



## Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 03:53 PM EST

PDB ID : 7LQG  
EMDB ID : EMD-23485  
Title : Cryo-EM of the KFE8 thinner nanotube (class 1, C2)  
Authors : Wang, F.; Gnewou, O.M.; Egelman, E.H.; Conticello, V.P.  
Deposited on : 2021-02-13  
Resolution : 3.40 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

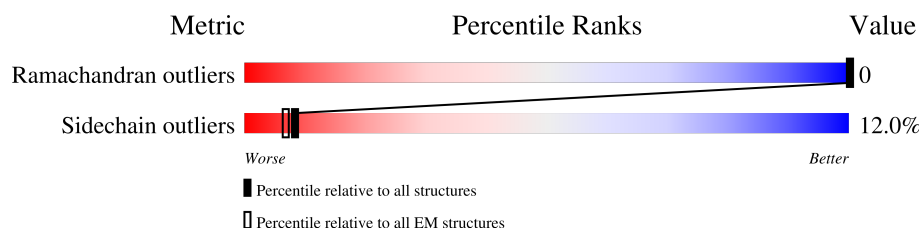
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson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

# 1 Overall quality at a glance

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	8	<div> <div>38%</div> <div>62%</div> <div>38%</div> </div>
1	0A	8	<div> <div>50%</div> <div>75%</div> <div>25%</div> </div>
1	1	8	<div> <div>38%</div> <div>50%</div> <div>50%</div> </div>
1	1A	8	<div> <div>75%</div> <div>75%</div> <div>25%</div> </div>
1	2	8	<div> <div>25%</div> <div>75%</div> <div>25%</div> </div>
1	2A	8	<div> <div>62%</div> <div>62%</div> <div>38%</div> </div>
1	3	8	<div> <div>25%</div> <div>62%</div> <div>38%</div> </div>
1	3A	8	<div> <div>50%</div> <div>75%</div> <div>25%</div> </div>
1	4	8	<div> <div>50%</div> <div>75%</div> <div>25%</div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	4A	8	
1	5	8	
1	5A	8	
1	6	8	
1	6A	8	
1	7	8	
1	7A	8	
1	8	8	
1	8A	8	
1	9	8	
1	9A	8	
1	A	8	
1	AA	8	
1	AB	8	
1	B	8	
1	BA	8	
1	BB	8	
1	C	8	
1	CA	8	
1	CB	8	
1	D	8	
1	DA	8	
1	DB	8	
1	E	8	
1	EA	8	

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	v	8	
1	vA	8	
1	w	8	
1	wA	8	
1	x	8	
1	xA	8	
1	y	8	
1	yA	8	
1	z	8	
1	zA	8	



## 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		

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms				AltConf	Trace
1	b	8	Total 84	C 60	N 11	O 13	0	0
1	aA	8	Total 84	C 60	N 11	O 13	0	0
1	bA	8	Total 84	C 60	N 11	O 13	0	0
1	cA	8	Total 84	C 60	N 11	O 13	0	0
1	dA	8	Total 84	C 60	N 11	O 13	0	0
1	eA	8	Total 84	C 60	N 11	O 13	0	0
1	fA	8	Total 84	C 60	N 11	O 13	0	0
1	gA	8	Total 84	C 60	N 11	O 13	0	0
1	c	8	Total 84	C 60	N 11	O 13	0	0
1	hA	8	Total 84	C 60	N 11	O 13	0	0
1	iA	8	Total 84	C 60	N 11	O 13	0	0
1	jA	8	Total 84	C 60	N 11	O 13	0	0
1	kA	8	Total 84	C 60	N 11	O 13	0	0
1	lA	8	Total 84	C 60	N 11	O 13	0	0
1	mA	8	Total 84	C 60	N 11	O 13	0	0
1	nA	8	Total 84	C 60	N 11	O 13	0	0
1	d	8	Total 84	C 60	N 11	O 13	0	0
1	oA	8	Total 84	C 60	N 11	O 13	0	0
1	pA	8	Total 84	C 60	N 11	O 13	0	0
1	qA	8	Total 84	C 60	N 11	O 13	0	0
1	rA	8	Total 84	C 60	N 11	O 13	0	0

*Continued on next page...*

*Continued from previous page...*

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		

*Continued on next page...*

*Continued from previous page...*

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		

*Continued on next page...*

*Continued from previous page...*

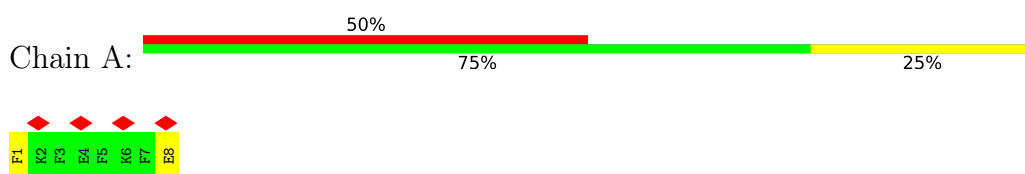
Mol	Chain	Residues	Atoms				AltConf	Trace
1	TB	8	Total	C	N	O	0	0
			84	60	11	13		



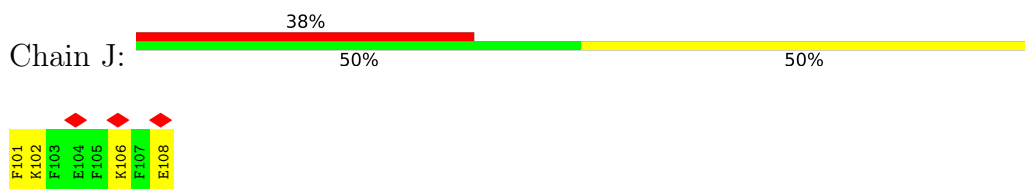
### 3 Residue-property plots [i](#)

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.

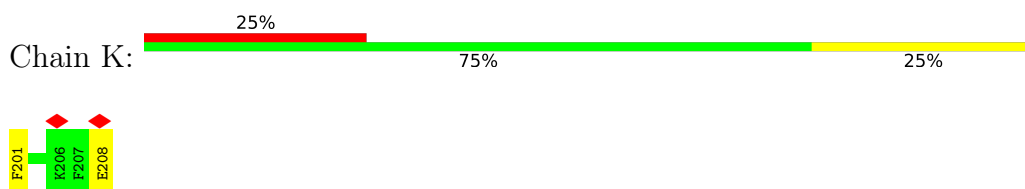
- Molecule 1: KFE8 peptide



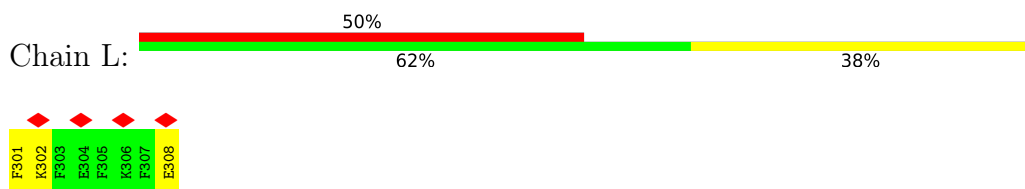
- Molecule 1: KFE8 peptide



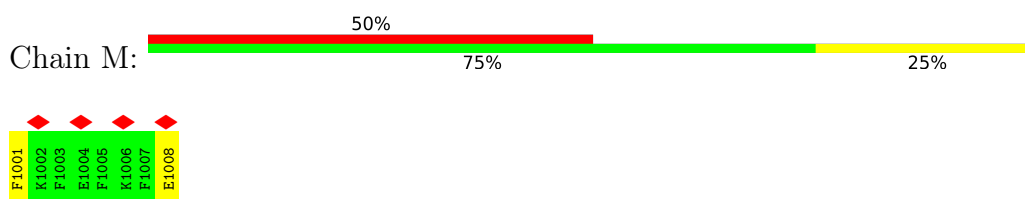
- Molecule 1: KFE8 peptide



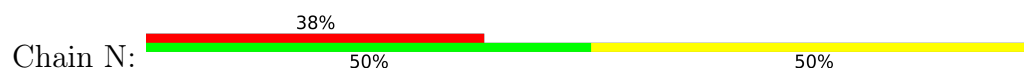
- Molecule 1: KFE8 peptide



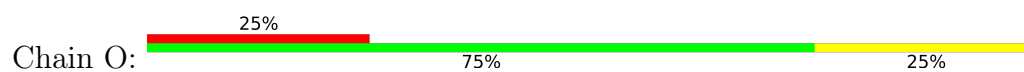
- Molecule 1: KFE8 peptide



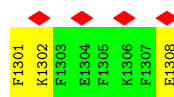
## ● Molecule 1: KFE8 peptide



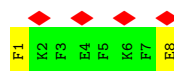
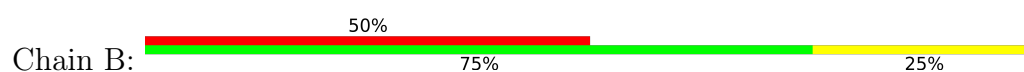
## ● Molecule 1: KFE8 peptide



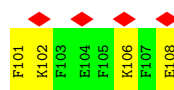
## ● Molecule 1: KFE8 peptide



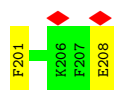
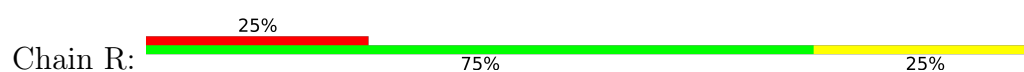
## ● Molecule 1: KFE8 peptide



## ● Molecule 1: KFE8 peptide

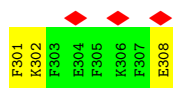


## ● Molecule 1: KFE8 peptide

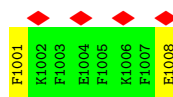
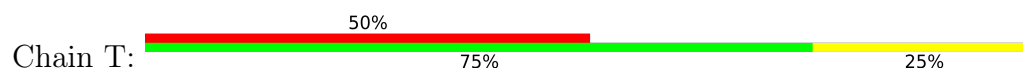


## ● Molecule 1: KFE8 peptide





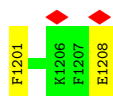
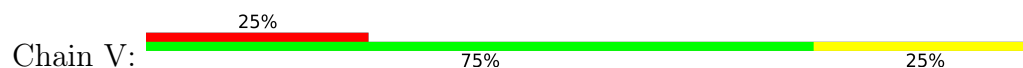
- Molecule 1: KFE8 peptide



- Molecule 1: KFE8 peptide



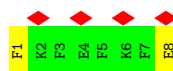
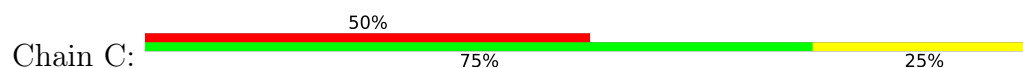
- Molecule 1: KFE8 peptide



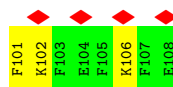
- Molecule 1: KFE8 peptide



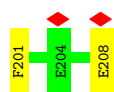
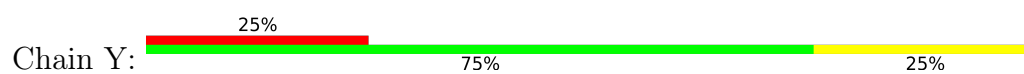
- Molecule 1: KFE8 peptide



- Molecule 1: KFE8 peptide



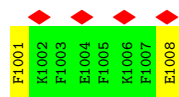
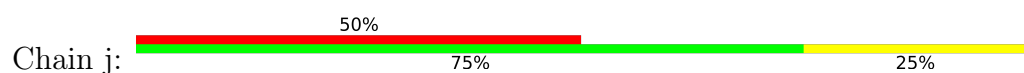
- Molecule 1: KFE8 peptide



- Molecule 1: KFE8 peptide



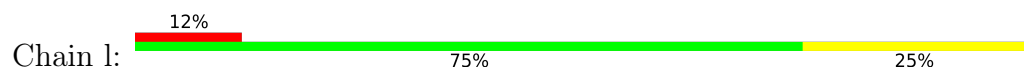
- Molecule 1: KFE8 peptide



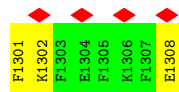
- Molecule 1: KFE8 peptide



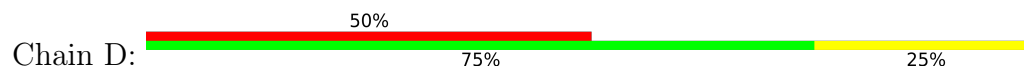
- Molecule 1: KFE8 peptide

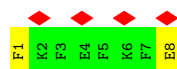


- Molecule 1: KFE8 peptide

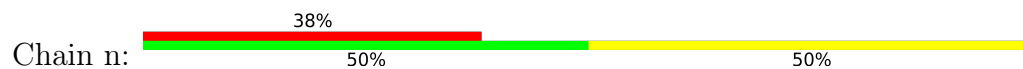


- Molecule 1: KFE8 peptide

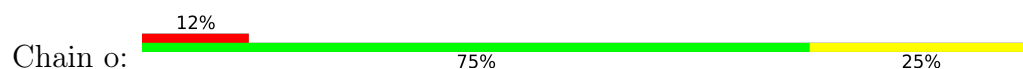




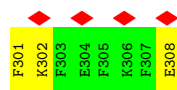
- Molecule 1: KFE8 peptide



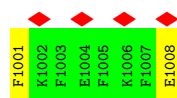
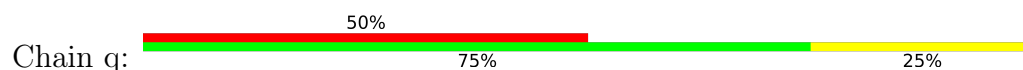
- Molecule 1: KFE8 peptide



