wwPDB EM Validation Summary Report

Nov 4, 2023 – 09:57 PM EDT

PDB ID	:	7LQH
EMDB ID	:	EMD-23486
Title	:	Cryo-EM of KFE8 thinner nanotube (class 2, 2-sub-1)
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 wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

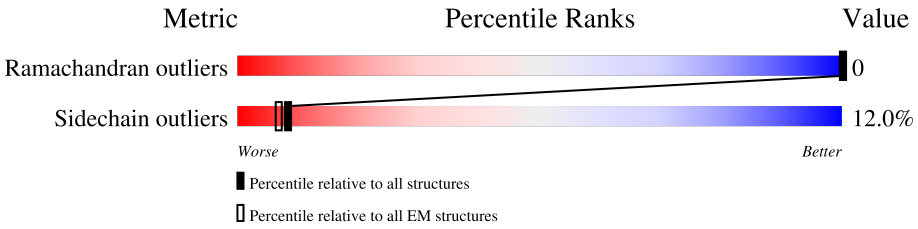
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (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 <=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	38% 62% 38%
1	0A	8	50% 75% 25%
1	1	8	50% 50% 50%
1	1A	8	88% 75% 25%
1	2	8	12% 75% 25%
1	2A	8	62% 62% 38%
1	3	8	38% 62% 38%
1	3A	8	50% 75% 25%
1	4	8	50% 75% 25%

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Mol	Chain	Length	Quality of chain
1	4A	8	62% 75% 25%
1	5	8	38% 50% 50%
1	5A	8	50% 50% 50%
1	6	8	12% 75% 25%
1	6A	8	75% 62% 38%
1	7	8	38% 62% 38%
1	7A	8	62% 75% 25%
1	8	8	50% 50% 50%
1	8A	8	88% 75% 25%
1	9	8	25% 75% 25%
1	9A	8	75% 62% 38%
1	A	8	50% 88% 12%
1	AA	8	38% 62% 38%
1	AB	8	50% 75% 25%
1	B	8	50% 75% 25%
1	BA	8	50% 88% 12%
1	BB	8	75% 75% 25%
1	C	8	50% 75% 25%
1	CA	8	50% 62% 38%
1	CB	8	50% 50% 50%
1	D	8	50% 88% 12%
1	DA	8	12% 75% 25%
1	DB	8	75% 62% 38%
1	E	8	50% 75% 25%
1	EA	8	38% 62% 38%

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Mol	Chain	Length	Quality of chain
1	EB	8	50% 75% 25%
1	F	8	50% 75% 25%
1	FA	8	50% 50% 50%
1	FB	8	88% 75% 25%
1	G	8	50% 88% 12%
1	GA	8	12% 75% 25%
1	GB	8	75% 62% 38%
1	H	8	50% 75% 25%
1	HA	8	38% 62% 38%
1	HB	8	50% 75% 25%
1	I	8	50% 75% 25%
1	IA	8	50% 88% 12%
1	IB	8	75% 75% 25%
1	J	8	50% 50% 50%
1	JA	8	50% 50% 50%
1	JB	8	62% 62% 38%
1	K	8	25% 75% 25%
1	KA	8	12% 75% 25%
1	KB	8	75% 62% 38%
1	L	8	38% 62% 38%
1	LA	8	38% 62% 38%
1	LB	8	50% 75% 25%
1	M	8	50% 75% 25%
1	MA	8	38% 50% 50%
1	MB	8	88% 75% 25%

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Mol	Chain	Length	Quality of chain
1	N	8	38% 50% 50%
1	NA	8	12% 75% 25%
1	NB	8	62% 62% 38%
1	O	8	12% 75% 25%
1	OA	8	38% 62% 38%
1	OB	8	50% 75% 25%
1	P	8	38% 62% 38%
1	PA	8	50% 75% 25%
1	PB	8	62% 75% 25%
1	Q	8	50% 50% 50%
1	QA	8	38% 50% 50%
1	QB	8	50% 50% 50%
1	R	8	12% 75% 25%
1	RA	8	12% 75% 25%
1	RB	8	75% 62% 38%
1	S	8	38% 62% 38%
1	SA	8	38% 62% 38%
1	SB	8	62% 75% 25%
1	T	8	50% 75% 25%
1	TA	8	62% 62% 38%
1	TB	8	88% 75% 25%
1	U	8	50% 50% 50%
1	UA	8	62% 75% 25%
1	V	8	25% 75% 25%
1	VA	8	62% 75% 25%

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Mol	Chain	Length	Quality of chain
1	W	8	38% 62% 38%
1	WA	8	50% 50% 50%
1	X	8	38% 62% 38%
1	XA	8	62% 62% 38%
1	Y	8	12% 75% 25%
1	YA	8	50% 75% 25%
1	Z	8	38% 62% 38%
1	ZA	8	75% 75% 25%
1	a	8	50% 50% 50%
1	aA	8	62% 62% 38%
1	b	8	50% 62% 38%
1	bA	8	50% 75% 25%
1	c	8	50% 50% 50%
1	cA	8	75% 75% 25%
1	d	8	62% 50% 50%
1	dA	8	62% 50% 50%
1	e	8	50% 50% 50%
1	eA	8	75% 62% 38%
1	f	8	62% 50% 50%
1	fA	8	50% 75% 25%
1	g	8	50% 50% 50%
1	gA	8	88% 75% 25%
1	h	8	50% 62% 38%
1	hA	8	62% 62% 38%
1	i	8	50% 50% 50%

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Mol	Chain	Length	Quality of chain
1	iA	8	50% 75% 25%
1	j	8	50% 75% 25%
1	jA	8	50% 75% 25%
1	k	8	50% 62% 38%
1	kA	8	62% 50% 50%
1	l	8	25% 75% 25%
1	lA	8	62% 62% 38%
1	m	8	38% 62% 38%
1	mA	8	50% 75% 25%
1	n	8	38% 50% 50%
1	nA	8	75% 75% 25%
1	o	8	25% 75% 25%
1	oA	8	88% 62% 38%
1	p	8	50% 62% 38%
1	pA	8	50% 75% 25%
1	q	8	50% 75% 25%
1	qA	8	50% 75% 25%
1	r	8	38% 50% 50%
1	rA	8	50% 50% 50%
1	s	8	12% 75% 25%
1	sA	8	75% 62% 38%
1	t	8	50% 62% 38%
1	tA	8	50% 75% 25%
1	u	8	38% 62% 38%
1	uA	8	88% 75% 25%

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Mol	Chain	Length	Quality of chain
1	v	8	12% 75% 25%
1	vA	8	62% 62% 38%
1	w	8	38% 62% 38%
1	wA	8	50% 75% 25%
1	x	8	50% 75% 25%
1	xA	8	62% 75% 25%
1	y	8	38% 62% 38%
1	yA	8	62% 62% 38%
1	z	8	25% 75% 25%
1	zA	8	75% 62% 38%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 12096 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
1	A	8	Total	C	N	O	0	0
			84	60	11	13		
1	J	8	Total	C	N	O	0	0
			84	60	11	13		
1	K	8	Total	C	N	O	0	0
			84	60	11	13		
1	L	8	Total	C	N	O	0	0
			84	60	11	13		
1	M	8	Total	C	N	O	0	0
			84	60	11	13		
1	N	8	Total	C	N	O	0	0
			84	60	11	13		
1	O	8	Total	C	N	O	0	0
			84	60	11	13		
1	P	8	Total	C	N	O	0	0
			84	60	11	13		
1	B	8	Total	C	N	O	0	0
			84	60	11	13		
1	Q	8	Total	C	N	O	0	0
			84	60	11	13		
1	R	8	Total	C	N	O	0	0
			84	60	11	13		
1	S	8	Total	C	N	O	0	0
			84	60	11	13		
1	T	8	Total	C	N	O	0	0
			84	60	11	13		
1	U	8	Total	C	N	O	0	0
			84	60	11	13		
1	V	8	Total	C	N	O	0	0
			84	60	11	13		
1	W	8	Total	C	N	O	0	0
			84	60	11	13		
1	C	8	Total	C	N	O	0	0
			84	60	11	13		

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	X	8	Total	C	N	O	0	0
			84	60	11	13		
1	Y	8	Total	C	N	O	0	0
			84	60	11	13		
1	Z	8	Total	C	N	O	0	0
			84	60	11	13		
1	j	8	Total	C	N	O	0	0
			84	60	11	13		
1	k	8	Total	C	N	O	0	0
			84	60	11	13		
1	l	8	Total	C	N	O	0	0
			84	60	11	13		
1	m	8	Total	C	N	O	0	0
			84	60	11	13		
1	D	8	Total	C	N	O	0	0
			84	60	11	13		
1	n	8	Total	C	N	O	0	0
			84	60	11	13		
1	o	8	Total	C	N	O	0	0
			84	60	11	13		
1	p	8	Total	C	N	O	0	0
			84	60	11	13		
1	q	8	Total	C	N	O	0	0
			84	60	11	13		
1	r	8	Total	C	N	O	0	0
			84	60	11	13		
1	s	8	Total	C	N	O	0	0
			84	60	11	13		
1	t	8	Total	C	N	O	0	0
			84	60	11	13		
1	E	8	Total	C	N	O	0	0
			84	60	11	13		
1	u	8	Total	C	N	O	0	0
			84	60	11	13		
1	v	8	Total	C	N	O	0	0
			84	60	11	13		
1	w	8	Total	C	N	O	0	0
			84	60	11	13		
1	x	8	Total	C	N	O	0	0
			84	60	11	13		
1	y	8	Total	C	N	O	0	0
			84	60	11	13		

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	z	8	Total	C	N	O	0	0
			84	60	11	13		
1	0	8	Total	C	N	O	0	0
			84	60	11	13		
1	F	8	Total	C	N	O	0	0
			84	60	11	13		
1	1	8	Total	C	N	O	0	0
			84	60	11	13		
1	2	8	Total	C	N	O	0	0
			84	60	11	13		
1	3	8	Total	C	N	O	0	0
			84	60	11	13		
1	4	8	Total	C	N	O	0	0
			84	60	11	13		
1	5	8	Total	C	N	O	0	0
			84	60	11	13		
1	6	8	Total	C	N	O	0	0
			84	60	11	13		
1	7	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	8	8	Total	C	N	O	0	0
			84	60	11	13		
1	9	8	Total	C	N	O	0	0
			84	60	11	13		
1	AA	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	EA	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	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		

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Mol	Chain	Residues	Atoms				AltConf	Trace
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		
1	KA	8	Total	C	N	O	0	0
			84	60	11	13		
1	LA	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	MA	8	Total	C	N	O	0	0
			84	60	11	13		
1	NA	8	Total	C	N	O	0	0
			84	60	11	13		
1	OA	8	Total	C	N	O	0	0
			84	60	11	13		
1	PA	8	Total	C	N	O	0	0
			84	60	11	13		
1	QA	8	Total	C	N	O	0	0
			84	60	11	13		
1	RA	8	Total	C	N	O	0	0
			84	60	11	13		
1	SA	8	Total	C	N	O	0	0
			84	60	11	13		
1	a	8	Total	C	N	O	0	0
			84	60	11	13		
1	TA	8	Total	C	N	O	0	0
			84	60	11	13		
1	UA	8	Total	C	N	O	0	0
			84	60	11	13		
1	VA	8	Total	C	N	O	0	0
			84	60	11	13		
1	WA	8	Total	C	N	O	0	0
			84	60	11	13		
1	XA	8	Total	C	N	O	0	0
			84	60	11	13		
1	YA	8	Total	C	N	O	0	0
			84	60	11	13		
1	ZA	8	Total	C	N	O	0	0
			84	60	11	13		

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	b	8	Total	C	N	O	0	0
			84	60	11	13		
1	aA	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	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	c	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		
1	kA	8	Total	C	N	O	0	0
			84	60	11	13		
1	lA	8	Total	C	N	O	0	0
			84	60	11	13		
1	mA	8	Total	C	N	O	0	0
			84	60	11	13		
1	nA	8	Total	C	N	O	0	0
			84	60	11	13		
1	d	8	Total	C	N	O	0	0
			84	60	11	13		
1	oA	8	Total	C	N	O	0	0
			84	60	11	13		
1	pA	8	Total	C	N	O	0	0
			84	60	11	13		
1	qA	8	Total	C	N	O	0	0
			84	60	11	13		
1	rA	8	Total	C	N	O	0	0
			84	60	11	13		

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	sA	8	Total	C	N	O	0	0
			84	60	11	13		
1	tA	8	Total	C	N	O	0	0
			84	60	11	13		
1	uA	8	Total	C	N	O	0	0
			84	60	11	13		
1	e	8	Total	C	N	O	0	0
			84	60	11	13		
1	vA	8	Total	C	N	O	0	0
			84	60	11	13		
1	wA	8	Total	C	N	O	0	0
			84	60	11	13		
1	xA	8	Total	C	N	O	0	0
			84	60	11	13		
1	yA	8	Total	C	N	O	0	0
			84	60	11	13		
1	zA	8	Total	C	N	O	0	0
			84	60	11	13		
1	0A	8	Total	C	N	O	0	0
			84	60	11	13		
1	1A	8	Total	C	N	O	0	0
			84	60	11	13		
1	f	8	Total	C	N	O	0	0
			84	60	11	13		
1	2A	8	Total	C	N	O	0	0
			84	60	11	13		
1	3A	8	Total	C	N	O	0	0
			84	60	11	13		
1	4A	8	Total	C	N	O	0	0
			84	60	11	13		
1	5A	8	Total	C	N	O	0	0
			84	60	11	13		
1	6A	8	Total	C	N	O	0	0
			84	60	11	13		
1	7A	8	Total	C	N	O	0	0
			84	60	11	13		
1	8A	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	9A	8	Total	C	N	O	0	0
			84	60	11	13		

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	AB	8	Total	C	N	O	0	0
			84	60	11	13		
1	BB	8	Total	C	N	O	0	0
			84	60	11	13		
1	CB	8	Total	C	N	O	0	0
			84	60	11	13		
1	DB	8	Total	C	N	O	0	0
			84	60	11	13		
1	EB	8	Total	C	N	O	0	0
			84	60	11	13		
1	FB	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	GB	8	Total	C	N	O	0	0
			84	60	11	13		
1	HB	8	Total	C	N	O	0	0
			84	60	11	13		
1	IB	8	Total	C	N	O	0	0
			84	60	11	13		
1	JB	8	Total	C	N	O	0	0
			84	60	11	13		
1	KB	8	Total	C	N	O	0	0
			84	60	11	13		
1	LB	8	Total	C	N	O	0	0
			84	60	11	13		
1	MB	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	NB	8	Total	C	N	O	0	0
			84	60	11	13		
1	OB	8	Total	C	N	O	0	0
			84	60	11	13		
1	PB	8	Total	C	N	O	0	0
			84	60	11	13		
1	QB	8	Total	C	N	O	0	0
			84	60	11	13		
1	RB	8	Total	C	N	O	0	0
			84	60	11	13		
1	SB	8	Total	C	N	O	0	0
			84	60	11	13		

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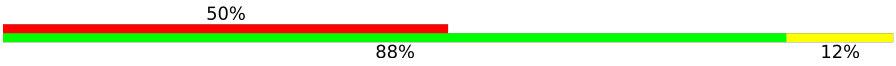
Mol	Chain	Residues	Atoms				AltConf	Trace
1	TB	8	Total	C	N	O	0	0
			84	60	11	13		

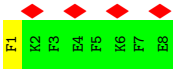
3 Residue-property plots (i)

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.

- Molecule 1: KFE8 peptide

Chain A:





- Molecule 1: KFE8 peptide

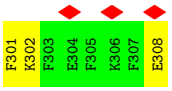
Chain J:

- Molecule 1: KFE8 peptide

Chain K:

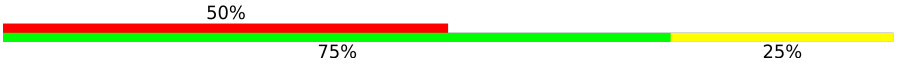
- Molecule 1: KFE8 peptide

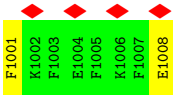
Chain L:



- Molecule 1: KFE8 peptide

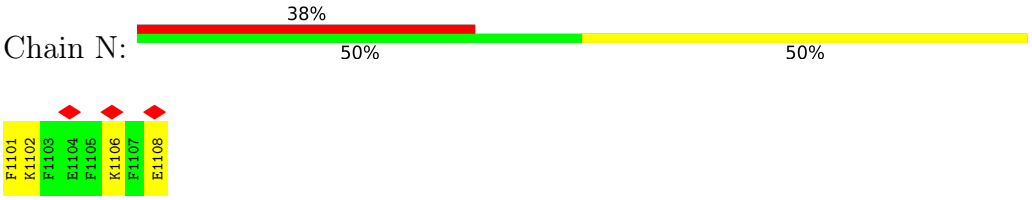
Chain M:





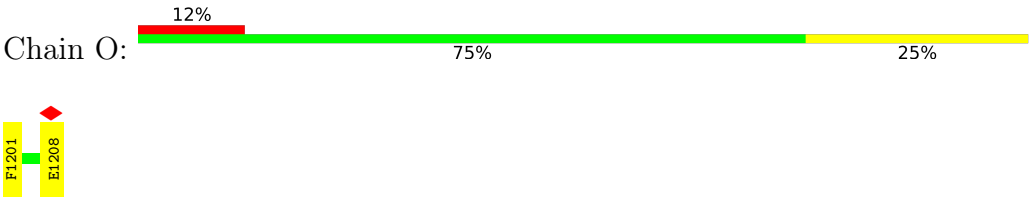
• Molecule 1: KFE8 peptide

Chain N:



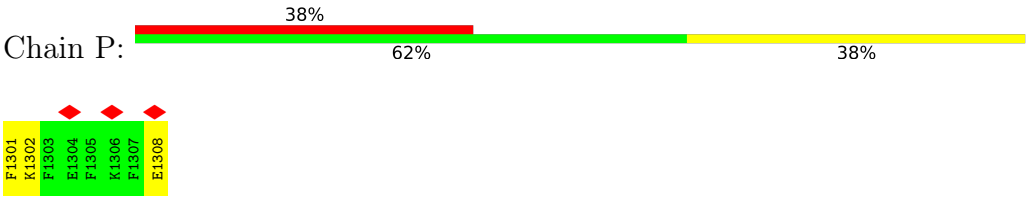
• Molecule 1: KFE8 peptide

Chain O:



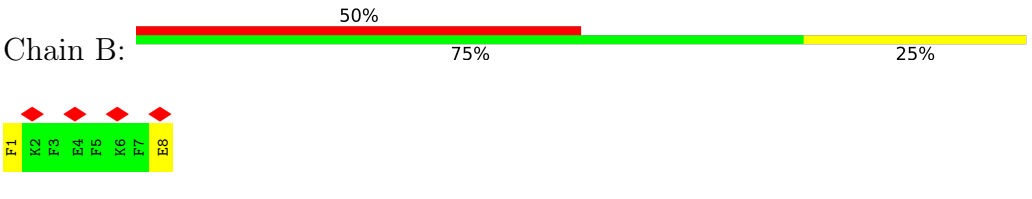
• Molecule 1: KFE8 peptide

Chain P:



