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Chain	Atom inclusion	Q-score
O	0.5480	0.4460
P	0.5590	0.4260
Q	0.5120	0.4830
R	0.5590	0.4480
S	0.5240	0.4210
T	0.5240	0.4660
U	0.5710	0.4500
V	0.5590	0.4330
W	0.5480	0.4760
X	0.5590	0.4380
Y	0.5360	0.4160
Z	0.5360	0.4790
a	0.5000	0.4430
b	0.4640	0.4340
c	0.4640	0.4510
d	0.4880	0.4420
e	0.4880	0.4360
f	0.5000	0.4430
g	0.4760	0.4490
h	0.5000	0.4250
i	0.4880	0.4420
j	0.5360	0.4500
k	0.5590	0.4260
l	0.5480	0.4790
m	0.5360	0.4320
n	0.5360	0.4230
o	0.5120	0.4580
p	0.5590	0.4430
q	0.5590	0.4170
r	0.5360	0.4770
s	0.5360	0.4350
t	0.4520	0.3960
u	0.5240	0.4440
v	0.4290	0.3380
w	0.4290	0.4030
x	0.5120	0.4580
y	0.4170	0.3500
z	0.4640	0.3980