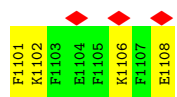
- Molecule 1: KFE8 peptide



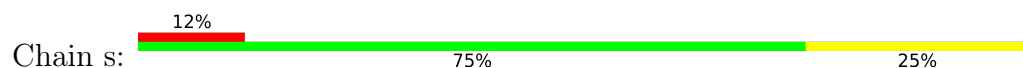
- Molecule 1: KFE8 peptide



- Molecule 1: KFE8 peptide



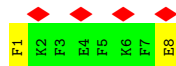
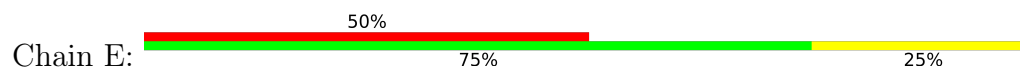
- Molecule 1: KFE8 peptide



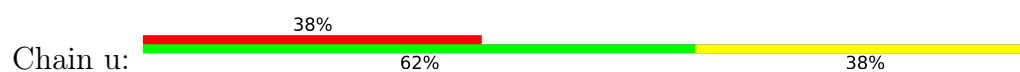
- Molecule 1: KFE8 peptide



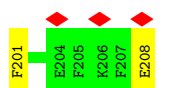
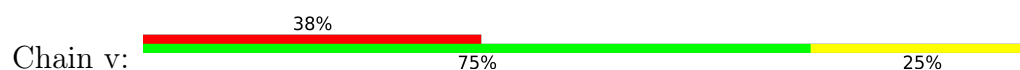
- Molecule 1: KFE8 peptide



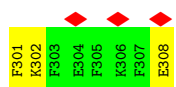
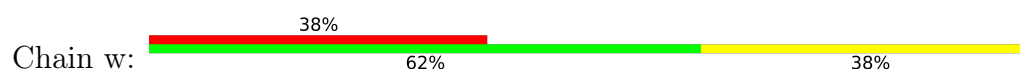
- Molecule 1: KFE8 peptide



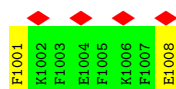
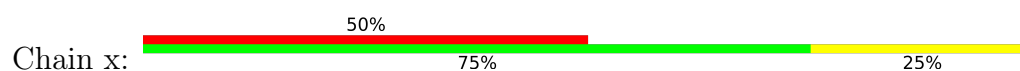
- Molecule 1: KFE8 peptide



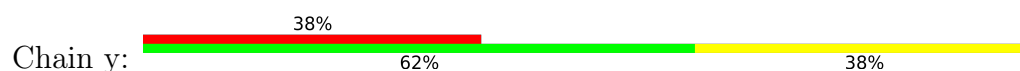
- Molecule 1: KFE8 peptide

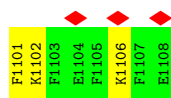


- Molecule 1: KFE8 peptide

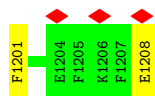
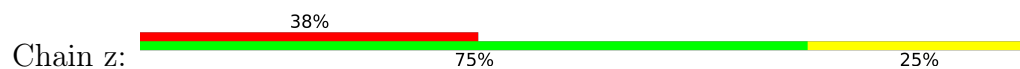


- Molecule 1: KFE8 peptide

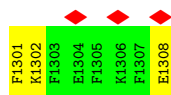
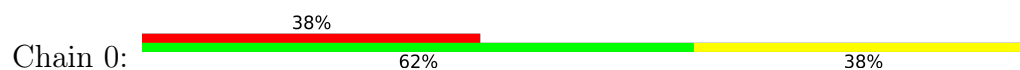




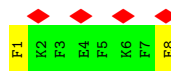
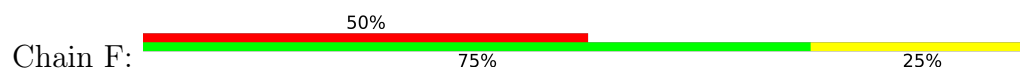
- Molecule 1: KFE8 peptide



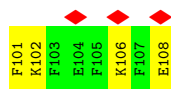
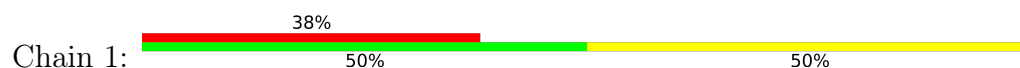
- Molecule 1: KFE8 peptide



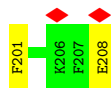
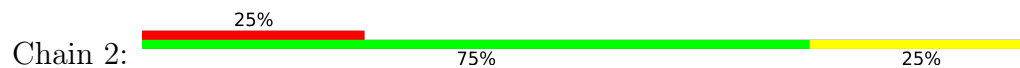
- Molecule 1: KFE8 peptide



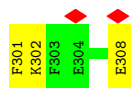
- Molecule 1: KFE8 peptide



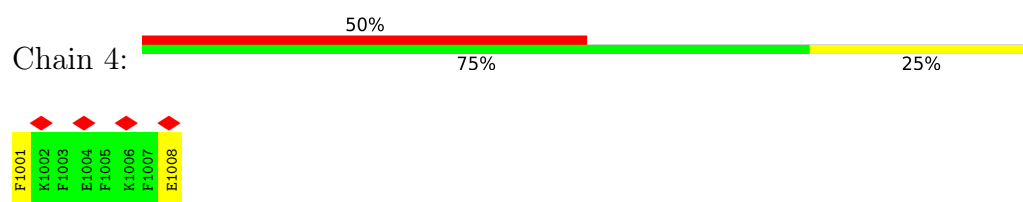
- Molecule 1: KFE8 peptide



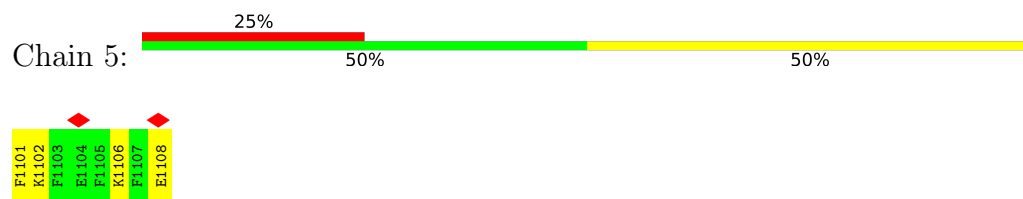
- Molecule 1: KFE8 peptide



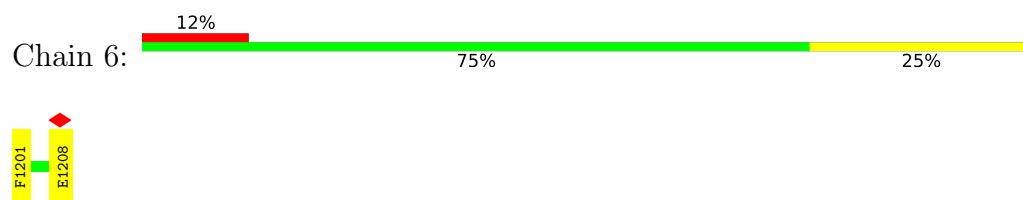
- Molecule 1: KFE8 peptide



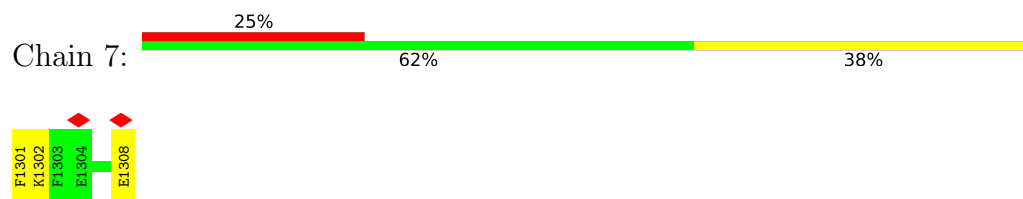
● Molecule 1: KFE8 peptide



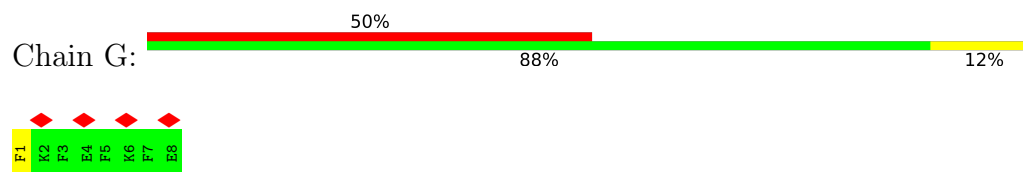
● Molecule 1: KFE8 peptide



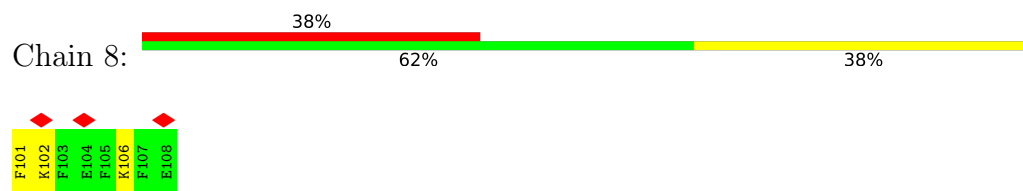
● Molecule 1: KFE8 peptide



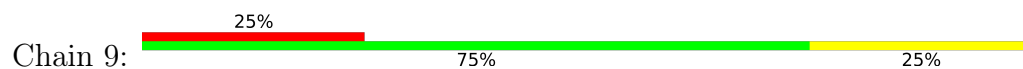
● Molecule 1: KFE8 peptide



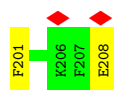
● Molecule 1: KFE8 peptide



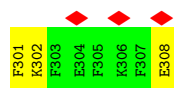
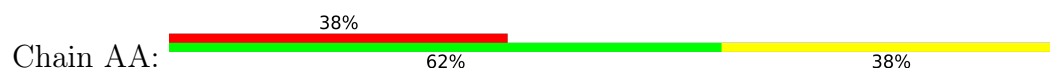
● Molecule 1: KFE8 peptide



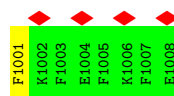




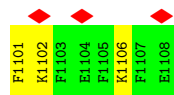
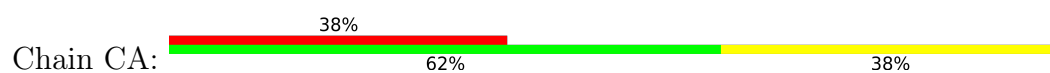
- Molecule 1: KFE8 peptide



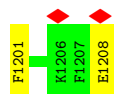
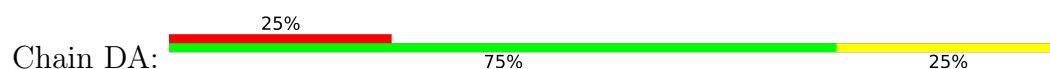
- Molecule 1: KFE8 peptide



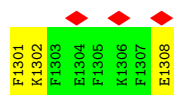
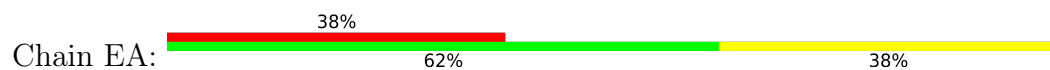
- Molecule 1: KFE8 peptide



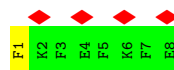
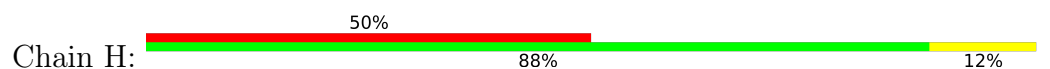
- Molecule 1: KFE8 peptide



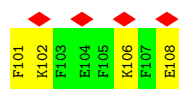
- Molecule 1: KFE8 peptide



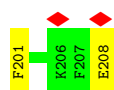
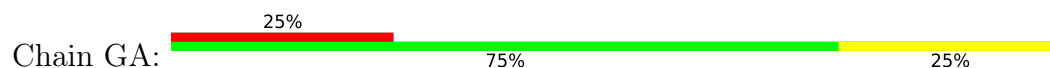
- Molecule 1: KFE8 peptide



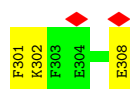
- Molecule 1: KFE8 peptide



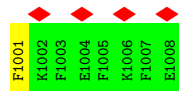
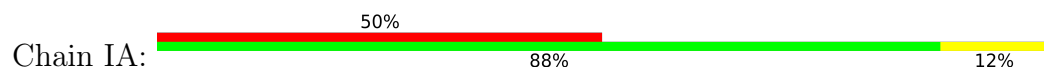
- Molecule 1: KFE8 peptide



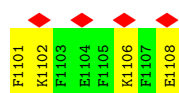
- Molecule 1: KFE8 peptide



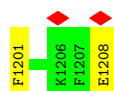
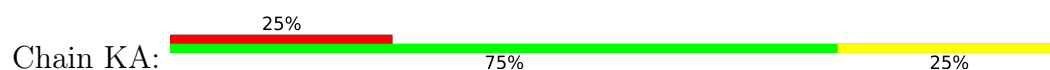
- Molecule 1: KFE8 peptide



- Molecule 1: KFE8 peptide

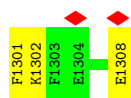


- Molecule 1: KFE8 peptide

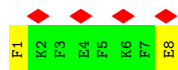
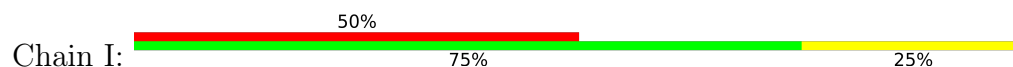