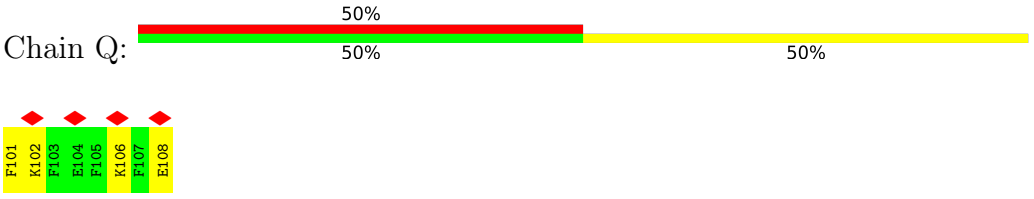
• Molecule 1: KFE8 peptide

Chain B:



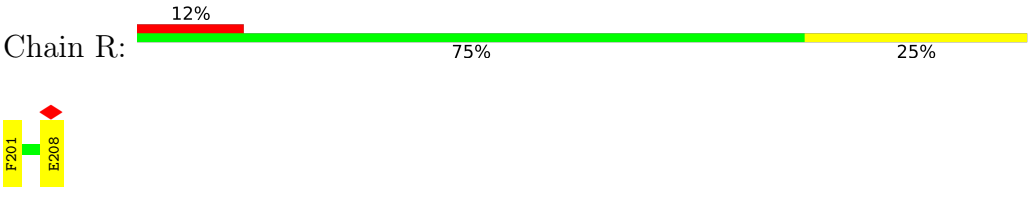
• Molecule 1: KFE8 peptide

Chain Q:



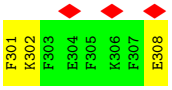
• Molecule 1: KFE8 peptide

Chain R:



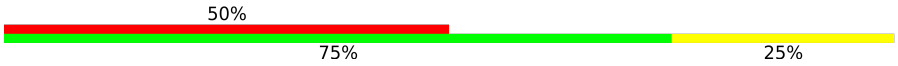
• Molecule 1: KFE8 peptide

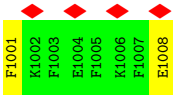
Chain S:



• Molecule 1: KFE8 peptide

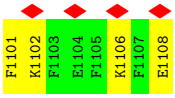
Chain T:





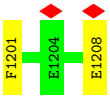
• Molecule 1: KFE8 peptide

Chain U:



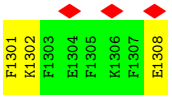
• Molecule 1: KFE8 peptide

Chain V:



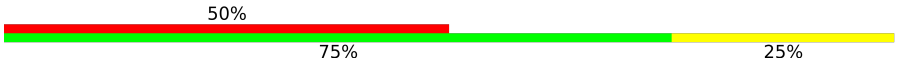
• Molecule 1: KFE8 peptide

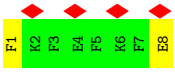
Chain W:



• Molecule 1: KFE8 peptide

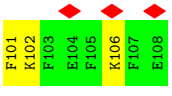
Chain C:





• Molecule 1: KFE8 peptide

Chain X:

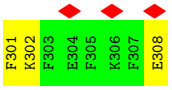


• Molecule 1: KFE8 peptide

Chain Y:

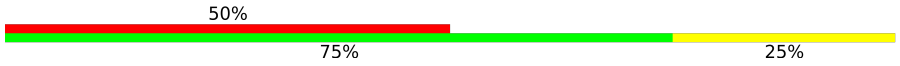
• Molecule 1: KFE8 peptide

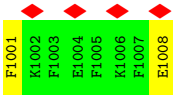
Chain Z:



• Molecule 1: KFE8 peptide

Chain j:



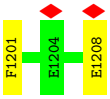


• Molecule 1: KFE8 peptide

Chain k:

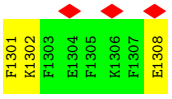
• Molecule 1: KFE8 peptide

Chain l:



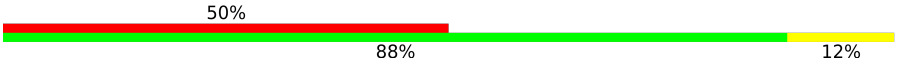
• Molecule 1: KFE8 peptide

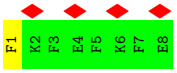
Chain m:



• Molecule 1: KFE8 peptide

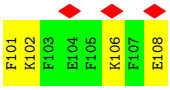
Chain D:





• Molecule 1: KFE8 peptide

Chain n:

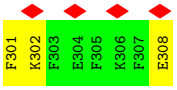


• Molecule 1: KFE8 peptide

Chain o:

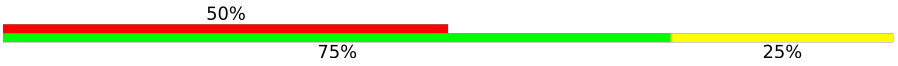
• Molecule 1: KFE8 peptide

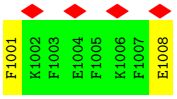
Chain p:



• Molecule 1: KFE8 peptide

Chain q:





• Molecule 1: KFE8 peptide

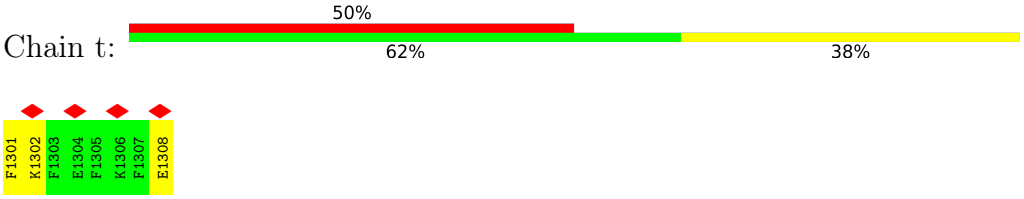
Chain r:

• Molecule 1: KFE8 peptide

Chain s:

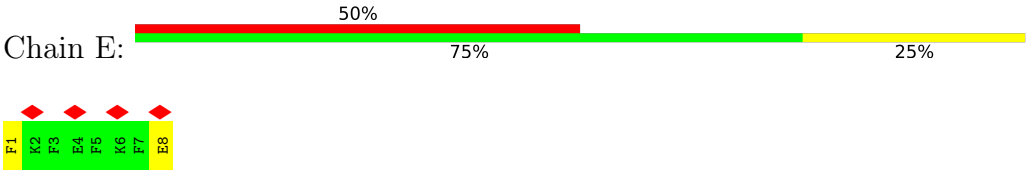
• Molecule 1: KFE8 peptide

Chain t:



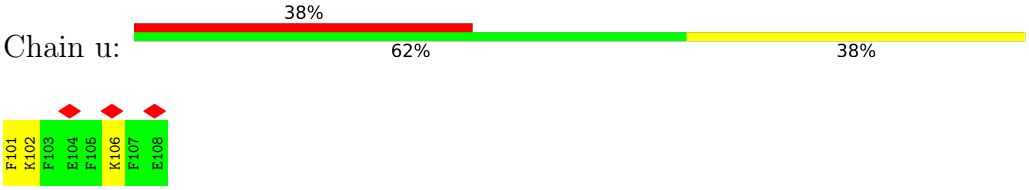
• Molecule 1: KFE8 peptide

Chain E:



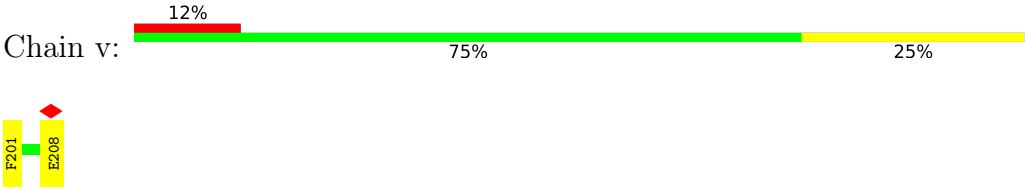
• Molecule 1: KFE8 peptide

Chain u:



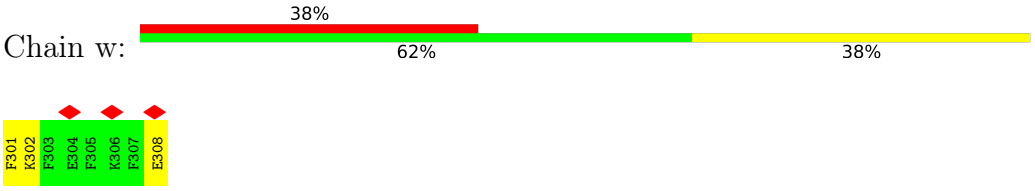
• Molecule 1: KFE8 peptide

Chain v:



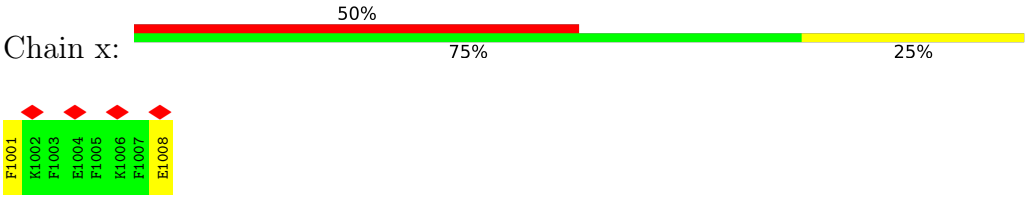
• Molecule 1: KFE8 peptide

Chain w:



• Molecule 1: KFE8 peptide

Chain x:

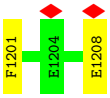


• Molecule 1: KFE8 peptide

Chain y:

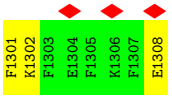
• Molecule 1: KFE8 peptide

Chain z:



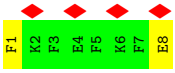
• Molecule 1: KFE8 peptide

Chain 0:



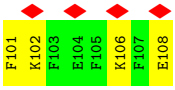
• Molecule 1: KFE8 peptide

Chain F:



• Molecule 1: KFE8 peptide

Chain 1:

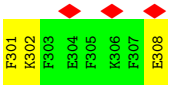


• Molecule 1: KFE8 peptide

Chain 2:

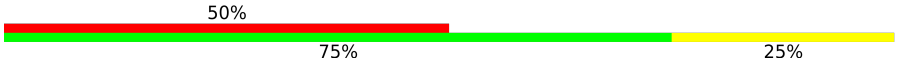
• Molecule 1: KFE8 peptide

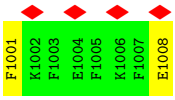
Chain 3:



• Molecule 1: KFE8 peptide

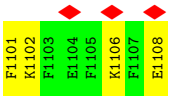
Chain 4:





• Molecule 1: KFE8 peptide

Chain 5:

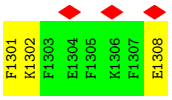


• Molecule 1: KFE8 peptide

Chain 6:

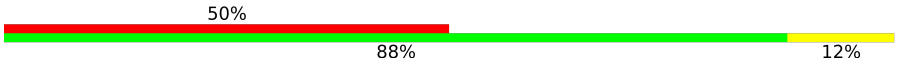
• Molecule 1: KFE8 peptide

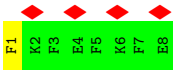
Chain 7:



• Molecule 1: KFE8 peptide

Chain G:





• Molecule 1: KFE8 peptide

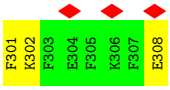
Chain 8:

• Molecule 1: KFE8 peptide

Chain 9:

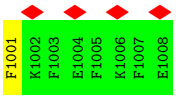
• Molecule 1: KFE8 peptide

Chain AA:



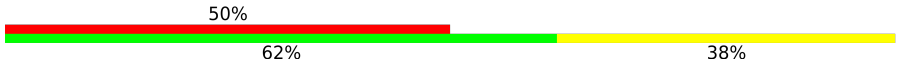
• Molecule 1: KFE8 peptide

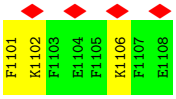
Chain BA:



• Molecule 1: KFE8 peptide

Chain CA:



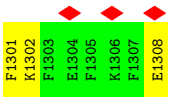


• Molecule 1: KFE8 peptide

Chain DA:

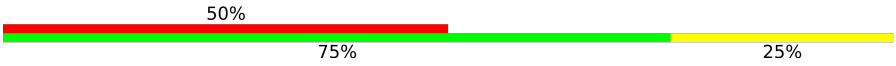
• Molecule 1: KFE8 peptide

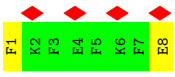
Chain EA:



• Molecule 1: KFE8 peptide

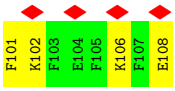
Chain H:





• Molecule 1: KFE8 peptide

Chain FA:

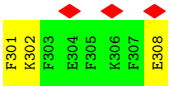


• Molecule 1: KFE8 peptide

Chain GA:

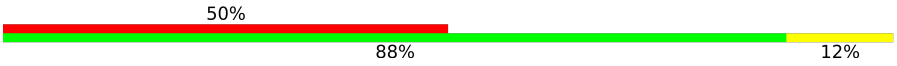
• Molecule 1: KFE8 peptide

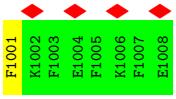
Chain HA:



• Molecule 1: KFE8 peptide

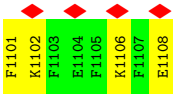
Chain IA:





• Molecule 1: KFE8 peptide

Chain JA:

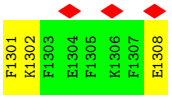


• Molecule 1: KFE8 peptide

Chain KA:

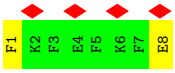
• Molecule 1: KFE8 peptide

Chain LA:



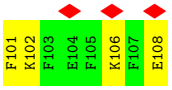
• Molecule 1: KFE8 peptide

Chain I:



• Molecule 1: KFE8 peptide

Chain MA:

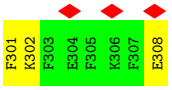


• Molecule 1: KFE8 peptide

Chain NA:

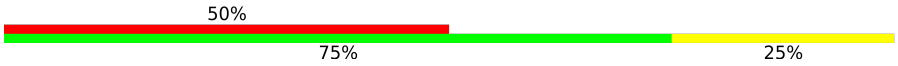
• Molecule 1: KFE8 peptide

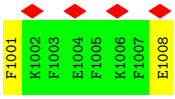
Chain OA:



• Molecule 1: KFE8 peptide

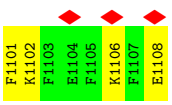
Chain PA:





• Molecule 1: KFE8 peptide

Chain QA:

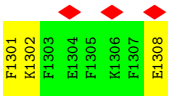


• Molecule 1: KFE8 peptide

Chain RA:

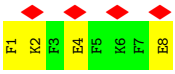
• Molecule 1: KFE8 peptide

Chain SA:



• Molecule 1: KFE8 peptide

Chain a:



• Molecule 1: KFE8 peptide

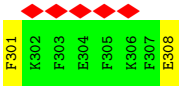
Chain TA:

• Molecule 1: KFE8 peptide

Chain UA:

• Molecule 1: KFE8 peptide

Chain VA:



• Molecule 1: KFE8 peptide

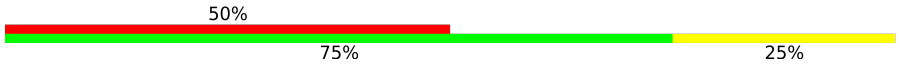
Chain WA:

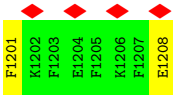
• Molecule 1: KFE8 peptide

Chain XA:

• Molecule 1: KFE8 peptide

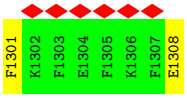
Chain YA:





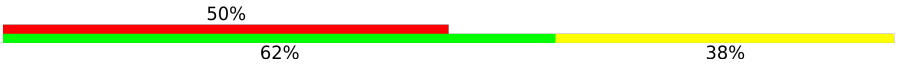
• Molecule 1: KFE8 peptide

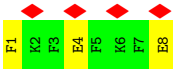
Chain ZA:



• Molecule 1: KFE8 peptide

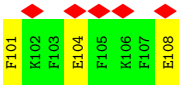
Chain b:





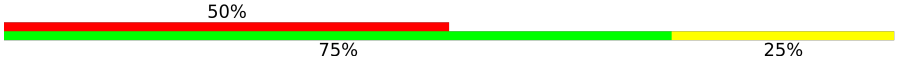
• Molecule 1: KFE8 peptide

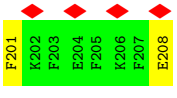
Chain aA:



• Molecule 1: KFE8 peptide

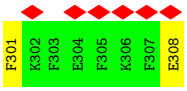
Chain bA:





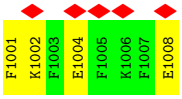
• Molecule 1: KFE8 peptide

Chain cA:



• Molecule 1: KFE8 peptide

Chain dA:

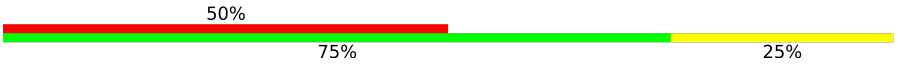


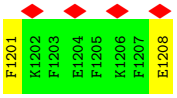
• Molecule 1: KFE8 peptide

Chain eA:

• Molecule 1: KFE8 peptide

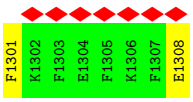
Chain fA:





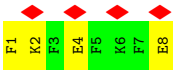
• Molecule 1: KFE8 peptide

Chain gA:



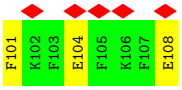
• Molecule 1: KFE8 peptide

Chain c:



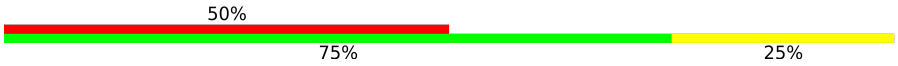
• Molecule 1: KFE8 peptide

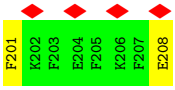
Chain hA:



• Molecule 1: KFE8 peptide

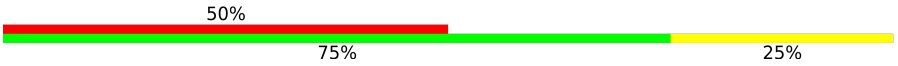
Chain iA:

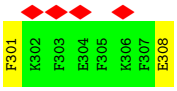




• Molecule 1: KFE8 peptide

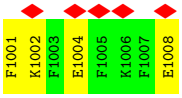
Chain jA:





• Molecule 1: KFE8 peptide

Chain kA:

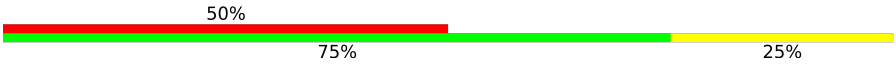


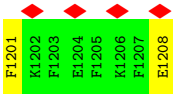
• Molecule 1: KFE8 peptide

Chain lA:

• Molecule 1: KFE8 peptide

Chain mA:



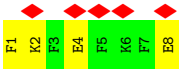


• Molecule 1: KFE8 peptide

Chain nA:

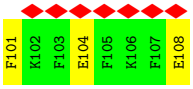
• Molecule 1: KFE8 peptide

Chain d:



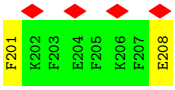
• Molecule 1: KFE8 peptide

Chain oA:



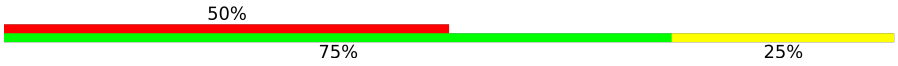
• Molecule 1: KFE8 peptide

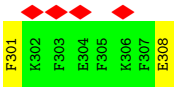
Chain pA:



• Molecule 1: KFE8 peptide

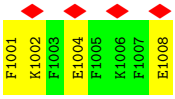
Chain qA:





• Molecule 1: KFE8 peptide

Chain rA:

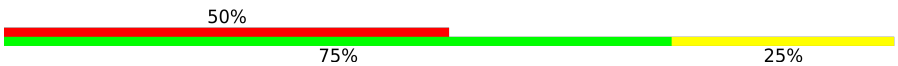


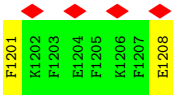
• Molecule 1: KFE8 peptide

Chain sA:

• Molecule 1: KFE8 peptide

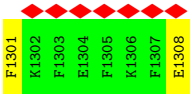
Chain tA:





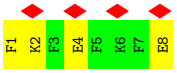
• Molecule 1: KFE8 peptide

Chain uA:



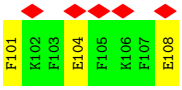
• Molecule 1: KFE8 peptide

Chain e:



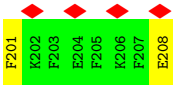
• Molecule 1: KFE8 peptide

Chain vA:



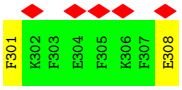
• Molecule 1: KFE8 peptide

Chain wA:



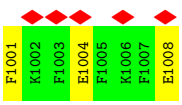
• Molecule 1: KFE8 peptide

Chain xA:



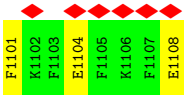
• Molecule 1: KFE8 peptide

Chain yA:



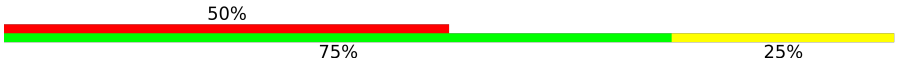
• Molecule 1: KFE8 peptide

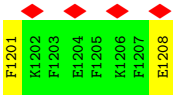
Chain zA:



• Molecule 1: KFE8 peptide

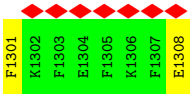
Chain 0A:





• Molecule 1: KFE8 peptide

Chain 1A:

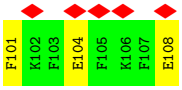


• Molecule 1: KFE8 peptide

Chain f:

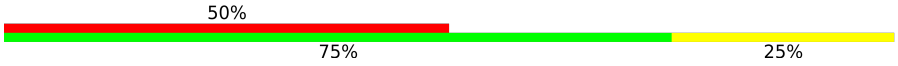
• Molecule 1: KFE8 peptide

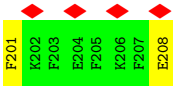
Chain 2A:



• Molecule 1: KFE8 peptide

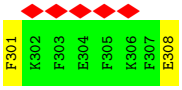
Chain 3A:





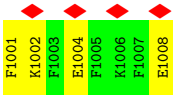
• Molecule 1: KFE8 peptide

Chain 4A:



• Molecule 1: KFE8 peptide

Chain 5A:

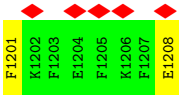


• Molecule 1: KFE8 peptide

Chain 6A:

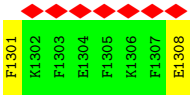
• Molecule 1: KFE8 peptide

Chain 7A:



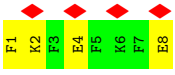
• Molecule 1: KFE8 peptide

Chain 8A:



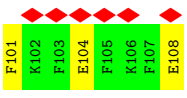
• Molecule 1: KFE8 peptide

Chain g:



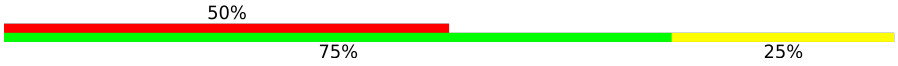
• Molecule 1: KFE8 peptide

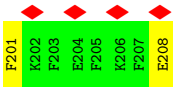
Chain 9A:



• Molecule 1: KFE8 peptide

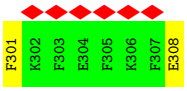
Chain AB:





• Molecule 1: KFE8 peptide

Chain BB:

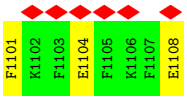


• Molecule 1: KFE8 peptide

Chain CB:

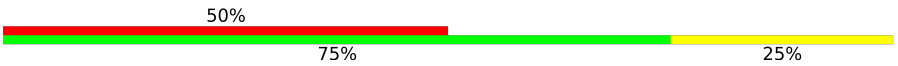
• Molecule 1: KFE8 peptide

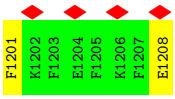
Chain DB:



• Molecule 1: KFE8 peptide

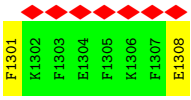
Chain EB:





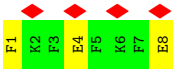
• Molecule 1: KFE8 peptide

Chain FB:



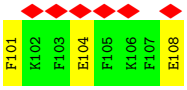
• Molecule 1: KFE8 peptide

Chain h:



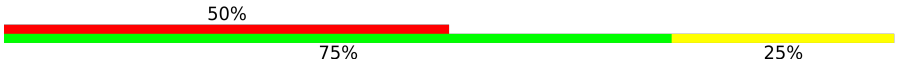
• Molecule 1: KFE8 peptide

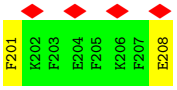
Chain GB:



• Molecule 1: KFE8 peptide

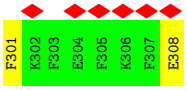
Chain HB:





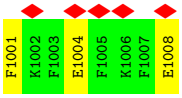
• Molecule 1: KFE8 peptide

Chain IB:



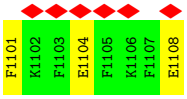
• Molecule 1: KFE8 peptide

Chain JB:



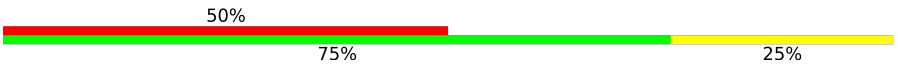
• Molecule 1: KFE8 peptide

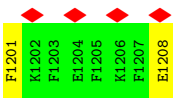
Chain KB:



• Molecule 1: KFE8 peptide

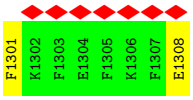
Chain LB:





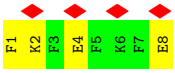
• Molecule 1: KFE8 peptide

Chain MB:



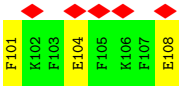
• Molecule 1: KFE8 peptide

Chain i:



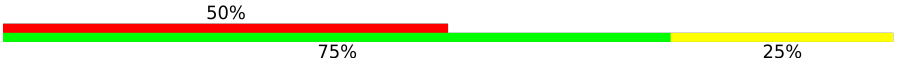
• Molecule 1: KFE8 peptide

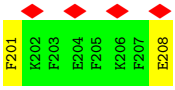
Chain NB:



• Molecule 1: KFE8 peptide

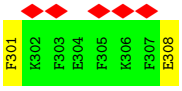
Chain OB:





• Molecule 1: KFE8 peptide

Chain PB:



• Molecule 1: KFE8 peptide

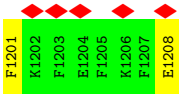
Chain QB:

• Molecule 1: KFE8 peptide

Chain RB:

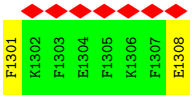
• Molecule 1: KFE8 peptide

Chain SB:



• Molecule 1: KFE8 peptide

Chain TB:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=172.1°, rise=3.97 Å, axial sym=C2	Depositor
Number of segments used	31760	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 ($e^-/Å^2$)	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	0.929	Depositor
Minimum map value	-0.001	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.273	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	0.55	0/62	0.37	0/79
1	0A	0.50	0/62	0.48	0/79
1	1	0.53	0/62	0.45	0/79
1	1A	0.50	0/62	0.48	0/79
1	2	0.59	0/62	0.42	0/79
1	2A	0.49	0/62	0.49	0/79
1	3	0.56	0/62	0.37	0/79
1	3A	0.50	0/62	0.48	0/79
1	4	0.55	0/62	0.45	0/79
1	4A	0.51	0/62	0.48	0/79
1	5	0.53	0/62	0.45	0/79
1	5A	0.54	0/62	0.60	0/79
1	6	0.60	0/62	0.42	0/79
1	6A	0.49	0/62	0.49	0/79
1	7	0.56	0/62	0.37	0/79
1	7A	0.51	0/62	0.48	0/79
1	8	0.54	0/62	0.44	0/79
1	8A	0.51	0/62	0.48	0/79
1	9	0.60	0/62	0.42	0/79
1	9A	0.49	0/62	0.50	0/79
1	A	0.55	0/62	0.45	0/79
1	AA	0.56	0/62	0.37	0/79
1	AB	0.50	0/62	0.48	0/79
1	B	0.55	0/62	0.45	0/79
1	BA	0.55	0/62	0.45	0/79
1	BB	0.51	0/62	0.48	0/79
1	C	0.54	0/62	0.46	0/79
1	CA	0.54	0/62	0.44	0/79
1	CB	0.55	0/62	0.60	0/79
1	D	0.55	0/62	0.45	0/79
1	DA	0.60	0/62	0.42	0/79
1	DB	0.49	0/62	0.50	0/79

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	E	0.55	0/62	0.45	0/79
1	EA	0.55	0/62	0.37	0/79
1	EB	0.50	0/62	0.48	0/79
1	F	0.55	0/62	0.45	0/79
1	FA	0.53	0/62	0.44	0/79
1	FB	0.51	0/62	0.48	0/79
1	G	0.55	0/62	0.45	0/79
1	GA	0.60	0/62	0.42	0/79
1	GB	0.49	0/62	0.49	0/79
1	H	0.54	0/62	0.45	0/79
1	HA	0.55	0/62	0.37	0/79
1	HB	0.50	0/62	0.48	0/79
1	I	0.55	0/62	0.45	0/79
1	IA	0.54	0/62	0.45	0/79
1	IB	0.50	0/62	0.48	0/79
1	J	0.53	0/62	0.45	0/79
1	JA	0.54	0/62	0.44	0/79
1	JB	0.55	0/62	0.60	0/79
1	K	0.60	0/62	0.42	0/79
1	KA	0.60	0/62	0.42	0/79
1	KB	0.50	0/62	0.49	0/79
1	L	0.55	0/62	0.37	0/79
1	LA	0.55	0/62	0.37	0/79
1	LB	0.50	0/62	0.48	0/79
1	M	0.55	0/62	0.45	0/79
1	MA	0.54	0/62	0.45	0/79
1	MB	0.50	0/62	0.48	0/79
1	N	0.53	0/62	0.45	0/79
1	NA	0.59	0/62	0.42	0/79
1	NB	0.49	0/62	0.50	0/79
1	O	0.60	0/62	0.42	0/79
1	OA	0.56	0/62	0.37	0/79
1	OB	0.51	0/62	0.47	0/79
1	P	0.55	0/62	0.37	0/79
1	PA	0.55	0/62	0.46	0/79
1	PB	0.50	0/62	0.48	0/79
1	Q	0.53	0/62	0.45	0/79
1	QA	0.54	0/62	0.45	0/79
1	QB	0.55	0/62	0.60	0/79
1	R	0.60	0/62	0.42	0/79
1	RA	0.59	0/62	0.42	0/79
1	RB	0.49	0/62	0.49	0/79
1	S	0.56	0/62	0.37	0/79

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	SA	0.56	0/62	0.37	0/79
1	SB	0.51	0/62	0.47	0/79
1	T	0.55	0/62	0.45	0/79
1	TA	0.48	0/62	0.49	0/79
1	TB	0.50	0/62	0.48	0/79
1	U	0.53	0/62	0.45	0/79
1	UA	0.51	0/62	0.48	0/79
1	V	0.60	0/62	0.42	0/79
1	VA	0.50	0/62	0.48	0/79
1	W	0.56	0/62	0.37	0/79
1	WA	0.55	0/62	0.60	0/79
1	X	0.53	0/62	0.45	0/79
1	XA	0.48	0/62	0.49	0/79
1	Y	0.60	0/62	0.42	0/79
1	YA	0.51	0/62	0.48	0/79
1	Z	0.55	0/62	0.37	0/79
1	ZA	0.50	0/62	0.48	0/79
1	a	0.55	0/62	0.60	0/79
1	aA	0.49	0/62	0.50	0/79
1	b	0.55	0/62	0.60	0/79
1	bA	0.50	0/62	0.47	0/79
1	c	0.55	0/62	0.60	0/79
1	cA	0.51	0/62	0.48	0/79
1	d	0.54	0/62	0.60	0/79
1	dA	0.55	0/62	0.60	0/79
1	e	0.54	0/62	0.60	0/79
1	eA	0.49	0/62	0.50	0/79
1	f	0.54	0/62	0.60	0/79
1	fA	0.50	0/62	0.47	0/79
1	g	0.55	0/62	0.59	0/79
1	gA	0.51	0/62	0.48	0/79
1	h	0.55	0/62	0.60	0/79
1	hA	0.49	0/62	0.49	0/79
1	i	0.55	0/62	0.60	0/79
1	iA	0.51	0/62	0.48	0/79
1	j	0.54	0/62	0.46	0/79
1	jA	0.50	0/62	0.48	0/79
1	k	0.53	0/62	0.45	0/79
1	kA	0.55	0/62	0.59	0/79
1	l	0.60	0/62	0.42	0/79
1	lA	0.49	0/62	0.49	0/79
1	m	0.55	0/62	0.36	0/79
1	mA	0.51	0/62	0.47	0/79

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	n	0.54	0/62	0.44	0/79
1	nA	0.50	0/62	0.48	0/79
1	o	0.60	0/62	0.42	0/79
1	oA	0.48	0/62	0.50	0/79
1	p	0.55	0/62	0.37	0/79
1	pA	0.50	0/62	0.48	0/79
1	q	0.55	0/62	0.45	0/79
1	qA	0.51	0/62	0.48	0/79
1	r	0.53	0/62	0.45	0/79
1	rA	0.55	0/62	0.60	0/79
1	s	0.60	0/62	0.42	0/79
1	sA	0.48	0/62	0.50	0/79
1	t	0.55	0/62	0.37	0/79
1	tA	0.50	0/62	0.48	0/79
1	u	0.53	0/62	0.45	0/79
1	uA	0.51	0/62	0.48	0/79
1	v	0.59	0/62	0.42	0/79
1	vA	0.49	0/62	0.50	0/79
1	w	0.55	0/62	0.37	0/79
1	wA	0.50	0/62	0.48	0/79
1	x	0.54	0/62	0.45	0/79
1	xA	0.51	0/62	0.48	0/79
1	y	0.53	0/62	0.44	0/79
1	yA	0.54	0/62	0.59	0/79
1	z	0.60	0/62	0.42	0/79
1	zA	0.49	0/62	0.50	0/79
All	All	0.54	0/8928	0.47	0/11376