- Molecule 1: KFE8 peptide

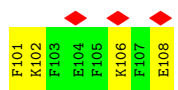




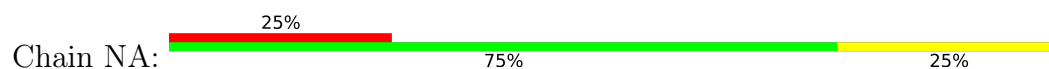
- Molecule 1: KFE8 peptide



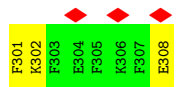
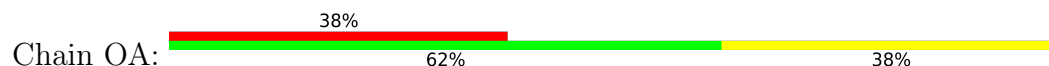
- Molecule 1: KFE8 peptide



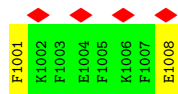
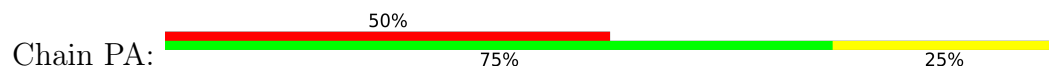
- Molecule 1: KFE8 peptide



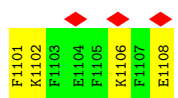
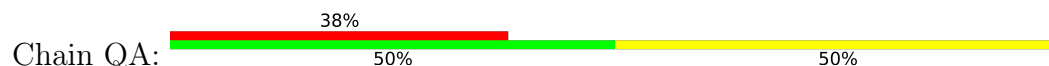
- Molecule 1: KFE8 peptide



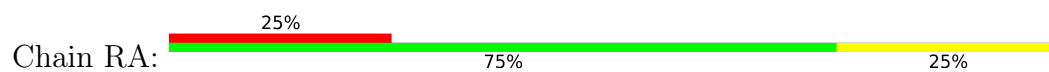
- Molecule 1: KFE8 peptide



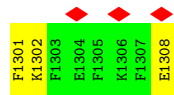
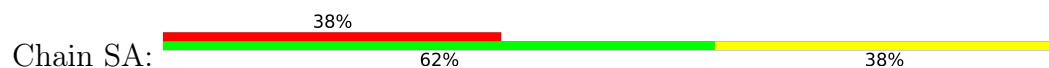
- Molecule 1: KFE8 peptide



- Molecule 1: KFE8 peptide



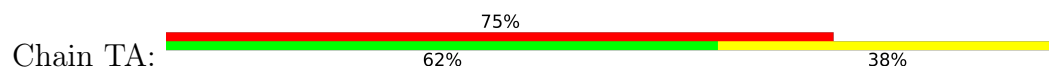
- Molecule 1: KFE8 peptide



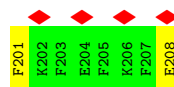
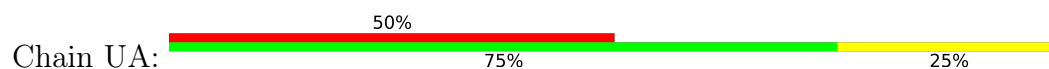
- Molecule 1: KFE8 peptide



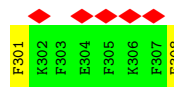
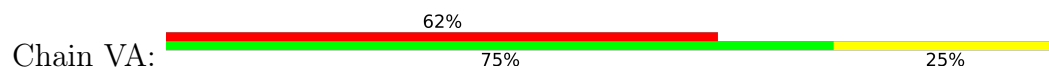
- Molecule 1: KFE8 peptide



- Molecule 1: KFE8 peptide

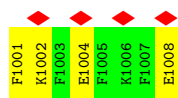


- Molecule 1: KFE8 peptide

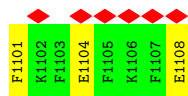
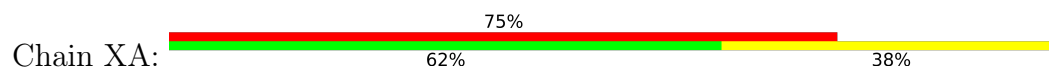


- Molecule 1: KFE8 peptide

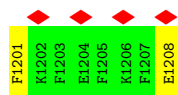




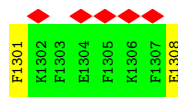
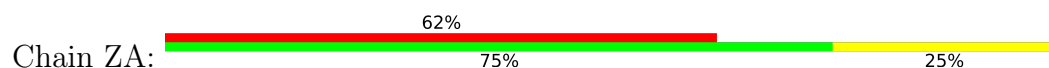
- Molecule 1: KFE8 peptide



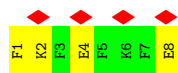
- Molecule 1: KFE8 peptide



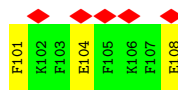
- Molecule 1: KFE8 peptide



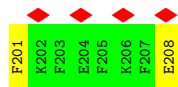
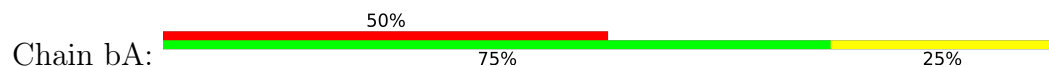
- Molecule 1: KFE8 peptide



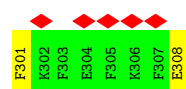
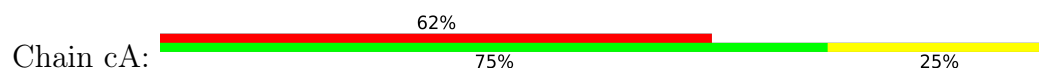
- Molecule 1: KFE8 peptide



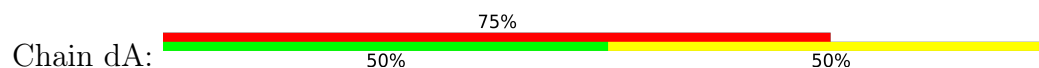
- Molecule 1: KFE8 peptide



- Molecule 1: KFE8 peptide



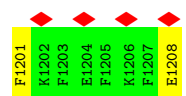
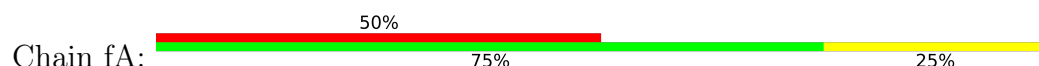
- Molecule 1: KFE8 peptide



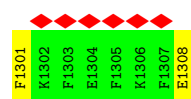
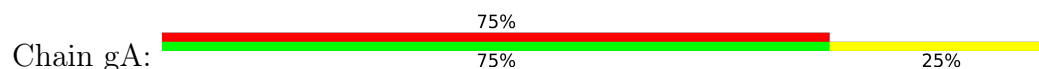
- Molecule 1: KFE8 peptide



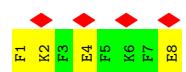
- Molecule 1: KFE8 peptide



- Molecule 1: KFE8 peptide

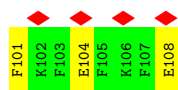


- Molecule 1: KFE8 peptide

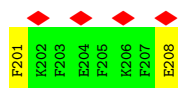
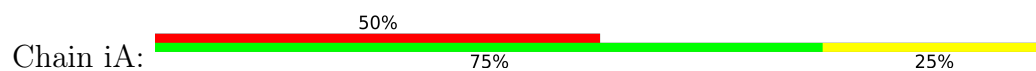


- Molecule 1: KFE8 peptide

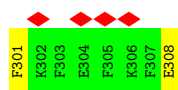
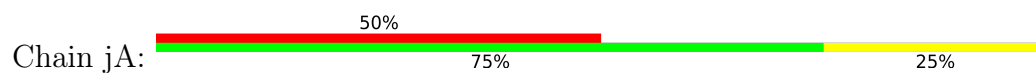




- Molecule 1: KFE8 peptide



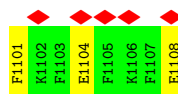
- Molecule 1: KFE8 peptide



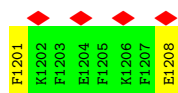
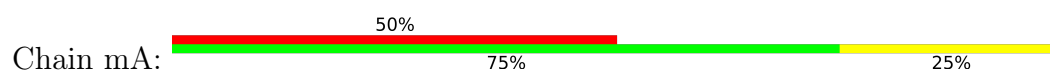
- Molecule 1: KFE8 peptide



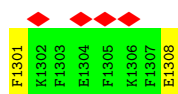
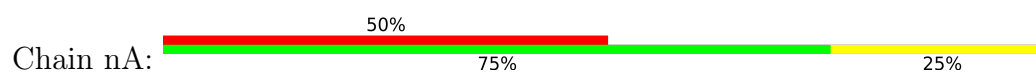
- Molecule 1: KFE8 peptide



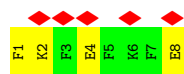
- Molecule 1: KFE8 peptide



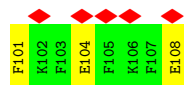
- Molecule 1: KFE8 peptide



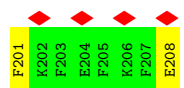
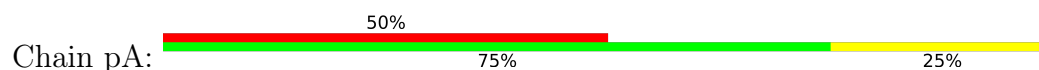
## • Molecule 1: KFE8 peptide



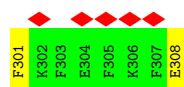
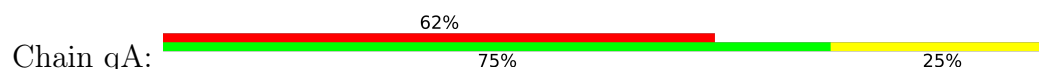
## • Molecule 1: KFE8 peptide



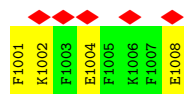
## • Molecule 1: KFE8 peptide



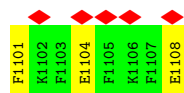
## • Molecule 1: KFE8 peptide



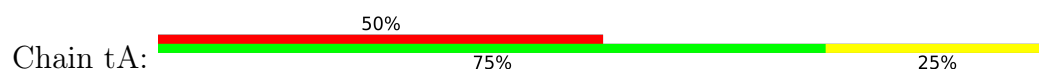
## • Molecule 1: KFE8 peptide



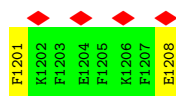
## • Molecule 1: KFE8 peptide



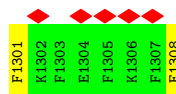
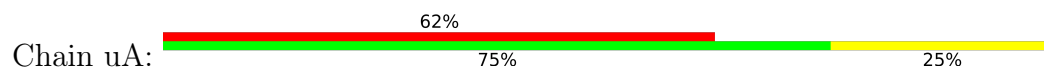
## • Molecule 1: KFE8 peptide



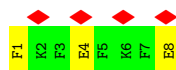




- Molecule 1: KFE8 peptide



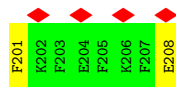
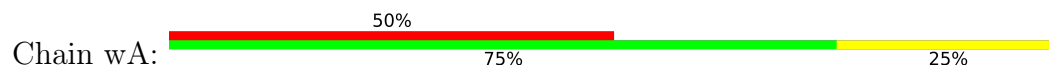
- Molecule 1: KFE8 peptide



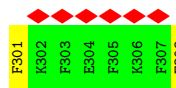
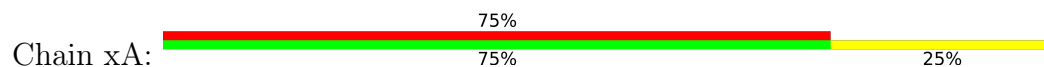
- Molecule 1: KFE8 peptide



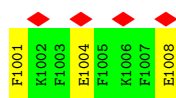
- Molecule 1: KFE8 peptide



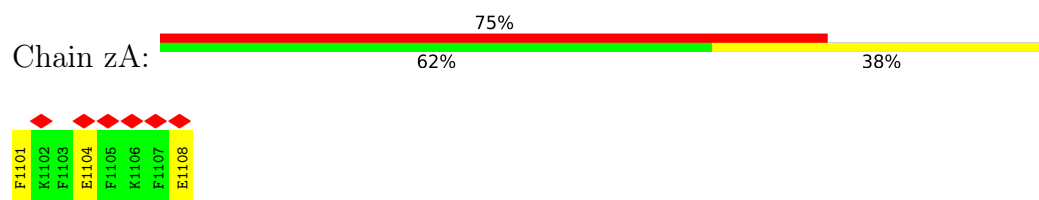
- Molecule 1: KFE8 peptide



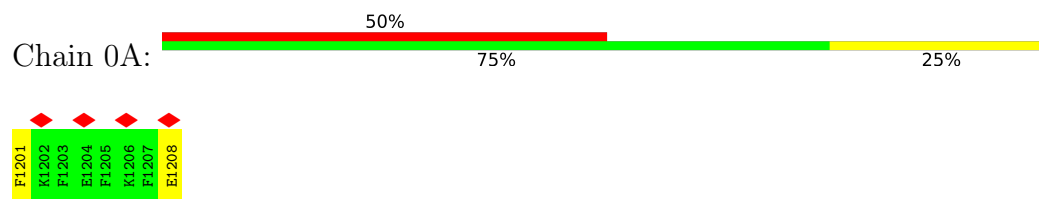
- Molecule 1: KFE8 peptide



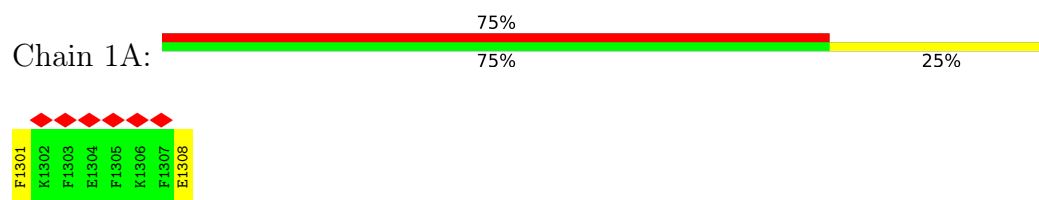
- Molecule 1: KFE8 peptide



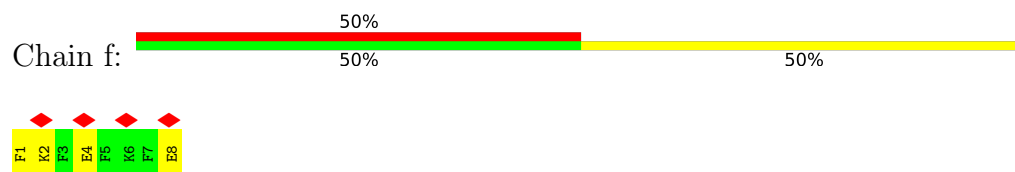
- Molecule 1: KFE8 peptide



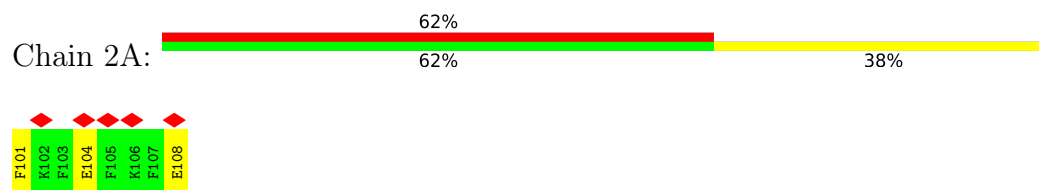
- Molecule 1: KFE8 peptide



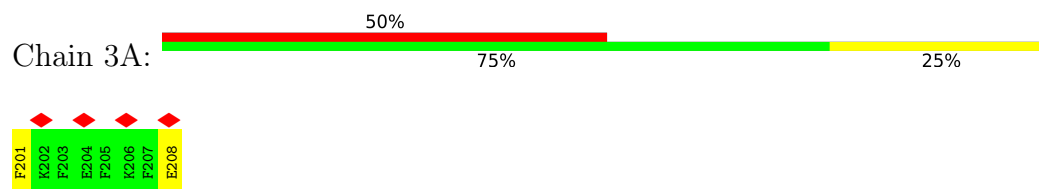
- Molecule 1: KFE8 peptide



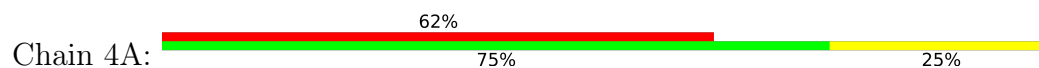
- Molecule 1: KFE8 peptide

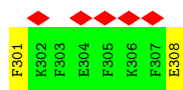


- Molecule 1: KFE8 peptide



- Molecule 1: KFE8 peptide

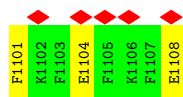




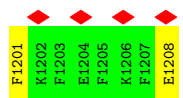
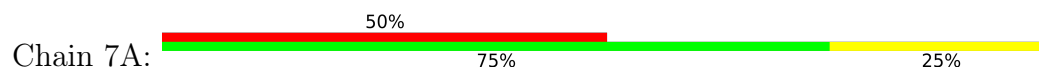
- Molecule 1: KFE8 peptide



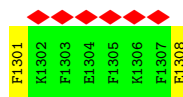
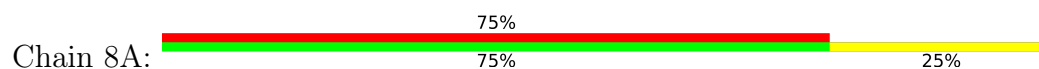
- Molecule 1: KFE8 peptide



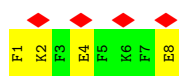
- Molecule 1: KFE8 peptide



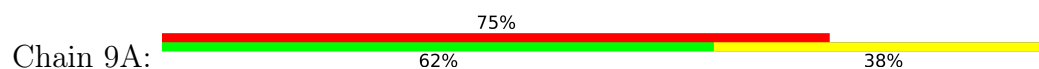
- Molecule 1: KFE8 peptide



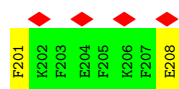
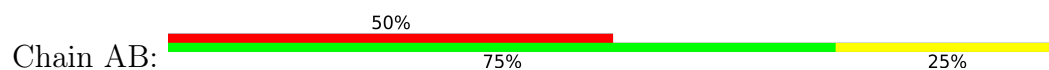
- Molecule 1: KFE8 peptide



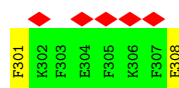
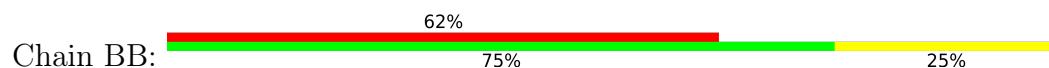
- Molecule 1: KFE8 peptide



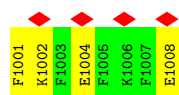
- Molecule 1: KFE8 peptide



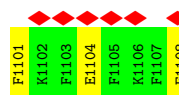
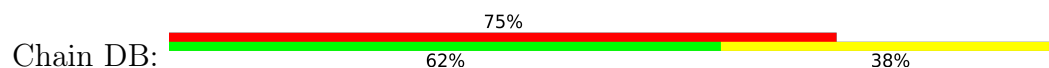
- Molecule 1: KFE8 peptide



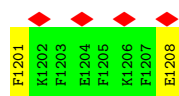
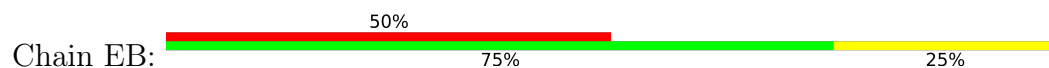
- Molecule 1: KFE8 peptide



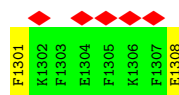
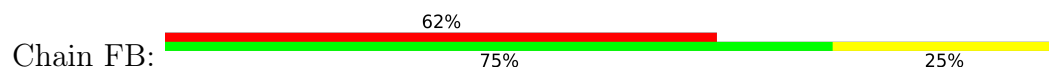
- Molecule 1: KFE8 peptide



- Molecule 1: KFE8 peptide

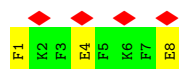


- Molecule 1: KFE8 peptide

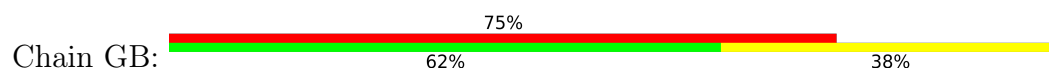


- Molecule 1: KFE8 peptide

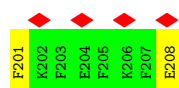
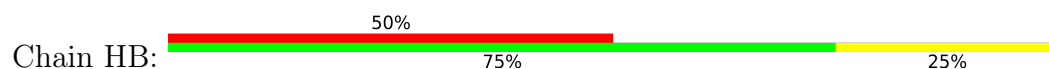




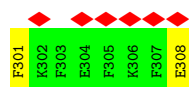
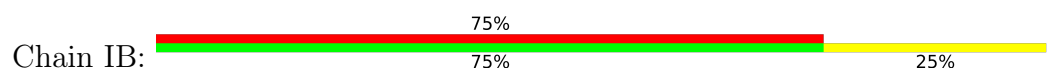
- Molecule 1: KFE8 peptide



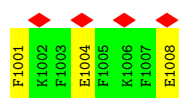
- Molecule 1: KFE8 peptide



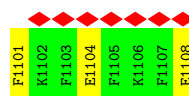
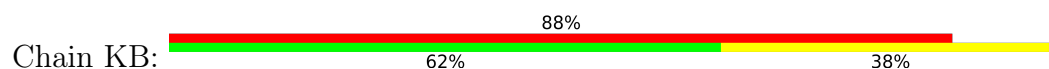
- Molecule 1: KFE8 peptide



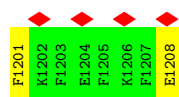
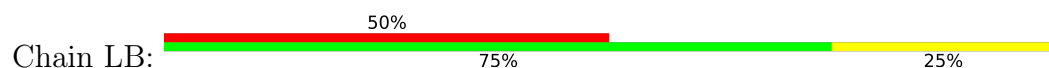
- Molecule 1: KFE8 peptide



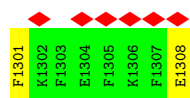
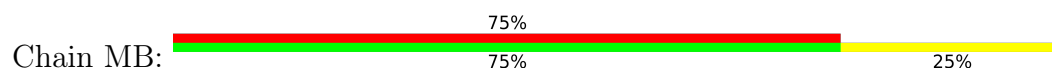
- Molecule 1: KFE8 peptide



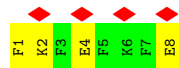
- Molecule 1: KFE8 peptide



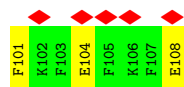
- Molecule 1: KFE8 peptide



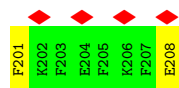
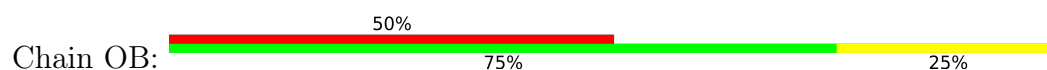
- Molecule 1: KFE8 peptide



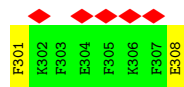
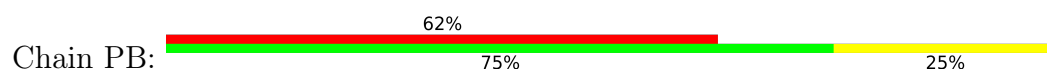
- Molecule 1: KFE8 peptide



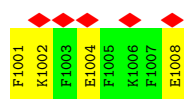
- Molecule 1: KFE8 peptide



- Molecule 1: KFE8 peptide

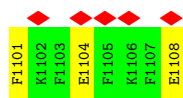


- Molecule 1: KFE8 peptide

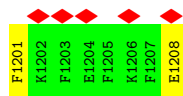
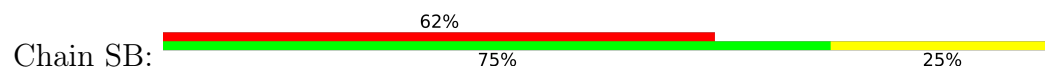


- Molecule 1: KFE8 peptide

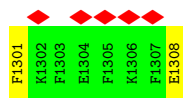
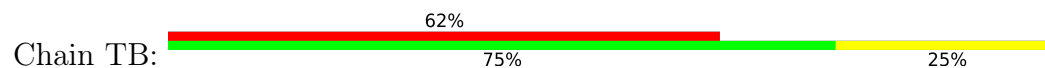




- Molecule 1: KFE8 peptide



- Molecule 1: KFE8 peptide



## 4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-15.8°, rise=7.93 Å, axial sym=C2	Depositor
Number of segments used	15486	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	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	0.881	Depositor
Minimum map value	-0.001	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.030	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	0.60	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	0.51	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	0.55	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	0.54	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	0.54	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	0.50	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	0.46	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	0.49	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	0.36	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	0.59	0/79
1	cA	0.51	0/62	0.48	0/79
1	d	0.55	0/62	0.60	0/79
1	dA	0.55	0/62	0.60	0/79
1	e	0.54	0/62	0.59	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	0.60	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	0.47	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	0.53	0/62	0.45	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	0.44	0/79
1	uA	0.51	0/62	0.48	0/79
1	v	0.60	0/62	0.42	0/79
1	vA	0.49	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	0.50	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 ⓘ

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

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*



*Continued from previous page...*

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 ⓘ

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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%)	4 (67%)	2 (33%)	0	1
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%)	5 (83%)	1 (17%)	2	8
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

*Continued on next page...*

*Continued from previous page...*

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

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	102	LYS
1	J	106	LYS
1	L	302	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	N	1102	LYS
1	N	1106	LYS
1	P	1302	LYS
1	Q	102	LYS
1	Q	106	LYS
1	S	302	LYS
1	U	1102	LYS
1	U	1106	LYS
1	W	1302	LYS
1	X	102	LYS
1	X	106	LYS
1	Z	302	LYS
1	k	1102	LYS
1	k	1106	LYS
1	m	1302	LYS
1	n	102	LYS
1	n	106	LYS
1	p	302	LYS
1	r	1102	LYS
1	r	1106	LYS
1	t	1302	LYS
1	u	102	LYS
1	u	106	LYS
1	w	302	LYS
1	y	1102	LYS
1	y	1106	LYS
1	0	1302	LYS
1	1	102	LYS
1	1	106	LYS
1	3	302	LYS
1	5	1102	LYS
1	5	1106	LYS
1	7	1302	LYS
1	8	102	LYS
1	8	106	LYS
1	AA	302	LYS
1	CA	1102	LYS
1	CA	1106	LYS
1	EA	1302	LYS
1	FA	102	LYS
1	FA	106	LYS
1	HA	302	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	JA	1102	LYS
1	JA	1106	LYS
1	LA	1302	LYS
1	MA	102	LYS
1	MA	106	LYS
1	OA	302	LYS
1	QA	1102	LYS
1	QA	1106	LYS
1	SA	1302	LYS
1	a	2	LYS
1	a	4	GLU
1	TA	104	GLU
1	WA	1002	LYS
1	WA	1004	GLU
1	XA	1104	GLU
1	b	2	LYS
1	b	4	GLU
1	aA	104	GLU
1	dA	1002	LYS
1	dA	1004	GLU
1	eA	1104	GLU
1	c	2	LYS
1	c	4	GLU
1	hA	104	GLU
1	kA	1002	LYS
1	kA	1004	GLU
1	lA	1104	GLU
1	d	2	LYS
1	d	4	GLU
1	oA	104	GLU
1	rA	1002	LYS
1	rA	1004	GLU
1	sA	1104	GLU
1	e	4	GLU
1	vA	104	GLU
1	yA	1004	GLU
1	zA	1104	GLU
1	f	2	LYS
1	f	4	GLU
1	2A	104	GLU
1	5A	1002	LYS
1	5A	1004	GLU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	6A	1104	GLU
1	g	2	LYS
1	g	4	GLU
1	9A	104	GLU
1	CB	1002	LYS
1	CB	1004	GLU
1	DB	1104	GLU
1	h	4	GLU
1	GB	104	GLU
1	JB	1004	GLU
1	KB	1104	GLU
1	i	2	LYS
1	i	4	GLU
1	NB	104	GLU
1	QB	1002	LYS
1	QB	1004	GLU
1	RB	1104	GLU