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%)	5 (83%)	1 (17%)	0	100	100
1	0A	6/8 (75%)	6 (100%)	0	0	100	100
1	1	6/8 (75%)	6 (100%)	0	0	100	100
1	1A	6/8 (75%)	6 (100%)	0	0	100	100
1	2	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	2A	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	3	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	3A	6/8 (75%)	6 (100%)	0	0	100	100
1	4	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	4A	6/8 (75%)	6 (100%)	0	0	100	100
1	5	6/8 (75%)	6 (100%)	0	0	100	100
1	5A	6/8 (75%)	6 (100%)	0	0	100	100
1	6	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	6A	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	7	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	7A	6/8 (75%)	6 (100%)	0	0	100	100
1	8	6/8 (75%)	6 (100%)	0	0	100	100
1	8A	6/8 (75%)	6 (100%)	0	0	100	100
1	9	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	9A	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	A	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	AA	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	AB	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BB	6/8 (75%)	6 (100%)	0	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	CB	6/8 (75%)	6 (100%)	0	0	100	100
1	D	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	DA	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	DB	6/8 (75%)	5 (83%)	1 (17%)	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	EB	6/8 (75%)	6 (100%)	0	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	FB	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%)	5 (83%)	1 (17%)	0	100	100
1	GB	6/8 (75%)	5 (83%)	1 (17%)	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	HB	6/8 (75%)	6 (100%)	0	0	100	100
1	I	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	IA	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	IB	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	JB	6/8 (75%)	6 (100%)	0	0	100	100
1	K	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	KA	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	KB	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	L	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	LA	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	LB	6/8 (75%)	6 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	MA	6/8 (75%)	6 (100%)	0	0	100	100
1	MB	6/8 (75%)	6 (100%)	0	0	100	100
1	N	6/8 (75%)	6 (100%)	0	0	100	100
1	NA	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	NB	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	O	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	OA	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	OB	6/8 (75%)	6 (100%)	0	0	100	100
1	P	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	PA	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	PB	6/8 (75%)	6 (100%)	0	0	100	100
1	Q	6/8 (75%)	6 (100%)	0	0	100	100
1	QA	6/8 (75%)	6 (100%)	0	0	100	100
1	QB	6/8 (75%)	6 (100%)	0	0	100	100
1	R	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	RA	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	RB	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	S	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	SA	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	SB	6/8 (75%)	6 (100%)	0	0	100	100
1	T	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	TA	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	TB	6/8 (75%)	6 (100%)	0	0	100	100
1	U	6/8 (75%)	6 (100%)	0	0	100	100
1	UA	6/8 (75%)	6 (100%)	0	0	100	100
1	V	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	VA	6/8 (75%)	6 (100%)	0	0	100	100
1	W	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	WA	6/8 (75%)	6 (100%)	0	0	100	100
1	X	6/8 (75%)	6 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	XA	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	Y	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	YA	6/8 (75%)	6 (100%)	0	0	100	100
1	Z	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	ZA	6/8 (75%)	6 (100%)	0	0	100	100
1	a	6/8 (75%)	6 (100%)	0	0	100	100
1	aA	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	b	6/8 (75%)	6 (100%)	0	0	100	100
1	bA	6/8 (75%)	6 (100%)	0	0	100	100
1	c	6/8 (75%)	6 (100%)	0	0	100	100
1	cA	6/8 (75%)	6 (100%)	0	0	100	100
1	d	6/8 (75%)	6 (100%)	0	0	100	100
1	dA	6/8 (75%)	6 (100%)	0	0	100	100
1	e	6/8 (75%)	6 (100%)	0	0	100	100
1	eA	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	f	6/8 (75%)	6 (100%)	0	0	100	100
1	fA	6/8 (75%)	6 (100%)	0	0	100	100
1	g	6/8 (75%)	6 (100%)	0	0	100	100
1	gA	6/8 (75%)	6 (100%)	0	0	100	100
1	h	6/8 (75%)	6 (100%)	0	0	100	100
1	hA	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	i	6/8 (75%)	6 (100%)	0	0	100	100
1	iA	6/8 (75%)	6 (100%)	0	0	100	100
1	j	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	jA	6/8 (75%)	6 (100%)	0	0	100	100
1	k	6/8 (75%)	6 (100%)	0	0	100	100
1	kA	6/8 (75%)	6 (100%)	0	0	100	100
1	l	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	lA	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	m	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	mA	6/8 (75%)	6 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	n	6/8 (75%)	6 (100%)	0	0	100	100
1	nA	6/8 (75%)	6 (100%)	0	0	100	100
1	o	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	oA	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	p	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	pA	6/8 (75%)	6 (100%)	0	0	100	100
1	q	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	qA	6/8 (75%)	6 (100%)	0	0	100	100
1	r	6/8 (75%)	6 (100%)	0	0	100	100
1	rA	6/8 (75%)	6 (100%)	0	0	100	100
1	s	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	sA	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	t	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	tA	6/8 (75%)	6 (100%)	0	0	100	100
1	u	6/8 (75%)	6 (100%)	0	0	100	100
1	uA	6/8 (75%)	6 (100%)	0	0	100	100
1	v	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	vA	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	w	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	wA	6/8 (75%)	6 (100%)	0	0	100	100
1	x	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	xA	6/8 (75%)	6 (100%)	0	0	100	100
1	y	6/8 (75%)	6 (100%)	0	0	100	100
1	yA	6/8 (75%)	6 (100%)	0	0	100	100
1	z	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	zA	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
All	All	864/1152 (75%)	792 (92%)	72 (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%)	5 (83%)	1 (17%)	2 8
1	0A	6/6 (100%)	6 (100%)	0	100 100
1	1	6/6 (100%)	4 (67%)	2 (33%)	0 1
1	1A	6/6 (100%)	6 (100%)	0	100 100
1	2	6/6 (100%)	6 (100%)	0	100 100
1	2A	6/6 (100%)	5 (83%)	1 (17%)	2 8
1	3	6/6 (100%)	5 (83%)	1 (17%)	2 8
1	3A	6/6 (100%)	6 (100%)	0	100 100
1	4	6/6 (100%)	6 (100%)	0	100 100
1	4A	6/6 (100%)	6 (100%)	0	100 100
1	5	6/6 (100%)	4 (67%)	2 (33%)	0 1
1	5A	6/6 (100%)	4 (67%)	2 (33%)	0 1
1	6	6/6 (100%)	6 (100%)	0	100 100
1	6A	6/6 (100%)	5 (83%)	1 (17%)	2 8
1	7	6/6 (100%)	5 (83%)	1 (17%)	2 8
1	7A	6/6 (100%)	6 (100%)	0	100 100
1	8	6/6 (100%)	4 (67%)	2 (33%)	0 1
1	8A	6/6 (100%)	6 (100%)	0	100 100
1	9	6/6 (100%)	6 (100%)	0	100 100
1	9A	6/6 (100%)	5 (83%)	1 (17%)	2 8
1	A	6/6 (100%)	6 (100%)	0	100 100
1	AA	6/6 (100%)	5 (83%)	1 (17%)	2 8
1	AB	6/6 (100%)	6 (100%)	0	100 100
1	B	6/6 (100%)	6 (100%)	0	100 100
1	BA	6/6 (100%)	6 (100%)	0	100 100
1	BB	6/6 (100%)	6 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	6/6 (100%)	6 (100%)	0	100 100
1	CA	6/6 (100%)	4 (67%)	2 (33%)	0 1
1	CB	6/6 (100%)	4 (67%)	2 (33%)	0 1
1	D	6/6 (100%)	6 (100%)	0	100 100
1	DA	6/6 (100%)	6 (100%)	0	100 100
1	DB	6/6 (100%)	5 (83%)	1 (17%)	2 8
1	E	6/6 (100%)	6 (100%)	0	100 100
1	EA	6/6 (100%)	5 (83%)	1 (17%)	2 8
1	EB	6/6 (100%)	6 (100%)	0	100 100
1	F	6/6 (100%)	6 (100%)	0	100 100
1	FA	6/6 (100%)	4 (67%)	2 (33%)	0 1
1	FB	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	GB	6/6 (100%)	5 (83%)	1 (17%)	2 8
1	H	6/6 (100%)	6 (100%)	0	100 100
1	HA	6/6 (100%)	5 (83%)	1 (17%)	2 8
1	HB	6/6 (100%)	6 (100%)	0	100 100
1	I	6/6 (100%)	6 (100%)	0	100 100
1	IA	6/6 (100%)	6 (100%)	0	100 100
1	IB	6/6 (100%)	6 (100%)	0	100 100
1	J	6/6 (100%)	4 (67%)	2 (33%)	0 1
1	JA	6/6 (100%)	4 (67%)	2 (33%)	0 1
1	JB	6/6 (100%)	5 (83%)	1 (17%)	2 8
1	K	6/6 (100%)	6 (100%)	0	100 100
1	KA	6/6 (100%)	6 (100%)	0	100 100
1	KB	6/6 (100%)	5 (83%)	1 (17%)	2 8
1	L	6/6 (100%)	5 (83%)	1 (17%)	2 8
1	LA	6/6 (100%)	5 (83%)	1 (17%)	2 8
1	LB	6/6 (100%)	6 (100%)	0	100 100
1	M	6/6 (100%)	6 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	MA	6/6 (100%)	4 (67%)	2 (33%)	0 1
1	MB	6/6 (100%)	6 (100%)	0	100 100
1	N	6/6 (100%)	4 (67%)	2 (33%)	0 1
1	NA	6/6 (100%)	6 (100%)	0	100 100
1	NB	6/6 (100%)	5 (83%)	1 (17%)	2 8
1	O	6/6 (100%)	6 (100%)	0	100 100
1	OA	6/6 (100%)	5 (83%)	1 (17%)	2 8
1	OB	6/6 (100%)	6 (100%)	0	100 100
1	P	6/6 (100%)	5 (83%)	1 (17%)	2 8
1	PA	6/6 (100%)	6 (100%)	0	100 100
1	PB	6/6 (100%)	6 (100%)	0	100 100
1	Q	6/6 (100%)	4 (67%)	2 (33%)	0 1
1	QA	6/6 (100%)	4 (67%)	2 (33%)	0 1
1	QB	6/6 (100%)	4 (67%)	2 (33%)	0 1
1	R	6/6 (100%)	6 (100%)	0	100 100
1	RA	6/6 (100%)	6 (100%)	0	100 100
1	RB	6/6 (100%)	5 (83%)	1 (17%)	2 8
1	S	6/6 (100%)	5 (83%)	1 (17%)	2 8
1	SA	6/6 (100%)	5 (83%)	1 (17%)	2 8
1	SB	6/6 (100%)	6 (100%)	0	100 100
1	T	6/6 (100%)	6 (100%)	0	100 100
1	TA	6/6 (100%)	5 (83%)	1 (17%)	2 8
1	TB	6/6 (100%)	6 (100%)	0	100 100
1	U	6/6 (100%)	4 (67%)	2 (33%)	0 1
1	UA	6/6 (100%)	6 (100%)	0	100 100
1	V	6/6 (100%)	6 (100%)	0	100 100
1	VA	6/6 (100%)	6 (100%)	0	100 100
1	W	6/6 (100%)	5 (83%)	1 (17%)	2 8
1	WA	6/6 (100%)	4 (67%)	2 (33%)	0 1
1	X	6/6 (100%)	4 (67%)	2 (33%)	0 1
1	XA	6/6 (100%)	5 (83%)	1 (17%)	2 8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	Y	6/6 (100%)	6 (100%)	0	100 100
1	YA	6/6 (100%)	6 (100%)	0	100 100
1	Z	6/6 (100%)	5 (83%)	1 (17%)	2 8
1	ZA	6/6 (100%)	6 (100%)	0	100 100
1	a	6/6 (100%)	4 (67%)	2 (33%)	0 1
1	aA	6/6 (100%)	5 (83%)	1 (17%)	2 8
1	b	6/6 (100%)	5 (83%)	1 (17%)	2 8
1	bA	6/6 (100%)	6 (100%)	0	100 100
1	c	6/6 (100%)	4 (67%)	2 (33%)	0 1
1	cA	6/6 (100%)	6 (100%)	0	100 100
1	d	6/6 (100%)	4 (67%)	2 (33%)	0 1
1	dA	6/6 (100%)	4 (67%)	2 (33%)	0 1
1	e	6/6 (100%)	4 (67%)	2 (33%)	0 1
1	eA	6/6 (100%)	5 (83%)	1 (17%)	2 8
1	f	6/6 (100%)	4 (67%)	2 (33%)	0 1
1	fA	6/6 (100%)	6 (100%)	0	100 100
1	g	6/6 (100%)	4 (67%)	2 (33%)	0 1
1	gA	6/6 (100%)	6 (100%)	0	100 100
1	h	6/6 (100%)	5 (83%)	1 (17%)	2 8
1	hA	6/6 (100%)	5 (83%)	1 (17%)	2 8
1	i	6/6 (100%)	4 (67%)	2 (33%)	0 1
1	iA	6/6 (100%)	6 (100%)	0	100 100
1	j	6/6 (100%)	6 (100%)	0	100 100
1	jA	6/6 (100%)	6 (100%)	0	100 100
1	k	6/6 (100%)	4 (67%)	2 (33%)	0 1
1	kA	6/6 (100%)	4 (67%)	2 (33%)	0 1
1	l	6/6 (100%)	6 (100%)	0	100 100
1	lA	6/6 (100%)	5 (83%)	1 (17%)	2 8
1	m	6/6 (100%)	5 (83%)	1 (17%)	2 8
1	mA	6/6 (100%)	6 (100%)	0	100 100
1	n	6/6 (100%)	4 (67%)	2 (33%)	0 1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	nA	6/6 (100%)	6 (100%)	0	100 100
1	o	6/6 (100%)	6 (100%)	0	100 100
1	oA	6/6 (100%)	5 (83%)	1 (17%)	2 8
1	p	6/6 (100%)	5 (83%)	1 (17%)	2 8
1	pA	6/6 (100%)	6 (100%)	0	100 100
1	q	6/6 (100%)	6 (100%)	0	100 100
1	qA	6/6 (100%)	6 (100%)	0	100 100
1	r	6/6 (100%)	4 (67%)	2 (33%)	0 1
1	rA	6/6 (100%)	4 (67%)	2 (33%)	0 1
1	s	6/6 (100%)	6 (100%)	0	100 100
1	sA	6/6 (100%)	5 (83%)	1 (17%)	2 8
1	t	6/6 (100%)	5 (83%)	1 (17%)	2 8
1	tA	6/6 (100%)	6 (100%)	0	100 100
1	u	6/6 (100%)	4 (67%)	2 (33%)	0 1
1	uA	6/6 (100%)	6 (100%)	0	100 100
1	v	6/6 (100%)	6 (100%)	0	100 100
1	vA	6/6 (100%)	5 (83%)	1 (17%)	2 8
1	w	6/6 (100%)	5 (83%)	1 (17%)	2 8
1	wA	6/6 (100%)	6 (100%)	0	100 100
1	x	6/6 (100%)	6 (100%)	0	100 100
1	xA	6/6 (100%)	6 (100%)	0	100 100
1	y	6/6 (100%)	4 (67%)	2 (33%)	0 1
1	yA	6/6 (100%)	5 (83%)	1 (17%)	2 8
1	z	6/6 (100%)	6 (100%)	0	100 100
1	zA	6/6 (100%)	5 (83%)	1 (17%)	2 8
All	All	864/864 (100%)	760 (88%)	104 (12%)	8 19

5 of 104 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	WA	1002	LYS
1	d	2	LYS
1	i	4	GLU

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Mol	Chain	Res	Type
1	XA	1104	GLU
1	c	2	LYS

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)