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	5CR	2A	101	1	13,14,15	1.21	1 (7%)	16,17,19	1.25	2 (12%)
1	5CR	XA	1101	1	13,14,15	1.21	1 (7%)	16,17,19	1.25	2 (12%)
1	GMA	BA	1008	1	9,9,9	1.13	0	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	MA	101	1	13,14,15	1.23	1 (7%)	16,17,19	1.51	2 (12%)
1	GMA	x	1008	1	9,9,9	1.16	1 (11%)	10,11,11	1.26	0
1	GMA	4A	308	1	9,9,9	1.14	1 (11%)	10,11,11	1.31	0
1	5CR	Q	101	1	13,14,15	1.22	1 (7%)	16,17,19	1.52	2 (12%)
1	GMA	aA	108	1	9,9,9	1.15	1 (11%)	10,11,11	1.20	0
1	5CR	RB	1101	1	13,14,15	1.21	1 (7%)	16,17,19	1.25	2 (12%)
1	GMA	H	8	1	9,9,9	1.15	0	10,11,11	1.26	0
1	GMA	xA	308	1	9,9,9	1.14	1 (11%)	10,11,11	1.32	0
1	5CR	AB	201	1	13,14,15	1.22	1 (7%)	16,17,19	1.14	1 (6%)
1	GMA	MA	108	1	9,9,9	1.15	1 (11%)	10,11,11	1.23	1 (10%)
1	GMA	NA	208	1	9,9,9	1.18	1 (11%)	10,11,11	1.28	2 (20%)
1	5CR	0	1301	1	13,14,15	1.24	2 (15%)	16,17,19	1.27	3 (18%)
1	GMA	T	1008	1	9,9,9	1.15	1 (11%)	10,11,11	1.26	1 (10%)
1	5CR	L	301	1	13,14,15	1.23	2 (15%)	16,17,19	1.28	3 (18%)
1	GMA	tA	1208	1	9,9,9	1.18	1 (11%)	10,11,11	1.13	0
1	5CR	sA	1101	1	13,14,15	1.21	1 (7%)	16,17,19	1.25	2 (12%)
1	5CR	BB	301	1	13,14,15	1.22	1 (7%)	16,17,19	1.03	1 (6%)
1	GMA	SA	1308	1	9,9,9	1.17	1 (11%)	10,11,11	1.24	0
1	GMA	2A	108	1	9,9,9	1.15	1 (11%)	10,11,11	1.18	0
1	GMA	7A	1208	1	9,9,9	1.18	1 (11%)	10,11,11	1.14	0
1	5CR	QB	1001	1	13,14,15	1.28	1 (7%)	16,17,19	1.74	4 (25%)
1	5CR	5	1101	1	13,14,15	1.23	1 (7%)	16,17,19	1.51	2 (12%)
1	GMA	h	8	1	9,9,9	1.18	1 (11%)	10,11,11	1.14	0
1	5CR	yA	1001	1	13,14,15	1.28	2 (15%)	16,17,19	1.73	4 (25%)
1	5CR	HA	301	1	13,14,15	1.21	2 (15%)	16,17,19	1.28	3 (18%)
1	5CR	x	1001	1	13,14,15	1.22	2 (15%)	16,17,19	1.69	3 (18%)
1	GMA	3	308	1	9,9,9	1.17	1 (11%)	10,11,11	1.24	0
1	GMA	3A	208	1	9,9,9	1.18	1 (11%)	10,11,11	1.14	0
1	GMA	V	1208	1	9,9,9	1.18	1 (11%)	10,11,11	1.26	1 (10%)
1	5CR	IA	1001	1	13,14,15	1.23	2 (15%)	16,17,19	1.69	3 (18%)
1	5CR	k	1101	1	13,14,15	1.23	1 (7%)	16,17,19	1.51	2 (12%)
1	5CR	rA	1001	1	13,14,15	1.29	2 (15%)	16,17,19	1.73	4 (25%)
1	GMA	w	308	1	9,9,9	1.15	1 (11%)	10,11,11	1.23	0
1	5CR	B	1	1	13,14,15	1.23	2 (15%)	16,17,19	1.70	3 (18%)
1	GMA	7	1308	1	9,9,9	1.17	1 (11%)	10,11,11	1.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	GMA	YA	1208	1	9,9,9	1.19	1 (11%)	10,11,11	1.14	0
1	GMA	bA	208	1	9,9,9	1.18	1 (11%)	10,11,11	1.11	0
1	GMA	HB	208	1	9,9,9	1.19	1 (11%)	10,11,11	1.14	0
1	GMA	JB	1008	1	9,9,9	1.18	1 (11%)	10,11,11	1.14	0
1	GMA	q	1008	1	9,9,9	1.16	1 (11%)	10,11,11	1.26	0
1	5CR	y	1101	1	13,14,15	1.23	1 (7%)	16,17,19	1.51	2 (12%)
1	5CR	MB	1301	1	13,14,15	1.23	1 (7%)	16,17,19	1.03	1 (6%)
1	GMA	G	8	1	9,9,9	1.13	0	10,11,11	1.25	0
1	GMA	zA	1108	1	9,9,9	1.15	1 (11%)	10,11,11	1.18	0
1	5CR	G	1	1	13,14,15	1.21	1 (7%)	16,17,19	1.70	3 (18%)
1	GMA	K	208	1	9,9,9	1.18	1 (11%)	10,11,11	1.27	0
1	GMA	AB	208	1	9,9,9	1.18	1 (11%)	10,11,11	1.13	0
1	5CR	lA	1101	1	13,14,15	1.22	1 (7%)	16,17,19	1.26	2 (12%)
1	GMA	j	1008	1	9,9,9	1.15	1 (11%)	10,11,11	1.26	0
1	GMA	k	1108	1	9,9,9	1.14	0	10,11,11	1.22	0
1	5CR	SB	1201	1	13,14,15	1.21	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	8A	1308	1	9,9,9	1.14	1 (11%)	10,11,11	1.31	0
1	5CR	dA	1001	1	13,14,15	1.27	2 (15%)	16,17,19	1.74	4 (25%)
1	5CR	7A	1201	1	13,14,15	1.23	1 (7%)	16,17,19	1.14	1 (6%)
1	GMA	LA	1308	1	9,9,9	1.17	1 (11%)	10,11,11	1.24	0
1	GMA	0	1308	1	9,9,9	1.15	1 (11%)	10,11,11	1.23	0
1	5CR	UA	201	1	13,14,15	1.22	1 (7%)	16,17,19	1.14	1 (6%)
1	GMA	c	8	1	9,9,9	1.18	1 (11%)	10,11,11	1.14	0
1	5CR	q	1001	1	13,14,15	1.22	2 (15%)	16,17,19	1.69	3 (18%)
1	5CR	zA	1101	1	13,14,15	1.21	1 (7%)	16,17,19	1.26	2 (12%)
1	GMA	g	8	1	9,9,9	1.19	1 (11%)	10,11,11	1.14	0
1	5CR	I	1	1	13,14,15	1.22	2 (15%)	16,17,19	1.71	3 (18%)
1	5CR	S	301	1	13,14,15	1.22	2 (15%)	16,17,19	1.28	3 (18%)
1	5CR	NA	201	1	13,14,15	1.24	1 (7%)	16,17,19	1.34	2 (12%)
1	GMA	J	108	1	9,9,9	1.15	1 (11%)	10,11,11	1.24	1 (10%)
1	GMA	d	8	1	9,9,9	1.19	1 (11%)	10,11,11	1.14	0
1	5CR	A	1	1	13,14,15	1.22	1 (7%)	16,17,19	1.70	3 (18%)
1	5CR	ZA	1301	1	13,14,15	1.23	1 (7%)	16,17,19	1.02	1 (6%)
1	5CR	5A	1001	1	13,14,15	1.28	2 (15%)	16,17,19	1.74	4 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	5CR	r	1101	1	13,14,15	1.22	1 (7%)	16,17,19	1.50	2 (12%)
1	5CR	vA	101	1	13,14,15	1.21	1 (7%)	16,17,19	1.26	2 (12%)
1	GMA	O	1208	1	9,9,9	1.18	1 (11%)	10,11,11	1.27	0
1	GMA	sA	1108	1	9,9,9	1.15	1 (11%)	10,11,11	1.18	0
1	5CR	U	1101	1	13,14,15	1.22	1 (7%)	16,17,19	1.52	2 (12%)
1	5CR	m	1301	1	13,14,15	1.24	2 (15%)	16,17,19	1.27	3 (18%)
1	GMA	P	1308	1	9,9,9	1.17	1 (11%)	10,11,11	1.24	0
1	5CR	nA	1301	1	13,14,15	1.23	1 (7%)	16,17,19	1.02	1 (6%)
1	GMA	lA	1108	1	9,9,9	1.14	1 (11%)	10,11,11	1.18	0
1	5CR	KA	1201	1	13,14,15	1.24	1 (7%)	16,17,19	1.34	3 (18%)
1	GMA	lA	1308	1	9,9,9	1.14	1 (11%)	10,11,11	1.32	0
1	5CR	JA	1101	1	13,14,15	1.23	1 (7%)	16,17,19	1.50	2 (12%)
1	5CR	iA	201	1	13,14,15	1.23	1 (7%)	16,17,19	1.14	1 (6%)
1	GMA	cA	308	1	9,9,9	1.15	1 (11%)	10,11,11	1.33	0
1	5CR	J	101	1	13,14,15	1.23	1 (7%)	16,17,19	1.51	2 (12%)
1	GMA	f	8	1	9,9,9	1.19	1 (11%)	10,11,11	1.15	0
1	GMA	fA	1208	1	9,9,9	1.18	1 (11%)	10,11,11	1.11	0
1	5CR	W	1301	1	13,14,15	1.22	2 (15%)	16,17,19	1.28	3 (18%)
1	5CR	C	1	1	13,14,15	1.22	2 (15%)	16,17,19	1.69	3 (18%)
1	5CR	b	1	1	13,14,15	1.27	2 (15%)	16,17,19	1.74	4 (25%)
1	5CR	xA	301	1	13,14,15	1.21	1 (7%)	16,17,19	1.03	1 (6%)
1	5CR	AA	301	1	13,14,15	1.22	2 (15%)	16,17,19	1.29	3 (18%)
1	GMA	v	208	1	9,9,9	1.17	1 (11%)	10,11,11	1.26	1 (10%)
1	5CR	TA	101	1	13,14,15	1.21	1 (7%)	16,17,19	1.25	2 (12%)
1	5CR	YA	1201	1	13,14,15	1.22	1 (7%)	16,17,19	1.14	1 (6%)
1	GMA	FA	108	1	9,9,9	1.14	1 (11%)	10,11,11	1.23	1 (10%)
1	5CR	CA	1101	1	13,14,15	1.24	1 (7%)	16,17,19	1.52	2 (12%)
1	GMA	IB	308	1	9,9,9	1.15	1 (11%)	10,11,11	1.33	0
1	5CR	WA	1001	1	13,14,15	1.28	2 (15%)	16,17,19	1.74	4 (25%)
1	5CR	jA	301	1	13,14,15	1.23	1 (7%)	16,17,19	1.02	1 (6%)
1	GMA	yA	1008	1	9,9,9	1.20	1 (11%)	10,11,11	1.16	0
1	GMA	FB	1308	1	9,9,9	1.14	1 (11%)	10,11,11	1.32	0
1	GMA	QB	1008	1	9,9,9	1.19	1 (11%)	10,11,11	1.15	0
1	5CR	Y	201	1	13,14,15	1.24	2 (15%)	16,17,19	1.34	2 (12%)
1	5CR	X	101	1	13,14,15	1.23	1 (7%)	16,17,19	1.51	2 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	GMA	VA	308	1	9,9,9	1.15	1 (11%)	10,11,11	1.32	0
1	5CR	3	301	1	13,14,15	1.23	2 (15%)	16,17,19	1.29	3 (18%)
1	GMA	t	1308	1	9,9,9	1.17	1 (11%)	10,11,11	1.24	0
1	GMA	JA	1108	1	9,9,9	1.14	1 (11%)	10,11,11	1.23	1 (10%)
1	5CR	JB	1001	1	13,14,15	1.28	1 (7%)	16,17,19	1.74	4 (25%)
1	GMA	u	108	1	9,9,9	1.14	0	10,11,11	1.22	0
1	5CR	F	1	1	13,14,15	1.22	1 (7%)	16,17,19	1.70	3 (18%)
1	5CR	LB	1201	1	13,14,15	1.22	1 (7%)	16,17,19	1.14	1 (6%)
1	5CR	g	1	1	13,14,15	1.28	2 (15%)	16,17,19	1.74	4 (25%)
1	GMA	Z	308	1	9,9,9	1.17	1 (11%)	10,11,11	1.24	0
1	5CR	eA	1101	1	13,14,15	1.21	1 (7%)	16,17,19	1.25	2 (12%)
1	5CR	DA	1201	1	13,14,15	1.24	1 (7%)	16,17,19	1.33	2 (12%)
1	GMA	TA	108	1	9,9,9	1.16	1 (11%)	10,11,11	1.19	0
1	5CR	NB	101	1	13,14,15	1.21	1 (7%)	16,17,19	1.25	2 (12%)
1	5CR	wA	201	1	13,14,15	1.22	1 (7%)	16,17,19	1.15	1 (6%)
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	5CR	E	1	1	13,14,15	1.22	2 (15%)	16,17,19	1.69	3 (18%)
1	GMA	jA	308	1	9,9,9	1.14	1 (11%)	10,11,11	1.33	0
1	5CR	OB	201	1	13,14,15	1.21	1 (7%)	16,17,19	1.14	1 (6%)
1	5CR	PB	301	1	13,14,15	1.22	1 (7%)	16,17,19	1.03	1 (6%)
1	GMA	e	8	1	9,9,9	1.20	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	5CR	o	201	1	13,14,15	1.24	1 (7%)	16,17,19	1.35	2 (12%)
1	5CR	n	101	1	13,14,15	1.22	1 (7%)	16,17,19	1.50	2 (12%)
1	5CR	P	1301	1	13,14,15	1.23	2 (15%)	16,17,19	1.28	3 (18%)
1	5CR	DB	1101	1	13,14,15	1.23	1 (7%)	16,17,19	1.25	2 (12%)
1	GMA	n	108	1	9,9,9	1.13	1 (11%)	10,11,11	1.22	1 (10%)
1	5CR	mA	1201	1	13,14,15	1.23	1 (7%)	16,17,19	1.14	1 (6%)
1	5CR	KB	1101	1	13,14,15	1.23	1 (7%)	16,17,19	1.24	2 (12%)
1	GMA	p	308	1	9,9,9	1.17	1 (11%)	10,11,11	1.24	0
1	GMA	CB	1008	1	9,9,9	1.19	1 (11%)	10,11,11	1.14	0
1	GMA	GA	208	1	9,9,9	1.18	1 (11%)	10,11,11	1.27	2 (20%)
1	5CR	LA	1301	1	13,14,15	1.21	2 (15%)	16,17,19	1.28	3 (18%)
1	GMA	iA	208	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	eA	1108	1	9,9,9	1.15	1 (11%)	10,11,11	1.20	0
1	5CR	CB	1001	1	13,14,15	1.28	2 (15%)	16,17,19	1.74	4 (25%)
1	GMA	GB	108	1	9,9,9	1.15	1 (11%)	10,11,11	1.18	0
1	GMA	6	1208	1	9,9,9	1.17	1 (11%)	10,11,11	1.26	1 (10%)
1	5CR	kA	1001	1	13,14,15	1.28	1 (7%)	16,17,19	1.73	4 (25%)
1	5CR	SA	1301	1	13,14,15	1.23	2 (15%)	16,17,19	1.28	3 (18%)
1	GMA	F	8	1	9,9,9	1.15	1 (11%)	10,11,11	1.27	1 (10%)
1	5CR	7	1301	1	13,14,15	1.23	2 (15%)	16,17,19	1.29	3 (18%)
1	GMA	B	8	1	9,9,9	1.15	1 (11%)	10,11,11	1.26	1 (10%)
1	GMA	gA	1308	1	9,9,9	1.15	1 (11%)	10,11,11	1.33	0
1	GMA	OB	208	1	9,9,9	1.19	1 (11%)	10,11,11	1.12	0
1	GMA	8	108	1	9,9,9	1.13	0	10,11,11	1.21	0
1	5CR	s	1201	1	13,14,15	1.24	1 (7%)	16,17,19	1.35	2 (12%)
1	GMA	HA	308	1	9,9,9	1.17	1 (11%)	10,11,11	1.24	0
1	5CR	a	1	1	13,14,15	1.28	2 (15%)	16,17,19	1.74	4 (25%)
1	5CR	2	201	1	13,14,15	1.25	2 (15%)	16,17,19	1.34	2 (12%)
1	GMA	W	1308	1	9,9,9	1.18	1 (11%)	10,11,11	1.25	0
1	GMA	S	308	1	9,9,9	1.18	1 (11%)	10,11,11	1.25	0
1	GMA	MB	1308	1	9,9,9	1.15	1 (11%)	10,11,11	1.33	0
1	5CR	pA	201	1	13,14,15	1.23	1 (7%)	16,17,19	1.14	1 (6%)
1	GMA	QA	1108	1	9,9,9	1.15	1 (11%)	10,11,11	1.23	1 (10%)
1	5CR	K	201	1	13,14,15	1.23	1 (7%)	16,17,19	1.33	2 (12%)
1	5CR	V	1201	1	13,14,15	1.24	1 (7%)	16,17,19	1.34	2 (12%)
1	5CR	c	1	1	13,14,15	1.28	1 (7%)	16,17,19	1.73	4 (25%)
1	GMA	9	208	1	9,9,9	1.19	1 (11%)	10,11,11	1.28	2 (20%)
1	5CR	aA	101	1	13,14,15	1.21	1 (7%)	16,17,19	1.25	2 (12%)
1	GMA	EA	1308	1	9,9,9	1.16	1 (11%)	10,11,11	1.25	0
1	5CR	f	1	1	13,14,15	1.28	2 (15%)	16,17,19	1.74	4 (25%)
1	GMA	CA	1108	1	9,9,9	1.13	0	10,11,11	1.21	0
1	5CR	0A	1201	1	13,14,15	1.22	1 (7%)	16,17,19	1.15	1 (6%)
1	GMA	uA	1308	1	9,9,9	1.14	1 (11%)	10,11,11	1.31	0
1	GMA	UA	208	1	9,9,9	1.19	1 (11%)	10,11,11	1.14	0
1	GMA	z	1208	1	9,9,9	1.17	1 (11%)	10,11,11	1.26	1 (10%)
1	GMA	s	1208	1	9,9,9	1.17	1 (11%)	10,11,11	1.26	1 (10%)
1	5CR	bA	201	1	13,14,15	1.22	1 (7%)	16,17,19	1.13	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	5CR	j	1001	1	13,14,15	1.22	2 (15%)	16,17,19	1.69	3 (18%)
1	GMA	EB	1208	1	9,9,9	1.18	1 (11%)	10,11,11	1.13	0
1	GMA	SB	1208	1	9,9,9	1.19	1 (11%)	10,11,11	1.12	0
1	GMA	NB	108	1	9,9,9	1.14	1 (11%)	10,11,11	1.17	0
1	5CR	QA	1101	1	13,14,15	1.23	1 (7%)	16,17,19	1.51	2 (12%)
1	GMA	R	208	1	9,9,9	1.18	1 (11%)	10,11,11	1.26	1 (10%)
1	GMA	r	1108	1	9,9,9	1.13	1 (11%)	10,11,11	1.22	1 (10%)
1	GMA	ZA	1308	1	9,9,9	1.15	1 (11%)	10,11,11	1.32	0
1	5CR	i	1	1	13,14,15	1.28	1 (7%)	16,17,19	1.74	4 (25%)
1	GMA	Y	208	1	9,9,9	1.18	1 (11%)	10,11,11	1.27	2 (20%)
1	GMA	qA	308	1	9,9,9	1.14	1 (11%)	10,11,11	1.31	0
1	GMA	rA	1008	1	9,9,9	1.19	1 (11%)	10,11,11	1.14	0
1	GMA	LB	1208	1	9,9,9	1.19	1 (11%)	10,11,11	1.14	0
1	5CR	M	1001	1	13,14,15	1.22	1 (7%)	16,17,19	1.70	3 (18%)
1	5CR	qA	301	1	13,14,15	1.23	1 (7%)	16,17,19	1.01	1 (6%)
1	GMA	X	108	1	9,9,9	1.14	0	10,11,11	1.22	0
1	GMA	b	8	1	9,9,9	1.18	1 (11%)	10,11,11	1.15	0
1	GMA	U	1108	1	9,9,9	1.14	1 (11%)	10,11,11	1.23	1 (10%)
1	GMA	RA	1208	1	9,9,9	1.18	1 (11%)	10,11,11	1.28	2 (20%)
1	5CR	D	1	1	13,14,15	1.22	2 (15%)	16,17,19	1.69	3 (18%)
1	GMA	l	1208	1	9,9,9	1.18	1 (11%)	10,11,11	1.27	2 (20%)
1	5CR	OA	301	1	13,14,15	1.23	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	5CR	hA	101	1	13,14,15	1.22	1 (7%)	16,17,19	1.26	2 (12%)
1	GMA	AA	308	1	9,9,9	1.16	1 (11%)	10,11,11	1.25	0
1	5CR	R	201	1	13,14,15	1.24	1 (7%)	16,17,19	1.34	2 (12%)
1	5CR	HB	201	1	13,14,15	1.22	1 (7%)	16,17,19	1.14	1 (6%)
1	GMA	I	8	1	9,9,9	1.16	1 (11%)	10,11,11	1.27	1 (10%)
1	GMA	6A	1108	1	9,9,9	1.15	1 (11%)	10,11,11	1.18	0
1	5CR	6	1201	1	13,14,15	1.25	2 (15%)	16,17,19	1.34	2 (12%)
1	5CR	4	1001	1	13,14,15	1.22	1 (7%)	16,17,19	1.70	3 (18%)
1	5CR	IB	301	1	13,14,15	1.23	1 (7%)	16,17,19	1.03	1 (6%)
1	GMA	RB	1108	1	9,9,9	1.14	1 (11%)	10,11,11	1.17	0
1	5CR	TB	1301	1	13,14,15	1.22	1 (7%)	16,17,19	1.03	1 (6%)
1	GMA	KA	1208	1	9,9,9	1.18	1 (11%)	10,11,11	1.27	2 (20%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	5CR	1	101	1	13,14,15	1.23	1 (7%)	16,17,19	1.51	2 (12%)
1	GMA	1	108	1	9,9,9	1.13	0	10,11,11	1.22	1 (10%)
1	5CR	3A	201	1	13,14,15	1.23	1 (7%)	16,17,19	1.14	1 (6%)
1	5CR	w	301	1	13,14,15	1.24	2 (15%)	16,17,19	1.27	3 (18%)
1	GMA	PA	1008	1	9,9,9	1.16	1 (11%)	10,11,11	1.27	1 (10%)
1	GMA	2	208	1	9,9,9	1.17	1 (11%)	10,11,11	1.26	1 (10%)
1	5CR	v	201	1	13,14,15	1.25	1 (7%)	16,17,19	1.33	2 (12%)
1	5CR	EA	1301	1	13,14,15	1.22	2 (15%)	16,17,19	1.29	3 (18%)
1	5CR	O	1201	1	13,14,15	1.23	1 (7%)	16,17,19	1.33	2 (12%)
1	5CR	FB	1301	1	13,14,15	1.22	1 (7%)	16,17,19	1.03	1 (6%)
1	GMA	IA	1008	1	9,9,9	1.15	0	10,11,11	1.26	0
1	GMA	pA	208	1	9,9,9	1.18	1 (11%)	10,11,11	1.13	0
1	5CR	8A	1301	1	13,14,15	1.22	1 (7%)	16,17,19	1.02	1 (6%)
1	5CR	p	301	1	13,14,15	1.22	2 (15%)	16,17,19	1.28	3 (18%)
1	GMA	C	8	1	9,9,9	1.15	1 (11%)	10,11,11	1.26	0
1	5CR	d	1	1	13,14,15	1.29	2 (15%)	16,17,19	1.73	4 (25%)
1	GMA	kA	1008	1	9,9,9	1.18	1 (11%)	10,11,11	1.14	0
1	GMA	wA	208	1	9,9,9	1.18	1 (11%)	10,11,11	1.14	0
1	5CR	h	1	1	13,14,15	1.28	1 (7%)	16,17,19	1.74	4 (25%)
1	GMA	y	1108	1	9,9,9	1.14	0	10,11,11	1.22	0
1	GMA	0A	1208	1	9,9,9	1.18	1 (11%)	10,11,11	1.14	0
1	5CR	l	1201	1	13,14,15	1.24	2 (15%)	16,17,19	1.34	2 (12%)
1	GMA	Q	108	1	9,9,9	1.14	1 (11%)	10,11,11	1.23	1 (10%)
1	5CR	z	1201	1	13,14,15	1.25	1 (7%)	16,17,19	1.33	2 (12%)
1	GMA	DA	1208	1	9,9,9	1.19	1 (11%)	10,11,11	1.28	2 (20%)
1	5CR	EB	1201	1	13,14,15	1.22	1 (7%)	16,17,19	1.14	1 (6%)
1	GMA	m	1308	1	9,9,9	1.17	1 (11%)	10,11,11	1.24	0
1	GMA	DB	1108	1	9,9,9	1.16	1 (11%)	10,11,11	1.19	0
1	5CR	FA	101	1	13,14,15	1.23	1 (7%)	16,17,19	1.50	2 (12%)
1	5CR	fA	1201	1	13,14,15	1.22	1 (7%)	16,17,19	1.13	1 (6%)
1	5CR	tA	1201	1	13,14,15	1.23	1 (7%)	16,17,19	1.14	1 (6%)
1	5CR	9A	101	1	13,14,15	1.23	1 (7%)	16,17,19	1.25	2 (12%)
1	GMA	dA	1008	1	9,9,9	1.18	1 (11%)	10,11,11	1.15	0
1	5CR	BA	1001	1	13,14,15	1.21	1 (7%)	16,17,19	1.70	3 (18%)
1	GMA	nA	1308	1	9,9,9	1.14	1 (11%)	10,11,11	1.33	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	GMA	i	8	1	9,9,9	1.19	1 (11%)	10,11,11	1.15	0
1	5CR	1A	1301	1	13,14,15	1.21	1 (7%)	16,17,19	1.03	1 (6%)
1	GMA	9A	108	1	9,9,9	1.16	1 (11%)	10,11,11	1.19	0
1	GMA	D	8	1	9,9,9	1.16	1 (11%)	10,11,11	1.26	0
1	5CR	RA	1201	1	13,14,15	1.24	1 (7%)	16,17,19	1.34	2 (12%)
1	5CR	VA	301	1	13,14,15	1.23	1 (7%)	16,17,19	1.02	1 (6%)
1	GMA	a	8	1	9,9,9	1.18	1 (11%)	10,11,11	1.14	0
1	5CR	6A	1101	1	13,14,15	1.21	1 (7%)	16,17,19	1.25	2 (12%)
1	5CR	PA	1001	1	13,14,15	1.22	2 (15%)	16,17,19	1.71	3 (18%)
1	GMA	WA	1008	1	9,9,9	1.18	1 (11%)	10,11,11	1.14	0
1	GMA	5A	1008	1	9,9,9	1.19	1 (11%)	10,11,11	1.15	0
1	5CR	N	1101	1	13,14,15	1.23	1 (7%)	16,17,19	1.51	2 (12%)
1	5CR	4A	301	1	13,14,15	1.22	1 (7%)	16,17,19	1.02	1 (6%)
1	GMA	mA	1208	1	9,9,9	1.19	1 (11%)	10,11,11	1.14	0
1	5CR	Z	301	1	13,14,15	1.24	2 (15%)	16,17,19	1.27	3 (18%)
1	GMA	vA	108	1	9,9,9	1.15	1 (11%)	10,11,11	1.18	0
1	GMA	hA	108	1	9,9,9	1.14	1 (11%)	10,11,11	1.18	0
1	GMA	BB	308	1	9,9,9	1.14	1 (11%)	10,11,11	1.32	0
1	GMA	E	8	1	9,9,9	1.16	1 (11%)	10,11,11	1.26	0
1	5CR	cA	301	1	13,14,15	1.22	1 (7%)	16,17,19	1.02	1 (6%)
1	GMA	N	1108	1	9,9,9	1.15	1 (11%)	10,11,11	1.24	1 (10%)
1	GMA	oA	108	1	9,9,9	1.15	1 (11%)	10,11,11	1.18	0
1	GMA	TB	1308	1	9,9,9	1.15	1 (11%)	10,11,11	1.33	0
1	GMA	A	8	1	9,9,9	1.14	1 (11%)	10,11,11	1.24	0
1	5CR	8	101	1	13,14,15	1.24	1 (7%)	16,17,19	1.52	2 (12%)
1	GMA	OA	308	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	1.24	0
1	GMA	M	1008	1	9,9,9	1.14	1 (11%)	10,11,11	1.24	0
1	GMA	PB	308	1	9,9,9	1.15	1 (11%)	10,11,11	1.33	0
1	5CR	oA	101	1	13,14,15	1.21	1 (7%)	16,17,19	1.25	2 (12%)
1	5CR	gA	1301	1	13,14,15	1.22	1 (7%)	16,17,19	1.02	1 (6%)
1	5CR	e	1	1	13,14,15	1.28	2 (15%)	16,17,19	1.73	4 (25%)
1	GMA	o	208	1	9,9,9	1.17	1 (11%)	10,11,11	1.26	1 (10%)
1	5CR	GA	201	1	13,14,15	1.24	1 (7%)	16,17,19	1.34	3 (18%)
1	5CR	u	101	1	13,14,15	1.23	1 (7%)	16,17,19	1.51	2 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	5CR	GB	101	1	13,14,15	1.23	1 (7%)	16,17,19	1.24	2 (12%)
1	5CR	H	1	1	13,14,15	1.23	2 (15%)	16,17,19	1.69	3 (18%)
1	5CR	t	1301	1	13,14,15	1.22	2 (15%)	16,17,19	1.28	3 (18%)
1	GMA	4	1008	1	9,9,9	1.15	1 (11%)	10,11,11	1.27	1 (10%)
1	5CR	T	1001	1	13,14,15	1.23	2 (15%)	16,17,19	1.70	3 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5CR	2A	101	1	-	1/9/10/12	0/1/1/1
1	5CR	XA	1101	1	-	1/9/10/12	0/1/1/1
1	GMA	BA	1008	1	-	1/9/9/9	-
1	5CR	MA	101	1	-	2/9/10/12	0/1/1/1
1	GMA	x	1008	1	-	1/9/9/9	-
1	GMA	4A	308	1	-	0/9/9/9	-
1	5CR	Q	101	1	-	2/9/10/12	0/1/1/1
1	GMA	aA	108	1	-	0/9/9/9	-
1	5CR	RB	1101	1	-	1/9/10/12	0/1/1/1
1	GMA	H	8	1	-	1/9/9/9	-
1	GMA	xA	308	1	-	0/9/9/9	-
1	5CR	AB	201	1	-	2/9/10/12	0/1/1/1
1	GMA	MA	108	1	-	3/9/9/9	-
1	GMA	NA	208	1	-	1/9/9/9	-
1	5CR	0	1301	1	-	3/9/10/12	0/1/1/1
1	GMA	T	1008	1	-	1/9/9/9	-
1	5CR	L	301	1	-	3/9/10/12	0/1/1/1
1	GMA	tA	1208	1	-	4/9/9/9	-
1	5CR	sA	1101	1	-	1/9/10/12	0/1/1/1
1	5CR	BB	301	1	-	4/9/10/12	0/1/1/1
1	GMA	SA	1308	1	-	1/9/9/9	-
1	GMA	2A	108	1	-	0/9/9/9	-
1	GMA	7A	1208	1	-	4/9/9/9	-
1	5CR	QB	1001	1	-	6/9/10/12	0/1/1/1
1	5CR	5	1101	1	-	2/9/10/12	0/1/1/1
1	GMA	h	8	1	-	8/9/9/9	-
1	5CR	yA	1001	1	-	6/9/10/12	0/1/1/1

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5CR	HA	301	1	-	3/9/10/12	0/1/1/1
1	5CR	x	1001	1	-	0/9/10/12	0/1/1/1
1	GMA	3	308	1	-	1/9/9/9	-
1	GMA	3A	208	1	-	4/9/9/9	-
1	GMA	V	1208	1	-	1/9/9/9	-
1	5CR	IA	1001	1	-	0/9/10/12	0/1/1/1
1	5CR	k	1101	1	-	2/9/10/12	0/1/1/1
1	5CR	rA	1001	1	-	6/9/10/12	0/1/1/1
1	GMA	w	308	1	-	1/9/9/9	-
1	5CR	B	1	1	-	0/9/10/12	0/1/1/1
1	GMA	7	1308	1	-	1/9/9/9	-
1	GMA	YA	1208	1	-	4/9/9/9	-
1	GMA	bA	208	1	-	4/9/9/9	-
1	GMA	HB	208	1	-	4/9/9/9	-
1	GMA	JB	1008	1	-	8/9/9/9	-
1	GMA	q	1008	1	-	1/9/9/9	-
1	5CR	y	1101	1	-	2/9/10/12	0/1/1/1
1	5CR	MB	1301	1	-	4/9/10/12	0/1/1/1
1	GMA	G	8	1	-	1/9/9/9	-
1	GMA	zA	1108	1	-	0/9/9/9	-
1	5CR	G	1	1	-	0/9/10/12	0/1/1/1
1	GMA	K	208	1	-	1/9/9/9	-
1	GMA	AB	208	1	-	4/9/9/9	-
1	5CR	lA	1101	1	-	1/9/10/12	0/1/1/1
1	GMA	j	1008	1	-	1/9/9/9	-
1	GMA	k	1108	1	-	3/9/9/9	-
1	5CR	SB	1201	1	-	2/9/10/12	0/1/1/1
1	5CR	uA	1301	1	-	4/9/10/12	0/1/1/1
1	GMA	8A	1308	1	-	0/9/9/9	-
1	5CR	dA	1001	1	-	6/9/10/12	0/1/1/1
1	5CR	7A	1201	1	-	2/9/10/12	0/1/1/1
1	GMA	LA	1308	1	-	1/9/9/9	-
1	GMA	0	1308	1	-	1/9/9/9	-
1	5CR	UA	201	1	-	2/9/10/12	0/1/1/1
1	GMA	c	8	1	-	8/9/9/9	-
1	5CR	q	1001	1	-	0/9/10/12	0/1/1/1
1	5CR	zA	1101	1	-	1/9/10/12	0/1/1/1
1	GMA	g	8	1	-	8/9/9/9	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5CR	I	1	1	-	0/9/10/12	0/1/1/1
1	5CR	S	301	1	-	3/9/10/12	0/1/1/1
1	5CR	NA	201	1	-	4/9/10/12	0/1/1/1
1	GMA	J	108	1	-	3/9/9/9	-
1	GMA	d	8	1	-	8/9/9/9	-
1	5CR	A	1	1	-	0/9/10/12	0/1/1/1
1	5CR	ZA	1301	1	-	4/9/10/12	0/1/1/1
1	5CR	5A	1001	1	-	6/9/10/12	0/1/1/1
1	5CR	r	1101	1	-	2/9/10/12	0/1/1/1
1	5CR	vA	101	1	-	1/9/10/12	0/1/1/1
1	GMA	O	1208	1	-	1/9/9/9	-
1	GMA	sA	1108	1	-	0/9/9/9	-
1	5CR	U	1101	1	-	2/9/10/12	0/1/1/1
1	5CR	m	1301	1	-	3/9/10/12	0/1/1/1
1	GMA	P	1308	1	-	1/9/9/9	-
1	5CR	nA	1301	1	-	4/9/10/12	0/1/1/1
1	GMA	lA	1108	1	-	0/9/9/9	-
1	5CR	KA	1201	1	-	4/9/10/12	0/1/1/1
1	GMA	1A	1308	1	-	0/9/9/9	-
1	5CR	JA	1101	1	-	2/9/10/12	0/1/1/1
1	5CR	iA	201	1	-	2/9/10/12	0/1/1/1
1	GMA	cA	308	1	-	0/9/9/9	-
1	5CR	J	101	1	-	2/9/10/12	0/1/1/1
1	GMA	f	8	1	-	8/9/9/9	-
1	GMA	fA	1208	1	-	4/9/9/9	-
1	5CR	W	1301	1	-	3/9/10/12	0/1/1/1
1	5CR	C	1	1	-	0/9/10/12	0/1/1/1
1	5CR	b	1	1	-	6/9/10/12	0/1/1/1
1	5CR	xA	301	1	-	4/9/10/12	0/1/1/1
1	5CR	AA	301	1	-	3/9/10/12	0/1/1/1
1	GMA	v	208	1	-	1/9/9/9	-
1	5CR	TA	101	1	-	1/9/10/12	0/1/1/1
1	5CR	YA	1201	1	-	2/9/10/12	0/1/1/1
1	GMA	FA	108	1	-	3/9/9/9	-
1	5CR	CA	1101	1	-	2/9/10/12	0/1/1/1
1	GMA	IB	308	1	-	0/9/9/9	-
1	5CR	WA	1001	1	-	6/9/10/12	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5CR	jA	301	1	-	4/9/10/12	0/1/1/1
1	GMA	yA	1008	1	-	8/9/9/9	-
1	GMA	FB	1308	1	-	0/9/9/9	-
1	GMA	QB	1008	1	-	8/9/9/9	-
1	5CR	Y	201	1	-	4/9/10/12	0/1/1/1
1	5CR	X	101	1	-	2/9/10/12	0/1/1/1
1	GMA	VA	308	1	-	0/9/9/9	-
1	5CR	3	301	1	-	3/9/10/12	0/1/1/1
1	GMA	t	1308	1	-	1/9/9/9	-
1	GMA	JA	1108	1	-	3/9/9/9	-
1	5CR	JB	1001	1	-	6/9/10/12	0/1/1/1
1	GMA	u	108	1	-	3/9/9/9	-
1	5CR	F	1	1	-	0/9/10/12	0/1/1/1
1	5CR	LB	1201	1	-	2/9/10/12	0/1/1/1
1	5CR	g	1	1	-	6/9/10/12	0/1/1/1
1	GMA	Z	308	1	-	1/9/9/9	-
1	5CR	eA	1101	1	-	1/9/10/12	0/1/1/1
1	5CR	DA	1201	1	-	4/9/10/12	0/1/1/1
1	GMA	TA	108	1	-	0/9/9/9	-
1	5CR	NB	101	1	-	1/9/10/12	0/1/1/1
1	5CR	wA	201	1	-	2/9/10/12	0/1/1/1
1	GMA	5	1108	1	-	3/9/9/9	-
1	5CR	9	201	1	-	4/9/10/12	0/1/1/1
1	5CR	E	1	1	-	0/9/10/12	0/1/1/1
1	GMA	jA	308	1	-	0/9/9/9	-
1	5CR	OB	201	1	-	2/9/10/12	0/1/1/1
1	5CR	PB	301	1	-	4/9/10/12	0/1/1/1
1	GMA	e	8	1	-	8/9/9/9	-
1	GMA	KB	1108	1	-	0/9/9/9	-
1	5CR	o	201	1	-	4/9/10/12	0/1/1/1
1	5CR	n	101	1	-	2/9/10/12	0/1/1/1
1	5CR	P	1301	1	-	3/9/10/12	0/1/1/1
1	5CR	DB	1101	1	-	1/9/10/12	0/1/1/1
1	GMA	n	108	1	-	3/9/9/9	-
1	5CR	mA	1201	1	-	2/9/10/12	0/1/1/1
1	5CR	KB	1101	1	-	1/9/10/12	0/1/1/1
1	GMA	p	308	1	-	1/9/9/9	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	GMA	CB	1008	1	-	8/9/9/9	-
1	GMA	GA	208	1	-	1/9/9/9	-
1	5CR	LA	1301	1	-	3/9/10/12	0/1/1/1
1	GMA	iA	208	1	-	4/9/9/9	-
1	GMA	eA	1108	1	-	0/9/9/9	-
1	5CR	CB	1001	1	-	6/9/10/12	0/1/1/1
1	GMA	GB	108	1	-	0/9/9/9	-
1	GMA	6	1208	1	-	1/9/9/9	-
1	5CR	kA	1001	1	-	6/9/10/12	0/1/1/1
1	5CR	SA	1301	1	-	3/9/10/12	0/1/1/1
1	GMA	F	8	1	-	1/9/9/9	-
1	5CR	7	1301	1	-	3/9/10/12	0/1/1/1
1	GMA	B	8	1	-	1/9/9/9	-
1	GMA	gA	1308	1	-	0/9/9/9	-
1	GMA	OB	208	1	-	4/9/9/9	-
1	GMA	8	108	1	-	3/9/9/9	-
1	5CR	s	1201	1	-	4/9/10/12	0/1/1/1
1	GMA	HA	308	1	-	1/9/9/9	-
1	5CR	a	1	1	-	6/9/10/12	0/1/1/1
1	5CR	2	201	1	-	4/9/10/12	0/1/1/1
1	GMA	W	1308	1	-	1/9/9/9	-
1	GMA	S	308	1	-	1/9/9/9	-
1	GMA	MB	1308	1	-	0/9/9/9	-
1	5CR	pA	201	1	-	2/9/10/12	0/1/1/1
1	GMA	QA	1108	1	-	3/9/9/9	-
1	5CR	K	201	1	-	4/9/10/12	0/1/1/1
1	5CR	V	1201	1	-	4/9/10/12	0/1/1/1
1	5CR	c	1	1	-	6/9/10/12	0/1/1/1
1	GMA	9	208	1	-	1/9/9/9	-
1	5CR	aA	101	1	-	1/9/10/12	0/1/1/1
1	GMA	EA	1308	1	-	1/9/9/9	-
1	5CR	f	1	1	-	6/9/10/12	0/1/1/1
1	GMA	CA	1108	1	-	3/9/9/9	-
1	5CR	0A	1201	1	-	2/9/10/12	0/1/1/1
1	GMA	uA	1308	1	-	0/9/9/9	-
1	GMA	UA	208	1	-	4/9/9/9	-
1	GMA	z	1208	1	-	1/9/9/9	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	GMA	s	1208	1	-	1/9/9/9	-
1	5CR	bA	201	1	-	2/9/10/12	0/1/1/1
1	5CR	j	1001	1	-	0/9/10/12	0/1/1/1
1	GMA	EB	1208	1	-	4/9/9/9	-
1	GMA	SB	1208	1	-	4/9/9/9	-
1	GMA	NB	108	1	-	0/9/9/9	-
1	5CR	QA	1101	1	-	2/9/10/12	0/1/1/1
1	GMA	R	208	1	-	1/9/9/9	-
1	GMA	r	1108	1	-	3/9/9/9	-
1	GMA	ZA	1308	1	-	0/9/9/9	-
1	5CR	i	1	1	-	6/9/10/12	0/1/1/1
1	GMA	Y	208	1	-	1/9/9/9	-
1	GMA	qA	308	1	-	0/9/9/9	-
1	GMA	rA	1008	1	-	8/9/9/9	-
1	GMA	LB	1208	1	-	4/9/9/9	-
1	5CR	M	1001	1	-	0/9/10/12	0/1/1/1
1	5CR	qA	301	1	-	4/9/10/12	0/1/1/1
1	GMA	X	108	1	-	3/9/9/9	-
1	GMA	b	8	1	-	8/9/9/9	-
1	GMA	U	1108	1	-	3/9/9/9	-
1	GMA	RA	1208	1	-	1/9/9/9	-
1	5CR	D	1	1	-	0/9/10/12	0/1/1/1
1	GMA	l	1208	1	-	1/9/9/9	-
1	5CR	OA	301	1	-	3/9/10/12	0/1/1/1
1	GMA	XA	1108	1	-	0/9/9/9	-
1	5CR	hA	101	1	-	1/9/10/12	0/1/1/1
1	GMA	AA	308	1	-	1/9/9/9	-
1	5CR	R	201	1	-	4/9/10/12	0/1/1/1
1	5CR	HB	201	1	-	2/9/10/12	0/1/1/1
1	GMA	I	8	1	-	1/9/9/9	-
1	GMA	6A	1108	1	-	0/9/9/9	-
1	5CR	6	1201	1	-	4/9/10/12	0/1/1/1
1	5CR	4	1001	1	-	0/9/10/12	0/1/1/1
1	5CR	IB	301	1	-	4/9/10/12	0/1/1/1
1	GMA	RB	1108	1	-	0/9/9/9	-
1	5CR	TB	1301	1	-	4/9/10/12	0/1/1/1
1	GMA	KA	1208	1	-	1/9/9/9	-
1	5CR	1	101	1	-	2/9/10/12	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	GMA	1	108	1	-	3/9/9/9	-
1	5CR	3A	201	1	-	2/9/10/12	0/1/1/1
1	5CR	w	301	1	-	3/9/10/12	0/1/1/1
1	GMA	PA	1008	1	-	1/9/9/9	-
1	GMA	2	208	1	-	1/9/9/9	-
1	5CR	v	201	1	-	4/9/10/12	0/1/1/1
1	5CR	EA	1301	1	-	3/9/10/12	0/1/1/1
1	5CR	O	1201	1	-	4/9/10/12	0/1/1/1
1	5CR	FB	1301	1	-	4/9/10/12	0/1/1/1
1	GMA	IA	1008	1	-	1/9/9/9	-
1	GMA	pA	208	1	-	4/9/9/9	-
1	5CR	8A	1301	1	-	4/9/10/12	0/1/1/1
1	5CR	p	301	1	-	3/9/10/12	0/1/1/1
1	GMA	C	8	1	-	1/9/9/9	-
1	5CR	d	1	1	-	6/9/10/12	0/1/1/1
1	GMA	kA	1008	1	-	8/9/9/9	-
1	GMA	wA	208	1	-	4/9/9/9	-
1	5CR	h	1	1	-	6/9/10/12	0/1/1/1
1	GMA	y	1108	1	-	3/9/9/9	-
1	GMA	0A	1208	1	-	4/9/9/9	-
1	5CR	l	1201	1	-	4/9/10/12	0/1/1/1
1	GMA	Q	108	1	-	3/9/9/9	-
1	5CR	z	1201	1	-	4/9/10/12	0/1/1/1
1	GMA	DA	1208	1	-	1/9/9/9	-
1	5CR	EB	1201	1	-	2/9/10/12	0/1/1/1
1	GMA	m	1308	1	-	1/9/9/9	-
1	GMA	DB	1108	1	-	0/9/9/9	-
1	5CR	FA	101	1	-	2/9/10/12	0/1/1/1
1	5CR	fA	1201	1	-	2/9/10/12	0/1/1/1
1	5CR	tA	1201	1	-	2/9/10/12	0/1/1/1
1	5CR	9A	101	1	-	1/9/10/12	0/1/1/1
1	GMA	dA	1008	1	-	8/9/9/9	-
1	5CR	BA	1001	1	-	0/9/10/12	0/1/1/1
1	GMA	nA	1308	1	-	0/9/9/9	-
1	GMA	i	8	1	-	8/9/9/9	-
1	5CR	1A	1301	1	-	4/9/10/12	0/1/1/1