288 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	GMA	AA	308	1	9,9,9	1.17	1 (11%)	10,11,11	1.26	0
1	5CR	sA	1101	1	13,14,15	1.21	1 (7%)	16,17,19	1.25	2 (12%)
1	5CR	tA	1201	1	13,14,15	1.23	1 (7%)	16,17,19	1.14	1 (6%)
1	5CR	f	1	1	13,14,15	1.28	2 (15%)	16,17,19	1.74	4 (25%)
1	5CR	AB	201	1	13,14,15	1.22	1 (7%)	16,17,19	1.15	1 (6%)
1	5CR	CB	1001	1	13,14,15	1.28	2 (15%)	16,17,19	1.74	4 (25%)
1	5CR	h	1	1	13,14,15	1.28	1 (7%)	16,17,19	1.73	4 (25%)
1	5CR	RB	1101	1	13,14,15	1.21	1 (7%)	16,17,19	1.25	2 (12%)
1	GMA	V	1208	1	9,9,9	1.18	1 (11%)	10,11,11	1.26	1 (10%)
1	GMA	1	108	1	9,9,9	1.13	1 (11%)	10,11,11	1.22	1 (10%)
1	GMA	5	1108	1	9,9,9	1.13	0	10,11,11	1.22	1 (10%)
1	5CR	9	201	1	13,14,15	1.24	1 (7%)	16,17,19	1.33	2 (12%)
1	GMA	FA	108	1	9,9,9	1.15	1 (11%)	10,11,11	1.24	1 (10%)
1	GMA	VA	308	1	9,9,9	1.16	1 (11%)	10,11,11	1.33	0
1	GMA	fA	1208	1	9,9,9	1.18	1 (11%)	10,11,11	1.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	GMA	vA	108	1	9,9,9	1.15	1 (11%)	10,11,11	1.18	0
1	5CR	5	1101	1	13,14,15	1.23	1 (7%)	16,17,19	1.51	2 (12%)
1	5CR	bA	201	1	13,14,15	1.21	1 (7%)	16,17,19	1.14	1 (6%)
1	GMA	B	8	1	9,9,9	1.15	1 (11%)	10,11,11	1.25	0
1	5CR	n	101	1	13,14,15	1.23	1 (7%)	16,17,19	1.51	2 (12%)
1	5CR	GB	101	1	13,14,15	1.23	1 (7%)	16,17,19	1.24	2 (12%)
1	5CR	U	1101	1	13,14,15	1.22	1 (7%)	16,17,19	1.52	2 (12%)
1	GMA	v	208	1	9,9,9	1.16	1 (11%)	10,11,11	1.25	0
1	GMA	2A	108	1	9,9,9	1.15	1 (11%)	10,11,11	1.17	0
1	5CR	P	1301	1	13,14,15	1.23	2 (15%)	16,17,19	1.28	3 (18%)
1	5CR	YA	1201	1	13,14,15	1.22	1 (7%)	16,17,19	1.14	1 (6%)
1	GMA	FB	1308	1	9,9,9	1.14	1 (11%)	10,11,11	1.32	0
1	5CR	zA	1101	1	13,14,15	1.21	1 (7%)	16,17,19	1.26	2 (12%)
1	5CR	LB	1201	1	13,14,15	1.22	1 (7%)	16,17,19	1.14	1 (6%)
1	GMA	z	1208	1	9,9,9	1.17	1 (11%)	10,11,11	1.26	1 (10%)
1	5CR	6	1201	1	13,14,15	1.25	2 (15%)	16,17,19	1.34	2 (12%)
1	5CR	x	1001	1	13,14,15	1.22	2 (15%)	16,17,19	1.69	3 (18%)
1	5CR	c	1	1	13,14,15	1.27	1 (7%)	16,17,19	1.73	4 (25%)
1	GMA	IA	1008	1	9,9,9	1.15	0	10,11,11	1.26	0
1	GMA	N	1108	1	9,9,9	1.15	1 (11%)	10,11,11	1.24	1 (10%)
1	5CR	8	101	1	13,14,15	1.24	1 (7%)	16,17,19	1.51	2 (12%)
1	GMA	I	8	1	9,9,9	1.16	1 (11%)	10,11,11	1.27	1 (10%)
1	GMA	bA	208	1	9,9,9	1.18	1 (11%)	10,11,11	1.12	0
1	GMA	b	8	1	9,9,9	1.19	1 (11%)	10,11,11	1.16	0
1	GMA	KB	1108	1	9,9,9	1.15	1 (11%)	10,11,11	1.18	0
1	GMA	RB	1108	1	9,9,9	1.14	1 (11%)	10,11,11	1.17	0
1	GMA	2	208	1	9,9,9	1.17	1 (11%)	10,11,11	1.26	1 (10%)
1	5CR	l	1201	1	13,14,15	1.24	2 (15%)	16,17,19	1.34	2 (12%)
1	5CR	y	1101	1	13,14,15	1.23	1 (7%)	16,17,19	1.51	2 (12%)
1	GMA	w	308	1	9,9,9	1.15	1 (11%)	10,11,11	1.23	0
1	GMA	R	208	1	9,9,9	1.18	1 (11%)	10,11,11	1.27	1 (10%)
1	5CR	AA	301	1	13,14,15	1.22	2 (15%)	16,17,19	1.28	3 (18%)
1	5CR	fA	1201	1	13,14,15	1.22	1 (7%)	16,17,19	1.13	1 (6%)
1	5CR	BB	301	1	13,14,15	1.22	1 (7%)	16,17,19	1.03	1 (6%)
1	GMA	CB	1008	1	9,9,9	1.19	1 (11%)	10,11,11	1.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	GMA	BA	1008	1	9,9,9	1.13	0	10,11,11	1.25	0
1	5CR	TB	1301	1	13,14,15	1.22	1 (7%)	16,17,19	1.03	1 (6%)
1	5CR	EA	1301	1	13,14,15	1.22	2 (15%)	16,17,19	1.29	3 (18%)
1	5CR	3A	201	1	13,14,15	1.23	1 (7%)	16,17,19	1.14	1 (6%)
1	GMA	KA	1208	1	9,9,9	1.18	1 (11%)	10,11,11	1.27	2 (20%)
1	5CR	E	1	1	13,14,15	1.22	1 (7%)	16,17,19	1.69	3 (18%)
1	5CR	W	1301	1	13,14,15	1.22	2 (15%)	16,17,19	1.28	3 (18%)
1	GMA	XA	1108	1	9,9,9	1.16	1 (11%)	10,11,11	1.19	0
1	GMA	6	1208	1	9,9,9	1.17	1 (11%)	10,11,11	1.26	1 (10%)
1	5CR	z	1201	1	13,14,15	1.25	1 (7%)	16,17,19	1.33	2 (12%)
1	GMA	zA	1108	1	9,9,9	1.15	1 (11%)	10,11,11	1.18	0
1	5CR	i	1	1	13,14,15	1.28	2 (15%)	16,17,19	1.73	4 (25%)
1	GMA	xA	308	1	9,9,9	1.14	1 (11%)	10,11,11	1.32	0
1	GMA	i	8	1	9,9,9	1.19	1 (11%)	10,11,11	1.16	0
1	5CR	Q	101	1	13,14,15	1.21	1 (7%)	16,17,19	1.52	2 (12%)
1	5CR	B	1	1	13,14,15	1.23	2 (15%)	16,17,19	1.70	3 (18%)
1	5CR	4	1001	1	13,14,15	1.22	1 (7%)	16,17,19	1.70	3 (18%)
1	5CR	SA	1301	1	13,14,15	1.23	2 (15%)	16,17,19	1.28	3 (18%)
1	5CR	hA	101	1	13,14,15	1.23	1 (7%)	16,17,19	1.26	2 (12%)
1	5CR	u	101	1	13,14,15	1.23	1 (7%)	16,17,19	1.51	2 (12%)
1	GMA	DB	1108	1	9,9,9	1.16	1 (11%)	10,11,11	1.19	0
1	5CR	C	1	1	13,14,15	1.22	2 (15%)	16,17,19	1.69	3 (18%)
1	5CR	SB	1201	1	13,14,15	1.21	1 (7%)	16,17,19	1.14	1 (6%)
1	5CR	V	1201	1	13,14,15	1.24	1 (7%)	16,17,19	1.34	2 (12%)
1	5CR	mA	1201	1	13,14,15	1.23	1 (7%)	16,17,19	1.14	1 (6%)
1	GMA	CA	1108	1	9,9,9	1.13	0	10,11,11	1.21	0
1	5CR	0	1301	1	13,14,15	1.24	2 (15%)	16,17,19	1.27	3 (18%)
1	GMA	sA	1108	1	9,9,9	1.15	1 (11%)	10,11,11	1.18	0
1	5CR	xA	301	1	13,14,15	1.21	1 (7%)	16,17,19	1.03	1 (6%)
1	5CR	JA	1101	1	13,14,15	1.23	1 (7%)	16,17,19	1.50	2 (12%)
1	5CR	w	301	1	13,14,15	1.23	2 (15%)	16,17,19	1.27	3 (18%)
1	5CR	IB	301	1	13,14,15	1.23	1 (7%)	16,17,19	1.02	1 (6%)
1	GMA	J	108	1	9,9,9	1.15	1 (11%)	10,11,11	1.23	1 (10%)
1	5CR	GA	201	1	13,14,15	1.23	1 (7%)	16,17,19	1.34	3 (18%)
1	GMA	EA	1308	1	9,9,9	1.16	1 (11%)	10,11,11	1.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	5CR	DB	1101	1	13,14,15	1.23	1 (7%)	16,17,19	1.25	2 (12%)
1	5CR	CA	1101	1	13,14,15	1.24	1 (7%)	16,17,19	1.52	2 (12%)
1	GMA	6A	1108	1	9,9,9	1.15	1 (11%)	10,11,11	1.18	0
1	GMA	y	1108	1	9,9,9	1.14	0	10,11,11	1.22	0
1	5CR	pA	201	1	13,14,15	1.23	1 (7%)	16,17,19	1.15	1 (6%)
1	5CR	EB	1201	1	13,14,15	1.22	1 (7%)	16,17,19	1.14	1 (6%)
1	GMA	d	8	1	9,9,9	1.18	1 (11%)	10,11,11	1.15	0
1	GMA	o	208	1	9,9,9	1.16	1 (11%)	10,11,11	1.26	0
1	5CR	O	1201	1	13,14,15	1.23	1 (7%)	16,17,19	1.33	2 (12%)
1	5CR	X	101	1	13,14,15	1.24	1 (7%)	16,17,19	1.51	2 (12%)
1	GMA	gA	1308	1	9,9,9	1.15	1 (11%)	10,11,11	1.33	0
1	GMA	p	308	1	9,9,9	1.16	1 (11%)	10,11,11	1.23	0
1	GMA	3	308	1	9,9,9	1.17	1 (11%)	10,11,11	1.24	0
1	GMA	HA	308	1	9,9,9	1.17	1 (11%)	10,11,11	1.24	0
1	5CR	2	201	1	13,14,15	1.25	2 (15%)	16,17,19	1.33	2 (12%)
1	5CR	yA	1001	1	13,14,15	1.28	2 (15%)	16,17,19	1.73	4 (25%)
1	GMA	s	1208	1	9,9,9	1.17	1 (11%)	10,11,11	1.26	1 (10%)
1	GMA	lA	1108	1	9,9,9	1.14	1 (11%)	10,11,11	1.18	0
1	5CR	OA	301	1	13,14,15	1.23	2 (15%)	16,17,19	1.28	3 (18%)
1	GMA	7A	1208	1	9,9,9	1.18	1 (11%)	10,11,11	1.14	0
1	5CR	BA	1001	1	13,14,15	1.21	1 (7%)	16,17,19	1.70	3 (18%)
1	GMA	kA	1008	1	9,9,9	1.18	1 (11%)	10,11,11	1.14	0
1	GMA	AB	208	1	9,9,9	1.18	1 (11%)	10,11,11	1.13	0
1	5CR	wA	201	1	13,14,15	1.21	1 (7%)	16,17,19	1.15	1 (6%)
1	5CR	DA	1201	1	13,14,15	1.24	1 (7%)	16,17,19	1.33	2 (12%)
1	5CR	m	1301	1	13,14,15	1.24	2 (15%)	16,17,19	1.27	3 (18%)
1	5CR	6A	1101	1	13,14,15	1.21	1 (7%)	16,17,19	1.25	2 (12%)
1	GMA	P	1308	1	9,9,9	1.17	1 (11%)	10,11,11	1.24	0
1	GMA	L	308	1	9,9,9	1.17	1 (11%)	10,11,11	1.25	0
1	GMA	x	1008	1	9,9,9	1.16	1 (11%)	10,11,11	1.26	0
1	5CR	K	201	1	13,14,15	1.24	1 (7%)	16,17,19	1.32	2 (12%)
1	5CR	aA	101	1	13,14,15	1.21	1 (7%)	16,17,19	1.25	2 (12%)
1	GMA	qA	308	1	9,9,9	1.14	1 (11%)	10,11,11	1.32	0
1	GMA	HB	208	1	9,9,9	1.19	1 (11%)	10,11,11	1.14	0
1	GMA	e	8	1	9,9,9	1.20	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	GMA	T	1008	1	9,9,9	1.15	1 (11%)	10,11,11	1.26	1 (10%)
1	GMA	LB	1208	1	9,9,9	1.19	1 (11%)	10,11,11	1.14	0
1	5CR	HA	301	1	13,14,15	1.21	2 (15%)	16,17,19	1.28	3 (18%)
1	GMA	JB	1008	1	9,9,9	1.18	1 (11%)	10,11,11	1.14	0
1	GMA	G	8	1	9,9,9	1.13	0	10,11,11	1.25	0
1	5CR	VA	301	1	13,14,15	1.23	1 (7%)	16,17,19	1.02	1 (6%)
1	GMA	hA	108	1	9,9,9	1.14	1 (11%)	10,11,11	1.18	0
1	5CR	WA	1001	1	13,14,15	1.28	2 (15%)	16,17,19	1.74	4 (25%)
1	5CR	dA	1001	1	13,14,15	1.27	2 (15%)	16,17,19	1.74	4 (25%)
1	GMA	eA	1108	1	9,9,9	1.15	1 (11%)	10,11,11	1.20	0
1	GMA	PA	1008	1	9,9,9	1.16	1 (11%)	10,11,11	1.27	1 (10%)
1	5CR	qA	301	1	13,14,15	1.24	1 (7%)	16,17,19	1.01	1 (6%)
1	GMA	M	1008	1	9,9,9	1.14	1 (11%)	10,11,11	1.24	0
1	GMA	SB	1208	1	9,9,9	1.19	1 (11%)	10,11,11	1.12	0
1	GMA	q	1008	1	9,9,9	1.16	1 (11%)	10,11,11	1.26	0
1	GMA	cA	308	1	9,9,9	1.16	1 (11%)	10,11,11	1.33	0
1	5CR	QA	1101	1	13,14,15	1.23	1 (7%)	16,17,19	1.51	2 (12%)
1	GMA	yA	1008	1	9,9,9	1.20	1 (11%)	10,11,11	1.16	0
1	GMA	SA	1308	1	9,9,9	1.17	1 (11%)	10,11,11	1.24	0
1	5CR	G	1	1	13,14,15	1.20	1 (7%)	16,17,19	1.70	3 (18%)
1	5CR	IA	1001	1	13,14,15	1.23	2 (15%)	16,17,19	1.69	3 (18%)
1	GMA	JA	1108	1	9,9,9	1.14	1 (11%)	10,11,11	1.23	1 (10%)
1	GMA	U	1108	1	9,9,9	1.14	1 (11%)	10,11,11	1.23	1 (10%)
1	5CR	T	1001	1	13,14,15	1.23	2 (15%)	16,17,19	1.70	3 (18%)
1	GMA	WA	1008	1	9,9,9	1.18	1 (11%)	10,11,11	1.14	0
1	GMA	rA	1008	1	9,9,9	1.19	1 (11%)	10,11,11	1.14	0
1	GMA	GB	108	1	9,9,9	1.15	1 (11%)	10,11,11	1.18	0
1	5CR	LA	1301	1	13,14,15	1.21	2 (15%)	16,17,19	1.28	3 (18%)
1	5CR	Y	201	1	13,14,15	1.24	2 (15%)	16,17,19	1.34	2 (12%)
1	5CR	b	1	1	13,14,15	1.27	2 (15%)	16,17,19	1.74	4 (25%)
1	5CR	ZA	1301	1	13,14,15	1.23	1 (7%)	16,17,19	1.02	1 (6%)
1	5CR	eA	1101	1	13,14,15	1.21	1 (7%)	16,17,19	1.25	2 (12%)
1	GMA	Q	108	1	9,9,9	1.15	1 (11%)	10,11,11	1.23	1 (10%)
1	GMA	W	1308	1	9,9,9	1.18	1 (11%)	10,11,11	1.25	0
1	5CR	7	1301	1	13,14,15	1.23	2 (15%)	16,17,19	1.29	3 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	GMA	j	1008	1	9,9,9	1.15	1 (11%)	10,11,11	1.26	0
1	GMA	n	108	1	9,9,9	1.13	1 (11%)	10,11,11	1.23	1 (10%)
1	GMA	UA	208	1	9,9,9	1.19	1 (11%)	10,11,11	1.14	0
1	5CR	PA	1001	1	13,14,15	1.22	2 (15%)	16,17,19	1.71	3 (18%)
1	5CR	NB	101	1	13,14,15	1.21	1 (7%)	16,17,19	1.24	2 (12%)
1	GMA	wA	208	1	9,9,9	1.18	1 (11%)	10,11,11	1.13	0
1	GMA	BB	308	1	9,9,9	1.14	1 (11%)	10,11,11	1.31	0
1	GMA	k	1108	1	9,9,9	1.14	0	10,11,11	1.22	0
1	5CR	MB	1301	1	13,14,15	1.23	1 (7%)	16,17,19	1.03	1 (6%)
1	5CR	HB	201	1	13,14,15	1.22	1 (7%)	16,17,19	1.14	1 (6%)
1	GMA	h	8	1	9,9,9	1.18	1 (11%)	10,11,11	1.13	0
1	5CR	q	1001	1	13,14,15	1.22	2 (15%)	16,17,19	1.69	3 (18%)
1	5CR	jA	301	1	13,14,15	1.23	1 (7%)	16,17,19	1.02	1 (6%)
1	5CR	a	1	1	13,14,15	1.28	2 (15%)	16,17,19	1.74	4 (25%)
1	5CR	UA	201	1	13,14,15	1.22	1 (7%)	16,17,19	1.14	1 (6%)
1	5CR	uA	1301	1	13,14,15	1.23	1 (7%)	16,17,19	1.01	1 (6%)
1	GMA	YA	1208	1	9,9,9	1.19	1 (11%)	10,11,11	1.14	0
1	5CR	d	1	1	13,14,15	1.29	1 (7%)	16,17,19	1.73	4 (25%)
1	GMA	NB	108	1	9,9,9	1.13	1 (11%)	10,11,11	1.17	0
1	5CR	s	1201	1	13,14,15	1.24	1 (7%)	16,17,19	1.35	2 (12%)
1	GMA	7	1308	1	9,9,9	1.17	1 (11%)	10,11,11	1.24	0
1	5CR	k	1101	1	13,14,15	1.23	1 (7%)	16,17,19	1.51	2 (12%)
1	5CR	5A	1001	1	13,14,15	1.28	2 (15%)	16,17,19	1.74	4 (25%)
1	GMA	C	8	1	9,9,9	1.15	1 (11%)	10,11,11	1.26	0
1	5CR	N	1101	1	13,14,15	1.23	1 (7%)	16,17,19	1.51	2 (12%)
1	5CR	lA	1101	1	13,14,15	1.22	1 (7%)	16,17,19	1.26	2 (12%)
1	5CR	OB	201	1	13,14,15	1.21	1 (7%)	16,17,19	1.14	1 (6%)
1	GMA	S	308	1	9,9,9	1.17	1 (11%)	10,11,11	1.24	0
1	GMA	Z	308	1	9,9,9	1.16	1 (11%)	10,11,11	1.24	0
1	5CR	KB	1101	1	13,14,15	1.23	1 (7%)	16,17,19	1.24	2 (12%)
1	GMA	g	8	1	9,9,9	1.19	1 (11%)	10,11,11	1.15	0
1	5CR	j	1001	1	13,14,15	1.22	2 (15%)	16,17,19	1.69	3 (18%)
1	GMA	PB	308	1	9,9,9	1.14	1 (11%)	10,11,11	1.32	0
1	GMA	TB	1308	1	9,9,9	1.15	1 (11%)	10,11,11	1.33	0
1	GMA	0	1308	1	9,9,9	1.15	1 (11%)	10,11,11	1.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	5CR	1A	1301	1	13,14,15	1.21	1 (7%)	16,17,19	1.03	1 (6%)
1	5CR	S	301	1	13,14,15	1.22	2 (15%)	16,17,19	1.29	3 (18%)
1	5CR	F	1	1	13,14,15	1.22	1 (7%)	16,17,19	1.69	3 (18%)
1	5CR	KA	1201	1	13,14,15	1.24	1 (7%)	16,17,19	1.34	3 (18%)
1	GMA	pA	208	1	9,9,9	1.18	1 (11%)	10,11,11	1.13	0
1	GMA	O	1208	1	9,9,9	1.18	1 (11%)	10,11,11	1.27	0
1	GMA	DA	1208	1	9,9,9	1.19	1 (11%)	10,11,11	1.28	2 (20%)
1	GMA	OA	308	1	9,9,9	1.18	1 (11%)	10,11,11	1.25	0
1	5CR	g	1	1	13,14,15	1.28	2 (15%)	16,17,19	1.74	4 (25%)
1	5CR	iA	201	1	13,14,15	1.23	1 (7%)	16,17,19	1.15	1 (6%)
1	GMA	iA	208	1	9,9,9	1.19	1 (11%)	10,11,11	1.14	0
1	5CR	H	1	1	13,14,15	1.23	2 (15%)	16,17,19	1.69	3 (18%)
1	5CR	v	201	1	13,14,15	1.24	1 (7%)	16,17,19	1.34	2 (12%)
1	GMA	QA	1108	1	9,9,9	1.15	1 (11%)	10,11,11	1.23	1 (10%)
1	5CR	gA	1301	1	13,14,15	1.22	1 (7%)	16,17,19	1.02	1 (6%)
1	GMA	dA	1008	1	9,9,9	1.18	1 (11%)	10,11,11	1.15	0
1	GMA	GA	208	1	9,9,9	1.17	1 (11%)	10,11,11	1.27	2 (20%)
1	GMA	TA	108	1	9,9,9	1.15	1 (11%)	10,11,11	1.19	0
1	GMA	ZA	1308	1	9,9,9	1.15	1 (11%)	10,11,11	1.32	0
1	5CR	vA	101	1	13,14,15	1.21	1 (7%)	16,17,19	1.26	2 (12%)
1	GMA	mA	1208	1	9,9,9	1.19	1 (11%)	10,11,11	1.14	0
1	GMA	4A	308	1	9,9,9	1.14	1 (11%)	10,11,11	1.30	0
1	5CR	r	1101	1	13,14,15	1.22	1 (7%)	16,17,19	1.50	2 (12%)
1	GMA	F	8	1	9,9,9	1.14	1 (11%)	10,11,11	1.26	0
1	GMA	Y	208	1	9,9,9	1.18	1 (11%)	10,11,11	1.27	2 (20%)
1	GMA	t	1308	1	9,9,9	1.17	1 (11%)	10,11,11	1.24	0
1	5CR	TA	101	1	13,14,15	1.21	1 (7%)	16,17,19	1.25	2 (12%)
1	GMA	f	8	1	9,9,9	1.20	1 (11%)	10,11,11	1.15	0
1	5CR	nA	1301	1	13,14,15	1.23	1 (7%)	16,17,19	1.02	1 (6%)
1	5CR	9A	101	1	13,14,15	1.23	1 (7%)	16,17,19	1.25	2 (12%)
1	GMA	A	8	1	9,9,9	1.14	0	10,11,11	1.24	0
1	5CR	t	1301	1	13,14,15	1.22	2 (15%)	16,17,19	1.28	3 (18%)
1	GMA	LA	1308	1	9,9,9	1.17	1 (11%)	10,11,11	1.24	0
1	5CR	4A	301	1	13,14,15	1.22	1 (7%)	16,17,19	1.02	1 (6%)
1	5CR	RA	1201	1	13,14,15	1.24	1 (7%)	16,17,19	1.34	2 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	5CR	0A	1201	1	13,14,15	1.22	1 (7%)	16,17,19	1.15	1 (6%)