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	GMA	9A	108	1	-	0/9/9/9	-
1	GMA	D	8	1	-	1/9/9/9	-
1	5CR	RA	1201	1	-	4/9/10/12	0/1/1/1
1	5CR	VA	301	1	-	4/9/10/12	0/1/1/1
1	GMA	a	8	1	-	8/9/9/9	-
1	5CR	6A	1101	1	-	1/9/10/12	0/1/1/1
1	5CR	PA	1001	1	-	0/9/10/12	0/1/1/1
1	GMA	WA	1008	1	-	8/9/9/9	-
1	GMA	5A	1008	1	-	8/9/9/9	-
1	5CR	N	1101	1	-	2/9/10/12	0/1/1/1
1	5CR	4A	301	1	-	4/9/10/12	0/1/1/1
1	GMA	mA	1208	1	-	4/9/9/9	-
1	5CR	Z	301	1	-	3/9/10/12	0/1/1/1
1	GMA	vA	108	1	-	0/9/9/9	-
1	GMA	hA	108	1	-	0/9/9/9	-
1	GMA	BB	308	1	-	0/9/9/9	-
1	GMA	E	8	1	-	1/9/9/9	-
1	5CR	cA	301	1	-	4/9/10/12	0/1/1/1
1	GMA	N	1108	1	-	3/9/9/9	-
1	GMA	oA	108	1	-	0/9/9/9	-
1	GMA	TB	1308	1	-	0/9/9/9	-
1	GMA	A	8	1	-	1/9/9/9	-
1	5CR	8	101	1	-	2/9/10/12	0/1/1/1
1	GMA	OA	308	1	-	1/9/9/9	-
1	GMA	L	308	1	-	1/9/9/9	-
1	GMA	M	1008	1	-	1/9/9/9	-
1	GMA	PB	308	1	-	0/9/9/9	-
1	5CR	oA	101	1	-	1/9/10/12	0/1/1/1
1	5CR	gA	1301	1	-	4/9/10/12	0/1/1/1
1	5CR	e	1	1	-	6/9/10/12	0/1/1/1
1	GMA	o	208	1	-	1/9/9/9	-
1	5CR	GA	201	1	-	4/9/10/12	0/1/1/1
1	5CR	u	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	H	1	1	-	0/9/10/12	0/1/1/1
1	5CR	t	1301	1	-	3/9/10/12	0/1/1/1
1	GMA	4	1008	1	-	1/9/9/9	-
1	5CR	T	1001	1	-	0/9/10/12	0/1/1/1