1	5CR	7A	1201	1	13,14,15	1.23	1 (7%)	16,17,19	1.14	1 (6%)
1	GMA	RA	1208	1	9,9,9	1.18	1 (11%)	10,11,11	1.28	2 (20%)
1	5CR	M	1001	1	13,14,15	1.22	1 (7%)	16,17,19	1.70	3 (18%)
1	5CR	R	201	1	13,14,15	1.24	2 (15%)	16,17,19	1.34	2 (12%)
1	5CR	p	301	1	13,14,15	1.22	2 (15%)	16,17,19	1.28	3 (18%)
1	5CR	e	1	1	13,14,15	1.29	2 (15%)	16,17,19	1.73	4 (25%)
1	GMA	nA	1308	1	9,9,9	1.14	1 (11%)	10,11,11	1.33	0
1	GMA	9A	108	1	9,9,9	1.15	1 (11%)	10,11,11	1.19	0
1	GMA	IB	308	1	9,9,9	1.16	1 (11%)	10,11,11	1.34	0
1	GMA	u	108	1	9,9,9	1.14	0	10,11,11	1.22	0
1	5CR	J	101	1	13,14,15	1.22	1 (7%)	16,17,19	1.51	2 (12%)
1	5CR	A	1	1	13,14,15	1.22	1 (7%)	16,17,19	1.71	3 (18%)
1	GMA	MA	108	1	9,9,9	1.15	1 (11%)	10,11,11	1.23	0
1	GMA	3A	208	1	9,9,9	1.18	1 (11%)	10,11,11	1.13	0
1	GMA	EB	1208	1	9,9,9	1.18	1 (11%)	10,11,11	1.13	0
1	GMA	uA	1308	1	9,9,9	1.14	1 (11%)	10,11,11	1.31	0
1	5CR	rA	1001	1	13,14,15	1.29	2 (15%)	16,17,19	1.73	4 (25%)
1	GMA	0A	1208	1	9,9,9	1.18	1 (11%)	10,11,11	1.14	0
1	GMA	l	1208	1	9,9,9	1.18	1 (11%)	10,11,11	1.27	2 (20%)
1	5CR	JB	1001	1	13,14,15	1.28	1 (7%)	16,17,19	1.74	4 (25%)
1	GMA	5A	1008	1	9,9,9	1.19	1 (11%)	10,11,11	1.15	0
1	GMA	D	8	1	9,9,9	1.16	0	10,11,11	1.26	0
1	5CR	QB	1001	1	13,14,15	1.28	1 (7%)	16,17,19	1.74	4 (25%)
1	GMA	a	8	1	9,9,9	1.18	1 (11%)	10,11,11	1.14	0
1	5CR	NA	201	1	13,14,15	1.24	1 (7%)	16,17,19	1.34	2 (12%)
1	GMA	MB	1308	1	9,9,9	1.15	1 (11%)	10,11,11	1.33	0
1	GMA	8A	1308	1	9,9,9	1.14	1 (11%)	10,11,11	1.31	0
1	5CR	o	201	1	13,14,15	1.24	1 (7%)	16,17,19	1.34	2 (12%)
1	5CR	cA	301	1	13,14,15	1.22	1 (7%)	16,17,19	1.01	1 (6%)
1	GMA	m	1308	1	9,9,9	1.17	1 (11%)	10,11,11	1.24	0
1	GMA	1A	1308	1	9,9,9	1.14	1 (11%)	10,11,11	1.32	0
1	5CR	kA	1001	1	13,14,15	1.28	1 (7%)	16,17,19	1.73	4 (25%)
1	5CR	D	1	1	13,14,15	1.22	2 (15%)	16,17,19	1.70	3 (18%)
1	5CR	oA	101	1	13,14,15	1.21	1 (7%)	16,17,19	1.25	2 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	GMA	4	1008	1	9,9,9	1.15	1 (11%)	10,11,11	1.27	1 (10%)
1	GMA	8	108	1	9,9,9	1.13	1 (11%)	10,11,11	1.22	0
1	GMA	tA	1208	1	9,9,9	1.18	1 (11%)	10,11,11	1.13	0
1	5CR	PB	301	1	13,14,15	1.22	1 (7%)	16,17,19	1.03	1 (6%)
1	GMA	X	108	1	9,9,9	1.13	0	10,11,11	1.22	0
1	GMA	c	8	1	9,9,9	1.18	1 (11%)	10,11,11	1.14	0
1	5CR	L	301	1	13,14,15	1.23	2 (15%)	16,17,19	1.28	3 (18%)
1	5CR	8A	1301	1	13,14,15	1.22	1 (7%)	16,17,19	1.02	1 (6%)
1	5CR	Z	301	1	13,14,15	1.24	2 (15%)	16,17,19	1.27	3 (18%)
1	5CR	FB	1301	1	13,14,15	1.22	1 (7%)	16,17,19	1.03	1 (6%)
1	GMA	aA	108	1	9,9,9	1.15	1 (11%)	10,11,11	1.21	0
1	5CR	3	301	1	13,14,15	1.24	2 (15%)	16,17,19	1.29	3 (18%)
1	GMA	QB	1008	1	9,9,9	1.19	1 (11%)	10,11,11	1.15	0
1	GMA	H	8	1	9,9,9	1.15	1 (11%)	10,11,11	1.26	0
1	5CR	I	1	1	13,14,15	1.22	1 (7%)	16,17,19	1.71	3 (18%)
1	GMA	oA	108	1	9,9,9	1.15	1 (11%)	10,11,11	1.18	0
1	5CR	XA	1101	1	13,14,15	1.21	1 (7%)	16,17,19	1.25	2 (12%)
1	5CR	MA	101	1	13,14,15	1.23	1 (7%)	16,17,19	1.51	2 (12%)
1	5CR	1	101	1	13,14,15	1.23	1 (7%)	16,17,19	1.51	2 (12%)
1	5CR	2A	101	1	13,14,15	1.21	1 (7%)	16,17,19	1.25	2 (12%)
1	GMA	jA	308	1	9,9,9	1.15	1 (11%)	10,11,11	1.34	0
1	GMA	OB	208	1	9,9,9	1.20	1 (11%)	10,11,11	1.13	0
1	GMA	r	1108	1	9,9,9	1.13	1 (11%)	10,11,11	1.22	1 (10%)
1	GMA	9	208	1	9,9,9	1.20	1 (11%)	10,11,11	1.28	2 (20%)
1	5CR	FA	101	1	13,14,15	1.23	1 (7%)	16,17,19	1.51	2 (12%)
1	GMA	NA	208	1	9,9,9	1.19	1 (11%)	10,11,11	1.29	2 (20%)
1	GMA	K	208	1	9,9,9	1.17	1 (11%)	10,11,11	1.26	0
1	GMA	E	8	1	9,9,9	1.17	1 (11%)	10,11,11	1.26	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	GMA	AA	308	1	-	1/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5CR	sA	1101	1	-	1/9/10/12	0/1/1/1
1	5CR	tA	1201	1	-	2/9/10/12	0/1/1/1
1	5CR	f	1	1	-	6/9/10/12	0/1/1/1
1	5CR	AB	201	1	-	2/9/10/12	0/1/1/1
1	5CR	CB	1001	1	-	6/9/10/12	0/1/1/1
1	5CR	h	1	1	-	6/9/10/12	0/1/1/1
1	5CR	RB	1101	1	-	1/9/10/12	0/1/1/1
1	GMA	V	1208	1	-	1/9/9/9	-
1	GMA	1	108	1	-	3/9/9/9	-
1	GMA	5	1108	1	-	3/9/9/9	-
1	5CR	9	201	1	-	4/9/10/12	0/1/1/1
1	GMA	FA	108	1	-	3/9/9/9	-
1	GMA	VA	308	1	-	0/9/9/9	-
1	GMA	fA	1208	1	-	4/9/9/9	-
1	GMA	vA	108	1	-	0/9/9/9	-
1	5CR	5	1101	1	-	2/9/10/12	0/1/1/1
1	5CR	bA	201	1	-	2/9/10/12	0/1/1/1
1	GMA	B	8	1	-	1/9/9/9	-
1	5CR	n	101	1	-	2/9/10/12	0/1/1/1
1	5CR	GB	101	1	-	1/9/10/12	0/1/1/1
1	5CR	U	1101	1	-	2/9/10/12	0/1/1/1
1	GMA	v	208	1	-	1/9/9/9	-
1	GMA	2A	108	1	-	0/9/9/9	-
1	5CR	P	1301	1	-	3/9/10/12	0/1/1/1
1	5CR	YA	1201	1	-	2/9/10/12	0/1/1/1
1	GMA	FB	1308	1	-	0/9/9/9	-
1	5CR	zA	1101	1	-	1/9/10/12	0/1/1/1
1	5CR	LB	1201	1	-	2/9/10/12	0/1/1/1
1	GMA	z	1208	1	-	1/9/9/9	-
1	5CR	6	1201	1	-	4/9/10/12	0/1/1/1
1	5CR	x	1001	1	-	0/9/10/12	0/1/1/1
1	5CR	c	1	1	-	6/9/10/12	0/1/1/1
1	GMA	IA	1008	1	-	1/9/9/9	-
1	GMA	N	1108	1	-	3/9/9/9	-
1	5CR	8	101	1	-	2/9/10/12	0/1/1/1
1	GMA	I	8	1	-	1/9/9/9	-
1	GMA	bA	208	1	-	4/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	GMA	b	8	1	-	8/9/9/9	-
1	GMA	KB	1108	1	-	0/9/9/9	-
1	GMA	RB	1108	1	-	0/9/9/9	-
1	GMA	2	208	1	-	1/9/9/9	-
1	5CR	l	1201	1	-	4/9/10/12	0/1/1/1
1	5CR	y	1101	1	-	2/9/10/12	0/1/1/1
1	GMA	w	308	1	-	1/9/9/9	-
1	GMA	R	208	1	-	1/9/9/9	-
1	5CR	AA	301	1	-	3/9/10/12	0/1/1/1
1	5CR	fA	1201	1	-	2/9/10/12	0/1/1/1
1	5CR	BB	301	1	-	4/9/10/12	0/1/1/1
1	GMA	CB	1008	1	-	8/9/9/9	-
1	GMA	BA	1008	1	-	1/9/9/9	-
1	5CR	TB	1301	1	-	4/9/10/12	0/1/1/1
1	5CR	EA	1301	1	-	3/9/10/12	0/1/1/1
1	5CR	3A	201	1	-	2/9/10/12	0/1/1/1
1	GMA	KA	1208	1	-	1/9/9/9	-
1	5CR	E	1	1	-	0/9/10/12	0/1/1/1
1	5CR	W	1301	1	-	3/9/10/12	0/1/1/1
1	GMA	XA	1108	1	-	0/9/9/9	-
1	GMA	6	1208	1	-	1/9/9/9	-
1	5CR	z	1201	1	-	4/9/10/12	0/1/1/1
1	GMA	zA	1108	1	-	0/9/9/9	-
1	5CR	i	1	1	-	6/9/10/12	0/1/1/1
1	GMA	xA	308	1	-	0/9/9/9	-
1	GMA	i	8	1	-	8/9/9/9	-
1	5CR	Q	101	1	-	2/9/10/12	0/1/1/1
1	5CR	B	1	1	-	0/9/10/12	0/1/1/1
1	5CR	4	1001	1	-	0/9/10/12	0/1/1/1
1	5CR	SA	1301	1	-	3/9/10/12	0/1/1/1
1	5CR	hA	101	1	-	1/9/10/12	0/1/1/1
1	5CR	u	101	1	-	2/9/10/12	0/1/1/1
1	GMA	DB	1108	1	-	0/9/9/9	-
1	5CR	C	1	1	-	0/9/10/12	0/1/1/1
1	5CR	SB	1201	1	-	2/9/10/12	0/1/1/1
1	5CR	V	1201	1	-	4/9/10/12	0/1/1/1
1	5CR	mA	1201	1	-	2/9/10/12	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	GMA	CA	1108	1	-	3/9/9/9	-
1	5CR	0	1301	1	-	3/9/10/12	0/1/1/1
1	GMA	sA	1108	1	-	0/9/9/9	-
1	5CR	xA	301	1	-	4/9/10/12	0/1/1/1
1	5CR	JA	1101	1	-	2/9/10/12	0/1/1/1
1	5CR	w	301	1	-	3/9/10/12	0/1/1/1
1	5CR	IB	301	1	-	4/9/10/12	0/1/1/1
1	GMA	J	108	1	-	3/9/9/9	-
1	5CR	GA	201	1	-	4/9/10/12	0/1/1/1
1	GMA	EA	1308	1	-	1/9/9/9	-
1	5CR	DB	1101	1	-	1/9/10/12	0/1/1/1
1	5CR	CA	1101	1	-	2/9/10/12	0/1/1/1
1	GMA	6A	1108	1	-	0/9/9/9	-
1	GMA	y	1108	1	-	3/9/9/9	-
1	5CR	pA	201	1	-	2/9/10/12	0/1/1/1
1	5CR	EB	1201	1	-	2/9/10/12	0/1/1/1
1	GMA	d	8	1	-	8/9/9/9	-
1	GMA	o	208	1	-	1/9/9/9	-
1	5CR	O	1201	1	-	4/9/10/12	0/1/1/1
1	5CR	X	101	1	-	2/9/10/12	0/1/1/1
1	GMA	gA	1308	1	-	0/9/9/9	-
1	GMA	p	308	1	-	1/9/9/9	-
1	GMA	3	308	1	-	1/9/9/9	-
1	GMA	HA	308	1	-	1/9/9/9	-
1	5CR	2	201	1	-	4/9/10/12	0/1/1/1
1	5CR	yA	1001	1	-	6/9/10/12	0/1/1/1
1	GMA	s	1208	1	-	1/9/9/9	-
1	GMA	lA	1108	1	-	0/9/9/9	-
1	5CR	OA	301	1	-	3/9/10/12	0/1/1/1
1	GMA	7A	1208	1	-	4/9/9/9	-
1	5CR	BA	1001	1	-	0/9/10/12	0/1/1/1
1	GMA	kA	1008	1	-	8/9/9/9	-
1	GMA	AB	208	1	-	4/9/9/9	-
1	5CR	wA	201	1	-	2/9/10/12	0/1/1/1
1	5CR	DA	1201	1	-	4/9/10/12	0/1/1/1
1	5CR	m	1301	1	-	3/9/10/12	0/1/1/1
1	5CR	6A	1101	1	-	1/9/10/12	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	GMA	P	1308	1	-	1/9/9/9	-
1	GMA	L	308	1	-	1/9/9/9	-
1	GMA	x	1008	1	-	1/9/9/9	-
1	5CR	K	201	1	-	4/9/10/12	0/1/1/1
1	5CR	aA	101	1	-	1/9/10/12	0/1/1/1
1	GMA	qA	308	1	-	0/9/9/9	-
1	GMA	HB	208	1	-	4/9/9/9	-
1	GMA	e	8	1	-	8/9/9/9	-
1	GMA	T	1008	1	-	1/9/9/9	-
1	GMA	LB	1208	1	-	4/9/9/9	-
1	5CR	HA	301	1	-	3/9/10/12	0/1/1/1
1	GMA	JB	1008	1	-	8/9/9/9	-
1	GMA	G	8	1	-	1/9/9/9	-
1	5CR	VA	301	1	-	4/9/10/12	0/1/1/1
1	GMA	hA	108	1	-	0/9/9/9	-
1	5CR	WA	1001	1	-	6/9/10/12	0/1/1/1
1	5CR	dA	1001	1	-	6/9/10/12	0/1/1/1
1	GMA	eA	1108	1	-	0/9/9/9	-
1	GMA	PA	1008	1	-	1/9/9/9	-
1	5CR	qA	301	1	-	4/9/10/12	0/1/1/1
1	GMA	M	1008	1	-	1/9/9/9	-
1	GMA	SB	1208	1	-	4/9/9/9	-
1	GMA	q	1008	1	-	1/9/9/9	-
1	GMA	cA	308	1	-	0/9/9/9	-
1	5CR	QA	1101	1	-	2/9/10/12	0/1/1/1
1	GMA	yA	1008	1	-	8/9/9/9	-
1	GMA	SA	1308	1	-	1/9/9/9	-
1	5CR	G	1	1	-	0/9/10/12	0/1/1/1
1	5CR	IA	1001	1	-	0/9/10/12	0/1/1/1
1	GMA	JA	1108	1	-	3/9/9/9	-
1	GMA	U	1108	1	-	3/9/9/9	-
1	5CR	T	1001	1	-	0/9/10/12	0/1/1/1
1	GMA	WA	1008	1	-	8/9/9/9	-
1	GMA	rA	1008	1	-	8/9/9/9	-
1	GMA	GB	108	1	-	0/9/9/9	-
1	5CR	LA	1301	1	-	3/9/10/12	0/1/1/1
1	5CR	Y	201	1	-	4/9/10/12	0/1/1/1
1	5CR	b	1	1	-	6/9/10/12	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5CR	ZA	1301	1	-	4/9/10/12	0/1/1/1
1	5CR	eA	1101	1	-	1/9/10/12	0/1/1/1
1	GMA	Q	108	1	-	3/9/9/9	-
1	GMA	W	1308	1	-	1/9/9/9	-
1	5CR	7	1301	1	-	3/9/10/12	0/1/1/1
1	GMA	j	1008	1	-	1/9/9/9	-
1	GMA	n	108	1	-	3/9/9/9	-
1	GMA	UA	208	1	-	4/9/9/9	-
1	5CR	PA	1001	1	-	0/9/10/12	0/1/1/1
1	5CR	NB	101	1	-	1/9/10/12	0/1/1/1
1	GMA	wA	208	1	-	4/9/9/9	-
1	GMA	BB	308	1	-	0/9/9/9	-
1	GMA	k	1108	1	-	3/9/9/9	-
1	5CR	MB	1301	1	-	4/9/10/12	0/1/1/1
1	5CR	HB	201	1	-	2/9/10/12	0/1/1/1
1	GMA	h	8	1	-	8/9/9/9	-
1	5CR	q	1001	1	-	0/9/10/12	0/1/1/1
1	5CR	jA	301	1	-	4/9/10/12	0/1/1/1
1	5CR	a	1	1	-	6/9/10/12	0/1/1/1
1	5CR	UA	201	1	-	2/9/10/12	0/1/1/1
1	5CR	uA	1301	1	-	4/9/10/12	0/1/1/1
1	GMA	YA	1208	1	-	4/9/9/9	-
1	5CR	d	1	1	-	6/9/10/12	0/1/1/1
1	GMA	NB	108	1	-	0/9/9/9	-
1	5CR	s	1201	1	-	4/9/10/12	0/1/1/1
1	GMA	7	1308	1	-	1/9/9/9	-
1	5CR	k	1101	1	-	2/9/10/12	0/1/1/1
1	5CR	5A	1001	1	-	6/9/10/12	0/1/1/1
1	GMA	C	8	1	-	1/9/9/9	-
1	5CR	N	1101	1	-	2/9/10/12	0/1/1/1
1	5CR	lA	1101	1	-	1/9/10/12	0/1/1/1
1	5CR	OB	201	1	-	2/9/10/12	0/1/1/1
1	GMA	S	308	1	-	1/9/9/9	-
1	GMA	Z	308	1	-	1/9/9/9	-
1	5CR	KB	1101	1	-	1/9/10/12	0/1/1/1
1	GMA	g	8	1	-	8/9/9/9	-
1	5CR	j	1001	1	-	0/9/10/12	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	GMA	PB	308	1	-	0/9/9/9	-
1	GMA	TB	1308	1	-	0/9/9/9	-
1	GMA	0	1308	1	-	1/9/9/9	-
1	5CR	1A	1301	1	-	4/9/10/12	0/1/1/1
1	5CR	S	301	1	-	3/9/10/12	0/1/1/1
1	5CR	F	1	1	-	0/9/10/12	0/1/1/1
1	5CR	KA	1201	1	-	4/9/10/12	0/1/1/1
1	GMA	pA	208	1	-	4/9/9/9	-
1	GMA	O	1208	1	-	1/9/9/9	-
1	GMA	DA	1208	1	-	1/9/9/9	-
1	GMA	OA	308	1	-	1/9/9/9	-
1	5CR	g	1	1	-	6/9/10/12	0/1/1/1
1	5CR	iA	201	1	-	2/9/10/12	0/1/1/1
1	GMA	iA	208	1	-	4/9/9/9	-
1	5CR	H	1	1	-	0/9/10/12	0/1/1/1
1	5CR	v	201	1	-	4/9/10/12	0/1/1/1
1	GMA	QA	1108	1	-	3/9/9/9	-
1	5CR	gA	1301	1	-	4/9/10/12	0/1/1/1
1	GMA	dA	1008	1	-	8/9/9/9	-
1	GMA	GA	208	1	-	1/9/9/9	-
1	GMA	TA	108	1	-	0/9/9/9	-
1	GMA	ZA	1308	1	-	0/9/9/9	-
1	5CR	vA	101	1	-	1/9/10/12	0/1/1/1
1	GMA	mA	1208	1	-	4/9/9/9	-
1	GMA	4A	308	1	-	0/9/9/9	-
1	5CR	r	1101	1	-	2/9/10/12	0/1/1/1
1	GMA	F	8	1	-	1/9/9/9	-
1	GMA	Y	208	1	-	1/9/9/9	-
1	GMA	t	1308	1	-	1/9/9/9	-
1	5CR	TA	101	1	-	1/9/10/12	0/1/1/1
1	GMA	f	8	1	-	8/9/9/9	-
1	5CR	nA	1301	1	-	4/9/10/12	0/1/1/1
1	5CR	9A	101	1	-	1/9/10/12	0/1/1/1
1	GMA	A	8	1	-	1/9/9/9	-
1	5CR	t	1301	1	-	3/9/10/12	0/1/1/1
1	GMA	LA	1308	1	-	1/9/9/9	-
1	5CR	4A	301	1	-	4/9/10/12	0/1/1/1
1	5CR	RA	1201	1	-	4/9/10/12	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5CR	0A	1201	1	-	2/9/10/12	0/1/1/1
1	5CR	7A	1201	1	-	2/9/10/12	0/1/1/1
1	GMA	RA	1208	1	-	1/9/9/9	-
1	5CR	M	1001	1	-	0/9/10/12	0/1/1/1
1	5CR	R	201	1	-	4/9/10/12	0/1/1/1
1	5CR	p	301	1	-	3/9/10/12	0/1/1/1
1	5CR	e	1	1	-	6/9/10/12	0/1/1/1
1	GMA	nA	1308	1	-	0/9/9/9	-
1	GMA	9A	108	1	-	0/9/9/9	-
1	GMA	IB	308	1	-	0/9/9/9	-
1	GMA	u	108	1	-	3/9/9/9	-
1	5CR	J	101	1	-	2/9/10/12	0/1/1/1
1	5CR	A	1	1	-	0/9/10/12	0/1/1/1
1	GMA	MA	108	1	-	3/9/9/9	-
1	GMA	3A	208	1	-	4/9/9/9	-
1	GMA	EB	1208	1	-	4/9/9/9	-
1	GMA	uA	1308	1	-	0/9/9/9	-
1	5CR	rA	1001	1	-	6/9/10/12	0/1/1/1
1	GMA	0A	1208	1	-	4/9/9/9	-
1	GMA	l	1208	1	-	1/9/9/9	-
1	5CR	JB	1001	1	-	6/9/10/12	0/1/1/1
1	GMA	5A	1008	1	-	8/9/9/9	-
1	GMA	D	8	1	-	1/9/9/9	-
1	5CR	QB	1001	1	-	6/9/10/12	0/1/1/1
1	GMA	a	8	1	-	8/9/9/9	-
1	5CR	NA	201	1	-	4/9/10/12	0/1/1/1
1	GMA	MB	1308	1	-	0/9/9/9	-
1	GMA	8A	1308	1	-	0/9/9/9	-
1	5CR	o	201	1	-	4/9/10/12	0/1/1/1
1	5CR	cA	301	1	-	4/9/10/12	0/1/1/1
1	GMA	m	1308	1	-	1/9/9/9	-
1	GMA	1A	1308	1	-	0/9/9/9	-
1	5CR	kA	1001	1	-	6/9/10/12	0/1/1/1
1	5CR	D	1	1	-	0/9/10/12	0/1/1/1
1	5CR	oA	101	1	-	1/9/10/12	0/1/1/1
1	GMA	4	1008	1	-	1/9/9/9	-
1	GMA	8	108	1	-	3/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	GMA	tA	1208	1	-	4/9/9/9	-
1	5CR	PB	301	1	-	4/9/10/12	0/1/1/1
1	GMA	X	108	1	-	3/9/9/9	-
1	GMA	c	8	1	-	8/9/9/9	-
1	5CR	L	301	1	-	3/9/10/12	0/1/1/1
1	5CR	8A	1301	1	-	4/9/10/12	0/1/1/1
1	5CR	Z	301	1	-	3/9/10/12	0/1/1/1
1	5CR	FB	1301	1	-	4/9/10/12	0/1/1/1
1	GMA	aA	108	1	-	0/9/9/9	-
1	5CR	3	301	1	-	3/9/10/12	0/1/1/1
1	GMA	QB	1008	1	-	8/9/9/9	-
1	GMA	H	8	1	-	1/9/9/9	-
1	5CR	I	1	1	-	0/9/10/12	0/1/1/1
1	GMA	oA	108	1	-	0/9/9/9	-
1	5CR	XA	1101	1	-	1/9/10/12	0/1/1/1
1	5CR	MA	101	1	-	2/9/10/12	0/1/1/1
1	5CR	1	101	1	-	2/9/10/12	0/1/1/1
1	5CR	2A	101	1	-	1/9/10/12	0/1/1/1
1	GMA	jA	308	1	-	0/9/9/9	-
1	GMA	OB	208	1	-	4/9/9/9	-
1	GMA	r	1108	1	-	3/9/9/9	-
1	GMA	9	208	1	-	1/9/9/9	-
1	5CR	FA	101	1	-	2/9/10/12	0/1/1/1
1	GMA	NA	208	1	-	1/9/9/9	-
1	GMA	K	208	1	-	1/9/9/9	-
1	GMA	E	8	1	-	1/9/9/9	-

The worst 5 of 322 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	d	1	5CR	CAL-N	3.50	1.46	1.34
1	e	1	5CR	CAL-N	3.49	1.46	1.34
1	rA	1001	5CR	CAL-N	3.49	1.46	1.34
1	yA	1001	5CR	CAL-N	3.48	1.46	1.34
1	i	1	5CR	CAL-N	3.48	1.46	1.34

The worst 5 of 363 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	b	1	5CR	CAA-CAL-N	5.15	124.81	116.10
1	f	1	5CR	CAA-CAL-N	5.14	124.80	116.10
1	5A	1001	5CR	CAA-CAL-N	5.13	124.79	116.10
1	a	1	5CR	CAA-CAL-N	5.13	124.79	116.10
1	WA	1001	5CR	CAA-CAL-N	5.13	124.79	116.10

There are no chirality outliers.

5 of 720 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

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.

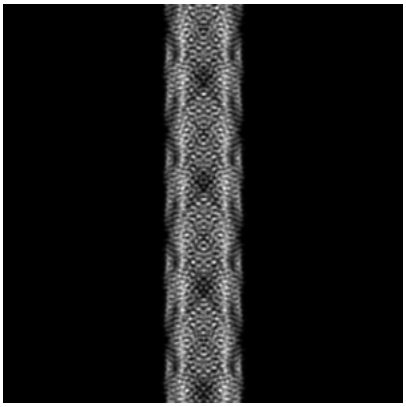
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23486. These allow visual inspection of the internal detail of the map and identification of artifacts.

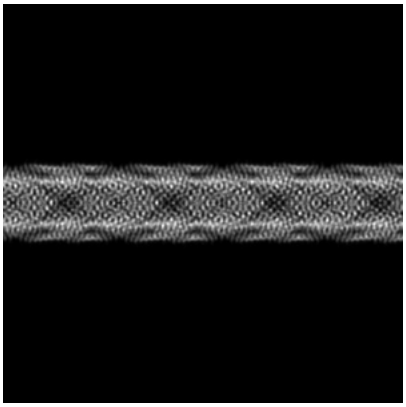
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

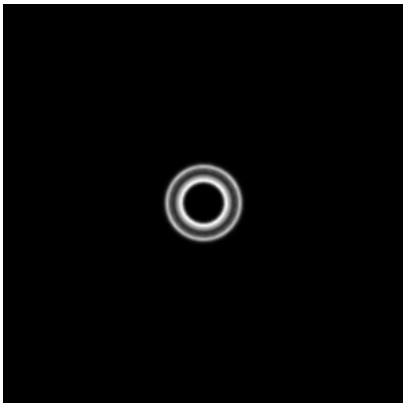
6.1.1 Primary map



X



Y

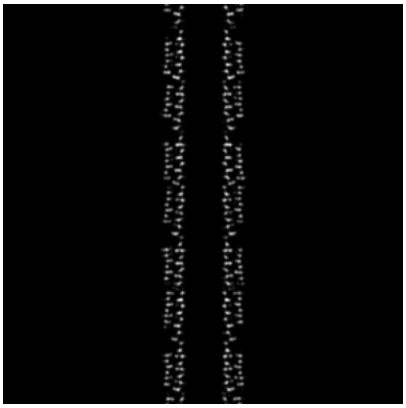


Z

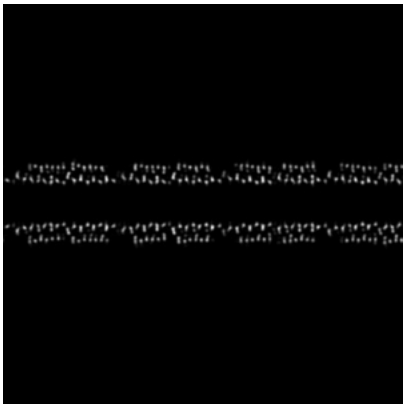
The images above show the map projected in three orthogonal directions.

6.2 Central slices

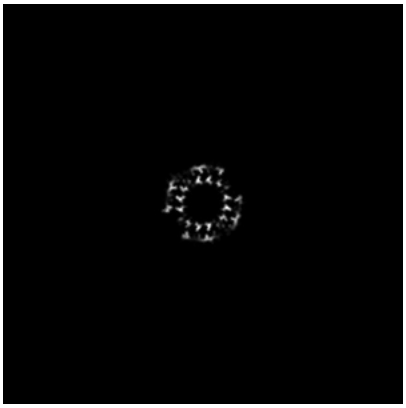
6.2.1 Primary map



X Index: 160



Y Index: 160

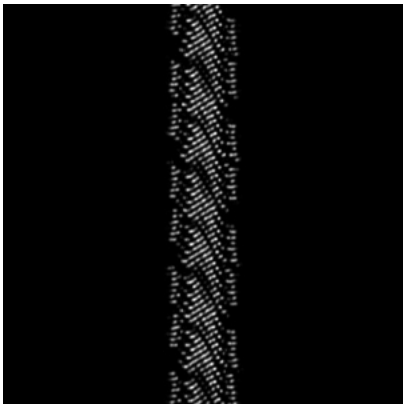


Z Index: 160

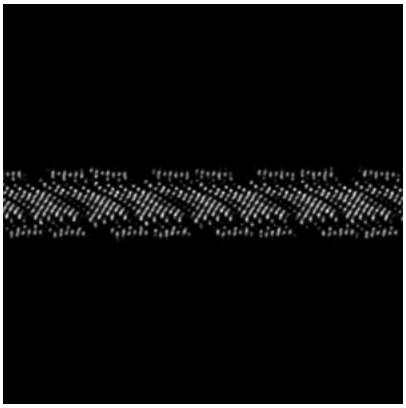
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

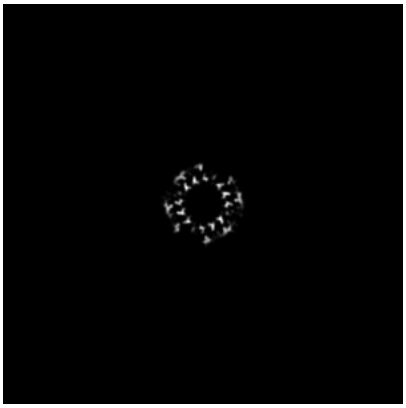
6.3.1 Primary map



X Index: 177



Y Index: 143

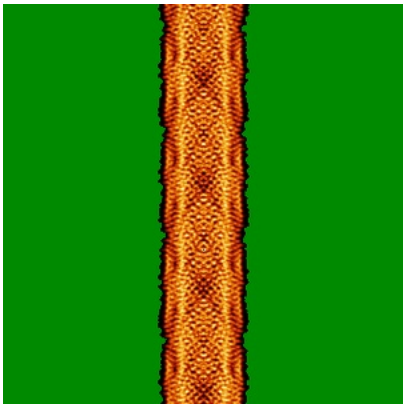


Z Index: 61

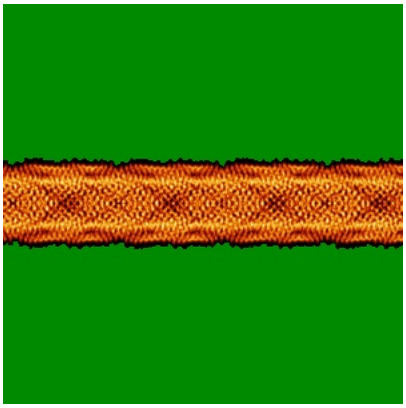
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

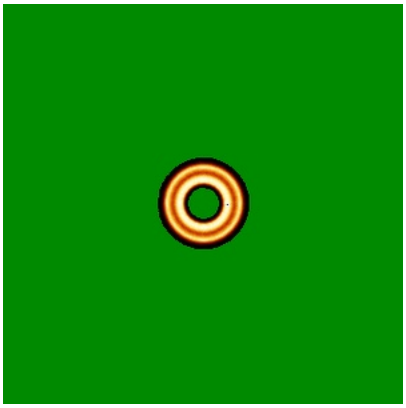
6.4.1 Primary map



X



Y

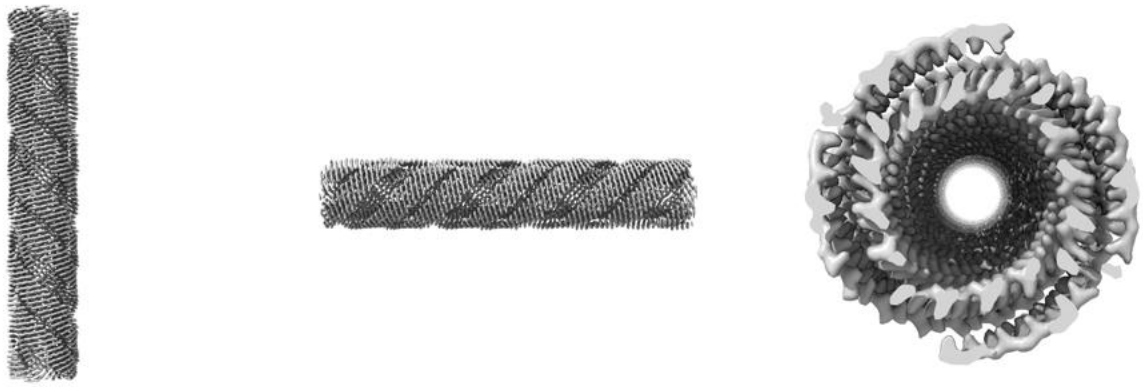


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.273. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

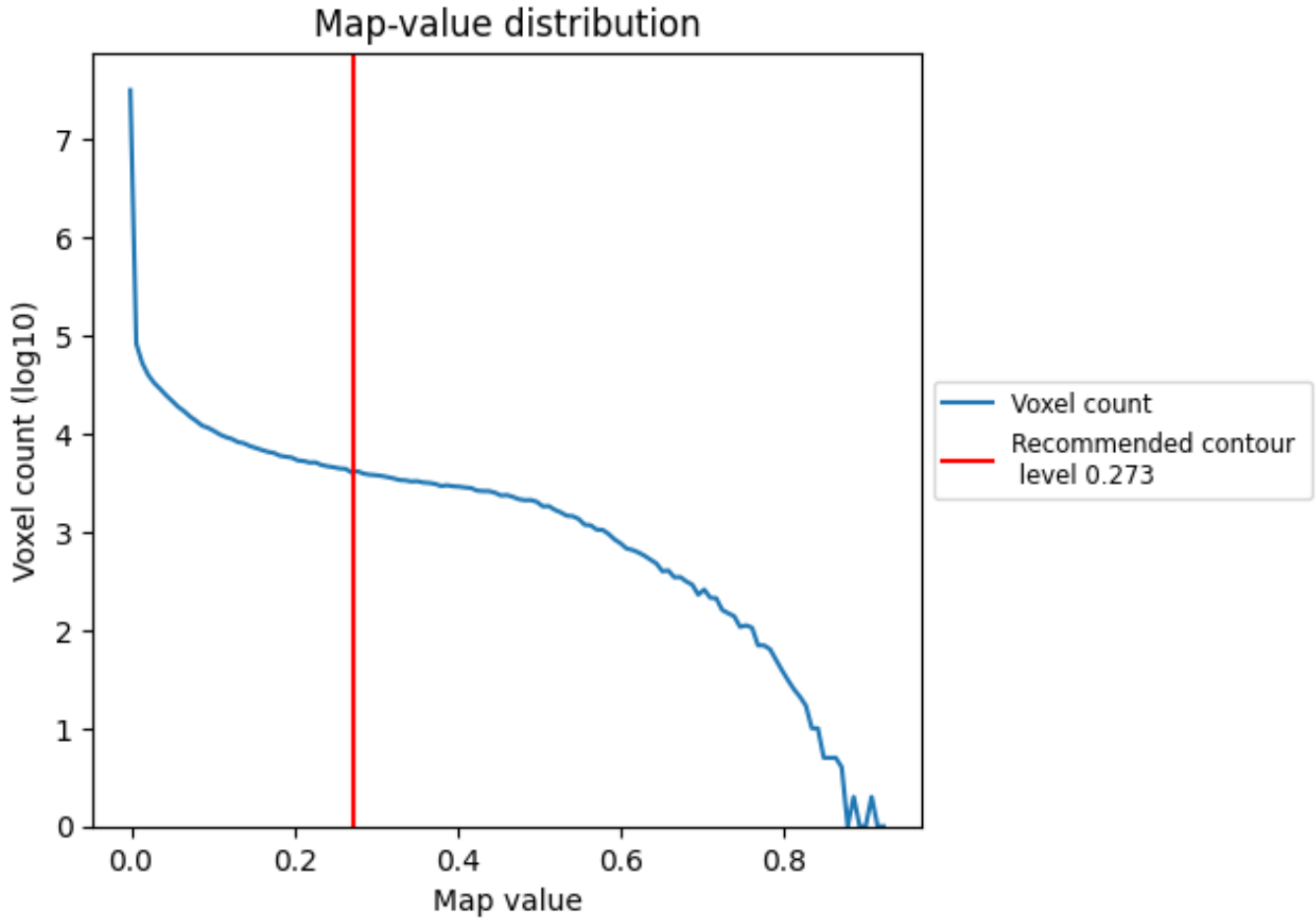
6.6 Mask visualisation (i)

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

7 Map analysis

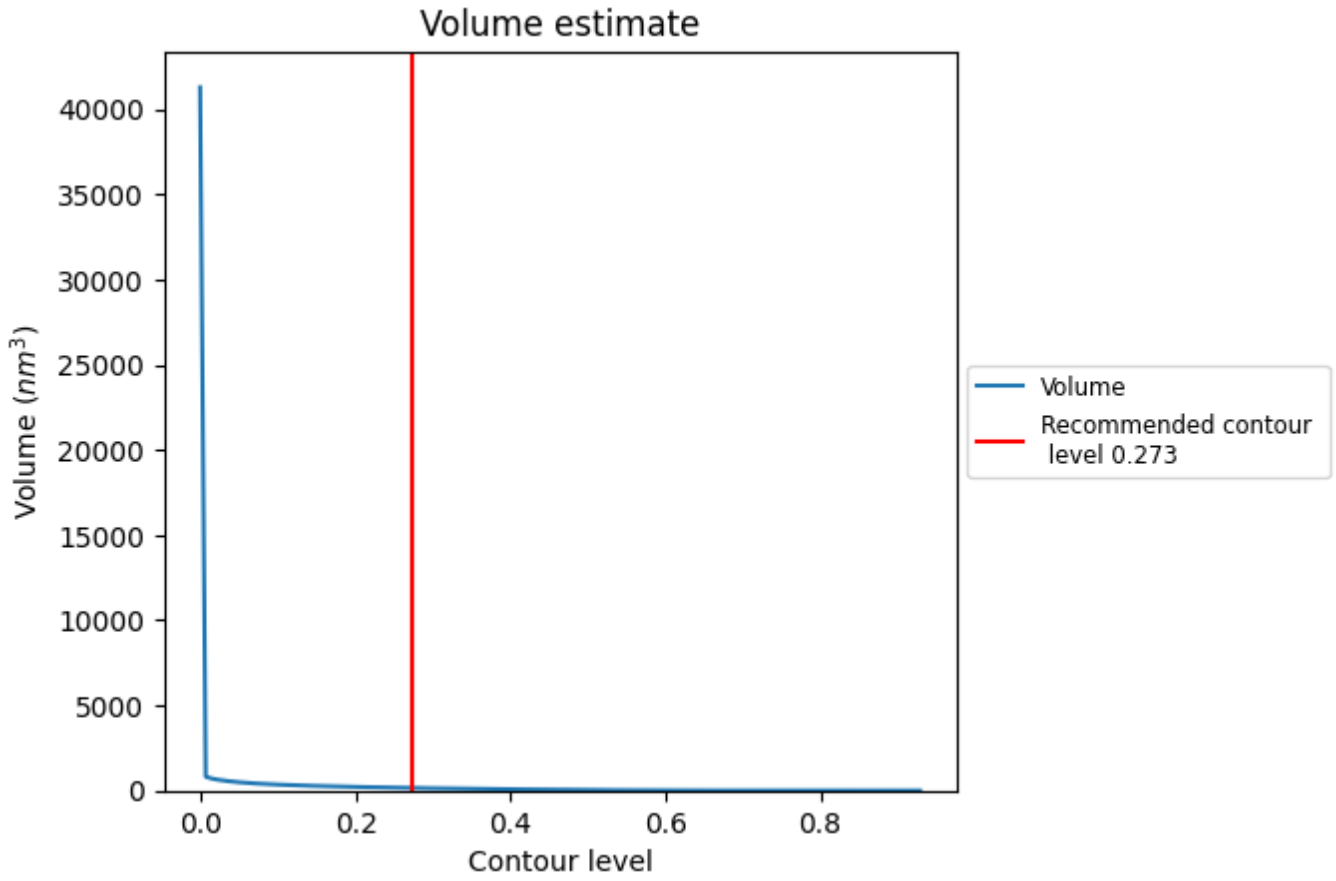
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

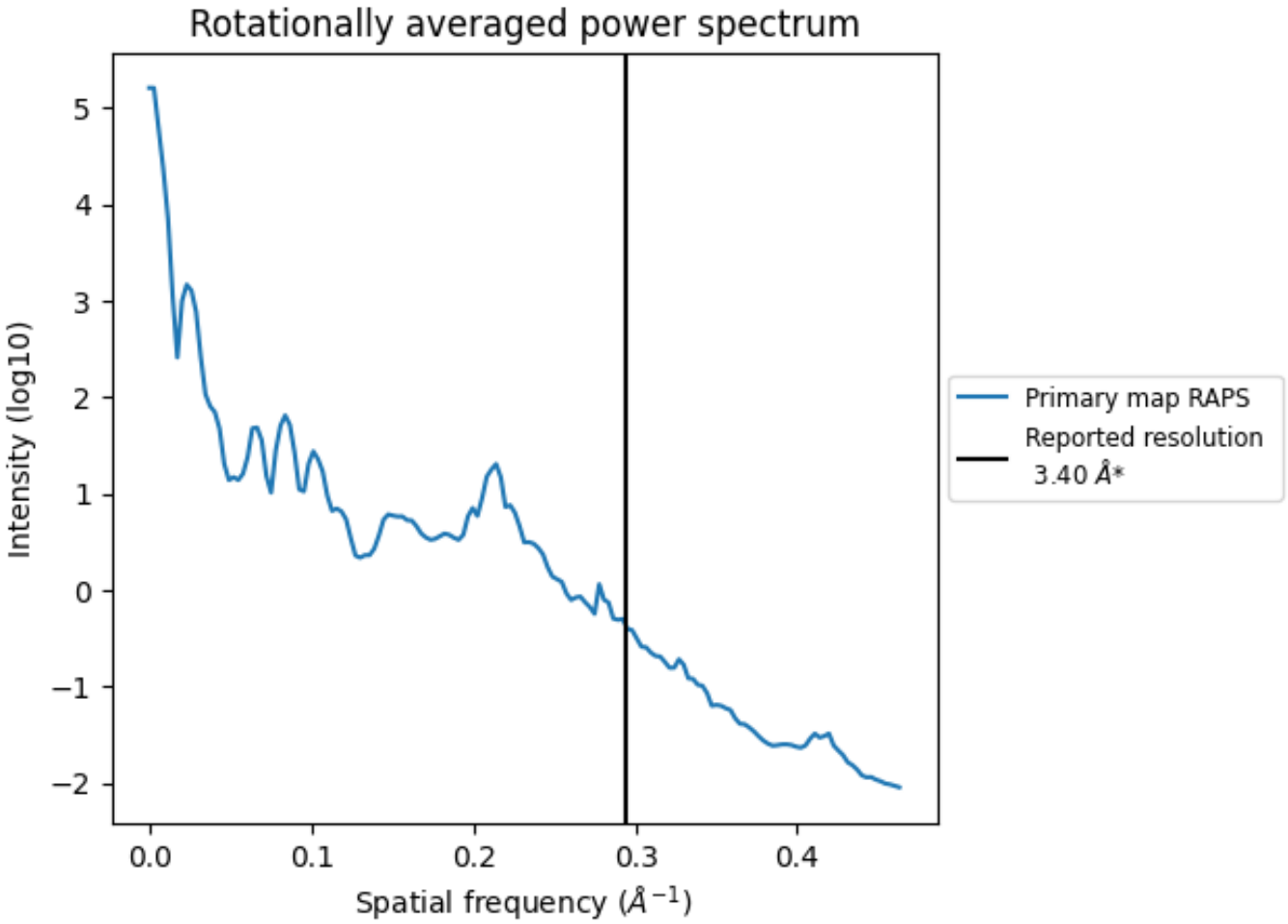
7.2 Volume estimate (i)



The volume at the recommended contour level is 153 nm^3; this corresponds to an approximate mass of 138 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}

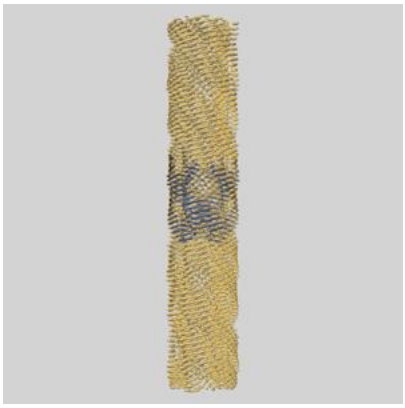
8 Fourier-Shell correlation (i)

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

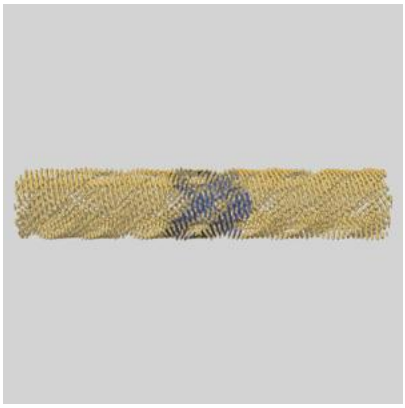
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-23486 and PDB model 7LQH. Per-residue inclusion information can be found in section 3 on page 17.

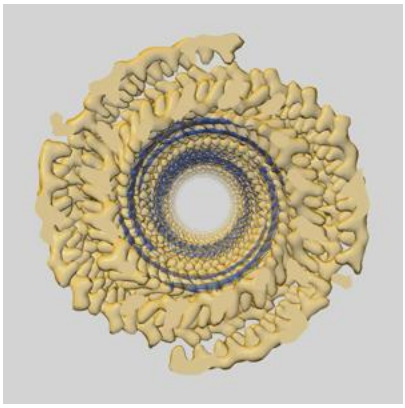
9.1 Map-model overlay



X



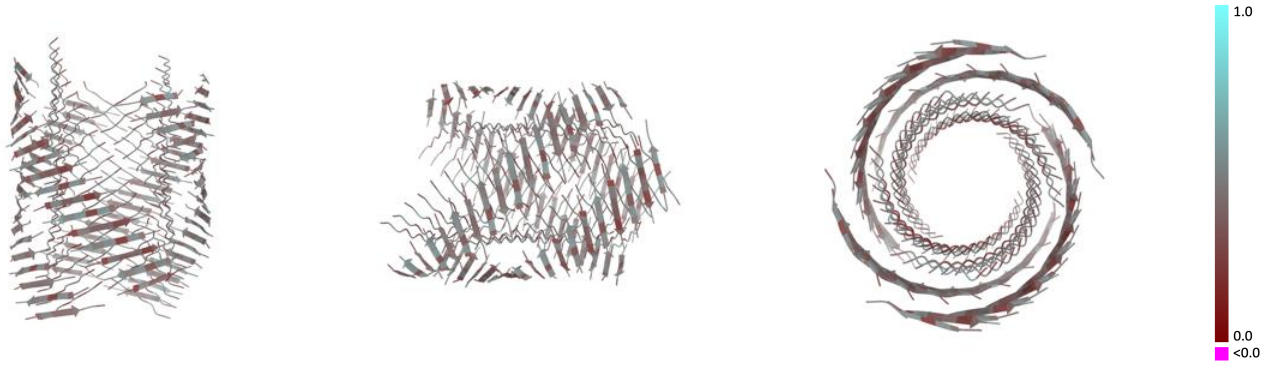
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.273 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.

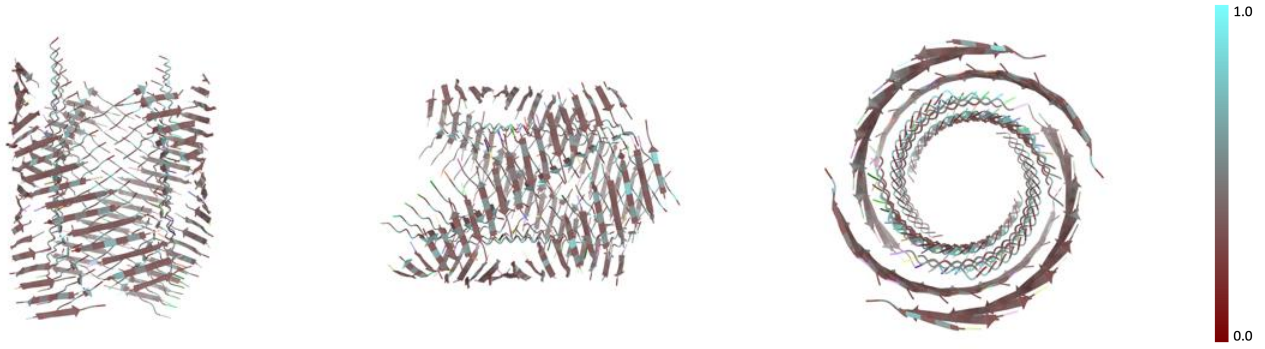
9.2 Q-score mapped to coordinate model



X Y Z

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

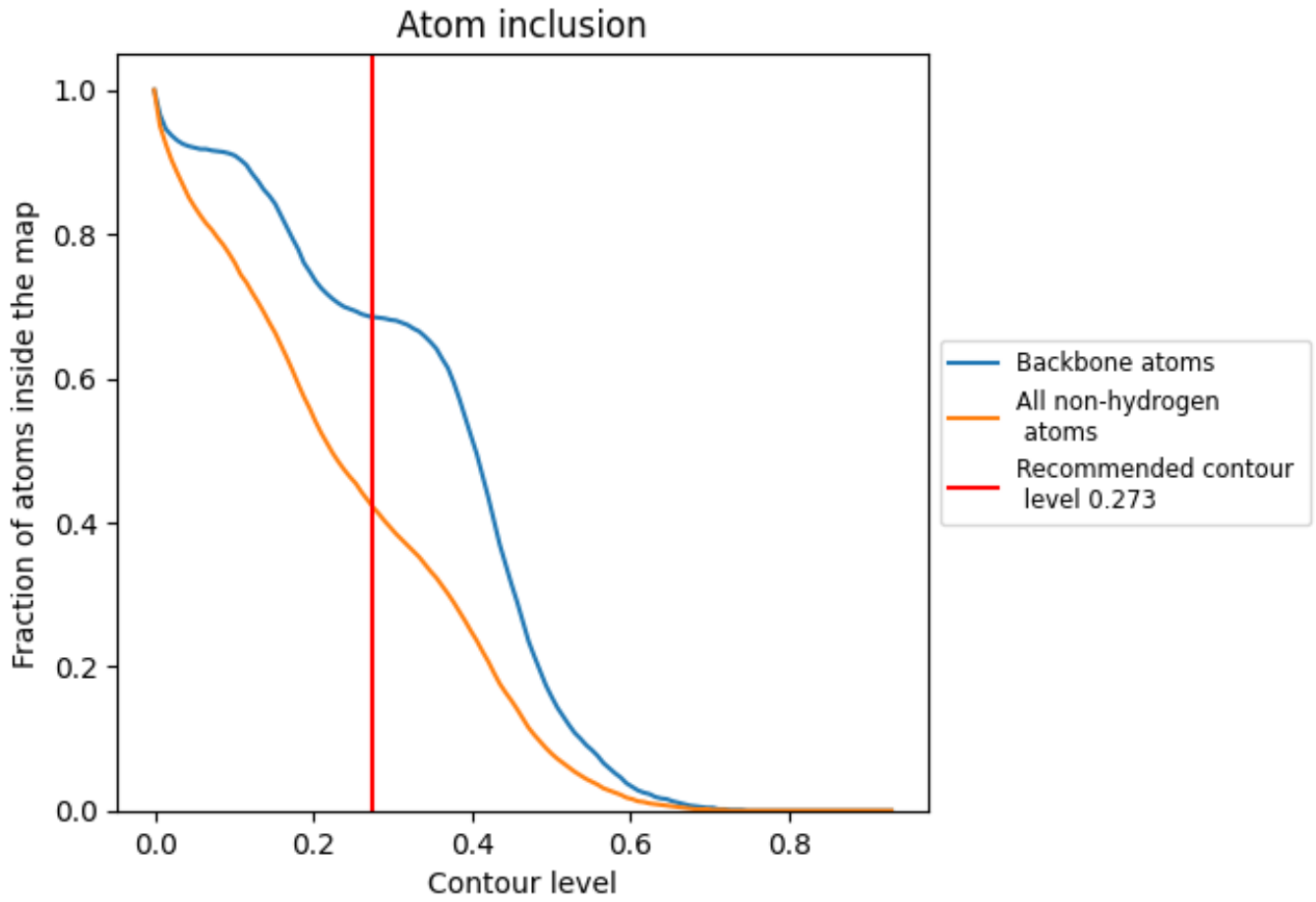
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.273).

9.4 Atom inclusion (i)



At the recommended contour level, 68% of all backbone atoms, 42% 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 (0.273) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4240	0.4250
0	0.4760	0.4280
0A	0.3810	0.4720
1	0.4640	0.4080
1A	0.3570	0.3700
2	0.5120	0.4480
2A	0.3810	0.4170
3	0.5000	0.4400
3A	0.4170	0.4720
4	0.4290	0.4290
4A	0.3690	0.3700
5	0.4410	0.4020
5A	0.3930	0.4440
6	0.5120	0.4570
6A	0.3570	0.4020
7	0.4880	0.4310
7A	0.3810	0.4510
8	0.4640	0.4030
8A	0.3330	0.3940
9	0.5000	0.4580
9A	0.3570	0.4260
A	0.4170	0.4240
AA	0.5240	0.4250
AB	0.4170	0.4470
B	0.4290	0.4130
BA	0.4050	0.3970
BB	0.3690	0.3980
C	0.4290	0.4190
CA	0.4170	0.3950
CB	0.3810	0.4370
D	0.4170	0.4170
DA	0.5590	0.4420
DB	0.3690	0.4080
E	0.4290	0.4240
EA	0.5000	0.4400

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Chain	Atom inclusion	Q-score
EB	0.3930	0.4530
F	0.4170	0.4240
FA	0.4410	0.4000
FB	0.3570	0.3740
G	0.4640	0.4260
GA	0.5240	0.4540
GB	0.3570	0.4140
H	0.4290	0.4210
HA	0.5120	0.4470
HB	0.4290	0.4600
I	0.4290	0.4190
IA	0.4290	0.4200
IB	0.3810	0.3890
J	0.4170	0.4060
JA	0.4410	0.3990
JB	0.3930	0.4170
K	0.5000	0.4440
KA	0.4760	0.4550
KB	0.3570	0.4100
L	0.5000	0.4450
LA	0.5000	0.4420
LB	0.4170	0.4380
M	0.4290	0.4120
MA	0.4410	0.3900
MB	0.3330	0.3890
N	0.4520	0.3940
NA	0.5240	0.4590
NB	0.3810	0.4100
O	0.4880	0.4430
OA	0.5000	0.4220
OB	0.4050	0.4590
P	0.5000	0.4450
PA	0.4170	0.4180
PB	0.3810	0.4000
Q	0.4410	0.4040
QA	0.4170	0.3850
QB	0.4170	0.4390
R	0.4760	0.4560
RA	0.4880	0.4450
RB	0.3570	0.3950
S	0.4760	0.4340
SA	0.5240	0.4480

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Chain	Atom inclusion	Q-score
SB	0.3810	0.4610
T	0.4410	0.4230
TA	0.3690	0.4300
TB	0.3570	0.3750
U	0.4290	0.4010
UA	0.3810	0.4770
V	0.5000	0.4470
VA	0.3810	0.3840
W	0.4880	0.4290
WA	0.3810	0.4290
X	0.4410	0.3970
XA	0.3930	0.4050
Y	0.5000	0.4430
YA	0.4050	0.4580
Z	0.5120	0.4230
ZA	0.3570	0.3800
a	0.3930	0.4520
aA	0.3810	0.4120
b	0.4050	0.4480
bA	0.4290	0.4580
c	0.4290	0.4450
cA	0.3810	0.3910
d	0.4170	0.4490
dA	0.3570	0.4400
e	0.3810	0.4410
eA	0.3570	0.4220
f	0.3810	0.4550
fA	0.3810	0.4560
g	0.4170	0.4590
gA	0.3450	0.3690
h	0.4290	0.4500
hA	0.3690	0.4140
i	0.4410	0.4660
iA	0.4170	0.4540
j	0.4290	0.4170
jA	0.3930	0.3680
k	0.4050	0.3840
kA	0.3810	0.4440
l	0.5000	0.4560
lA	0.3810	0.3960
m	0.5120	0.4470
mA	0.3690	0.4550

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Chain	Atom inclusion	Q-score
n	0.4290	0.4070
nA	0.3810	0.3840
o	0.5000	0.4560
oA	0.3570	0.4040
p	0.5120	0.4470
pA	0.4170	0.4580
q	0.4170	0.4150
qA	0.3930	0.3860
r	0.4410	0.3930
rA	0.3930	0.4360
s	0.5000	0.4430
sA	0.3570	0.4020
t	0.4640	0.4350
tA	0.3690	0.4600
u	0.4410	0.3940
uA	0.3330	0.3710
v	0.5000	0.4390
vA	0.3690	0.4240
w	0.5360	0.4180
wA	0.3810	0.4590
x	0.4290	0.4060
xA	0.3810	0.3930
y	0.4520	0.3930
yA	0.3570	0.4460
z	0.4640	0.4490
zA	0.3450	0.4120