All (322) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	d	1	5CR	CAL-N	3.49	1.46	1.34
1	rA	1001	5CR	CAL-N	3.49	1.46	1.34
1	e	1	5CR	CAL-N	3.48	1.46	1.34
1	yA	1001	5CR	CAL-N	3.48	1.46	1.34
1	i	1	5CR	CAL-N	3.47	1.46	1.34
1	QB	1001	5CR	CAL-N	3.47	1.46	1.34
1	a	1	5CR	CAL-N	3.47	1.46	1.34
1	WA	1001	5CR	CAL-N	3.47	1.46	1.34
1	f	1	5CR	CAL-N	3.47	1.46	1.34
1	5A	1001	5CR	CAL-N	3.47	1.46	1.34
1	h	1	5CR	CAL-N	3.46	1.46	1.34
1	JB	1001	5CR	CAL-N	3.46	1.46	1.34
1	g	1	5CR	CAL-N	3.46	1.46	1.34
1	CB	1001	5CR	CAL-N	3.46	1.46	1.34
1	c	1	5CR	CAL-N	3.45	1.46	1.34
1	kA	1001	5CR	CAL-N	3.45	1.46	1.34
1	b	1	5CR	CAL-N	3.45	1.46	1.34
1	dA	1001	5CR	CAL-N	3.45	1.46	1.34
1	X	101	5CR	CAL-N	3.24	1.45	1.34
1	k	1101	5CR	CAL-N	3.24	1.45	1.34
1	1	101	5CR	CAL-N	3.23	1.45	1.34
1	5	1101	5CR	CAL-N	3.23	1.45	1.34
1	8	101	5CR	CAL-N	3.22	1.45	1.34
1	CA	1101	5CR	CAL-N	3.22	1.45	1.34
1	FA	101	5CR	CAL-N	3.22	1.45	1.34
1	JA	1101	5CR	CAL-N	3.22	1.45	1.34
1	n	101	5CR	CAL-N	3.22	1.45	1.34
1	r	1101	5CR	CAL-N	3.22	1.45	1.34
1	MA	101	5CR	CAL-N	3.22	1.45	1.34
1	QA	1101	5CR	CAL-N	3.22	1.45	1.34
1	HB	201	5CR	CAL-N	3.22	1.45	1.34
1	LB	1201	5CR	CAL-N	3.22	1.45	1.34
1	u	101	5CR	CAL-N	3.22	1.45	1.34
1	y	1101	5CR	CAL-N	3.22	1.45	1.34
1	J	101	5CR	CAL-N	3.21	1.45	1.34
1	N	1101	5CR	CAL-N	3.21	1.45	1.34
1	pA	201	5CR	CAL-N	3.21	1.45	1.34
1	tA	1201	5CR	CAL-N	3.21	1.45	1.34
1	GB	101	5CR	CAL-N	3.20	1.45	1.34
1	KB	1101	5CR	CAL-N	3.20	1.45	1.34
1	9A	101	5CR	CAL-N	3.20	1.45	1.34
1	DB	1101	5CR	CAL-N	3.20	1.45	1.34

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	101	5CR	CAL-N	3.20	1.45	1.34
1	U	1101	5CR	CAL-N	3.20	1.45	1.34
1	wA	201	5CR	CAL-N	3.20	1.45	1.34
1	0A	1201	5CR	CAL-N	3.20	1.45	1.34
1	hA	101	5CR	CAL-N	3.20	1.45	1.34
1	lA	1101	5CR	CAL-N	3.20	1.45	1.34
1	IB	301	5CR	CAL-N	3.20	1.45	1.34
1	MB	1301	5CR	CAL-N	3.20	1.45	1.34
1	OB	201	5CR	CAL-N	3.20	1.45	1.34
1	SB	1201	5CR	CAL-N	3.20	1.45	1.34
1	NB	101	5CR	CAL-N	3.20	1.45	1.34
1	RB	1101	5CR	CAL-N	3.20	1.45	1.34
1	qA	301	5CR	CAL-N	3.20	1.45	1.34
1	uA	1301	5CR	CAL-N	3.20	1.45	1.34
1	UA	201	5CR	CAL-N	3.19	1.45	1.34
1	YA	1201	5CR	CAL-N	3.19	1.45	1.34
1	iA	201	5CR	CAL-N	3.19	1.45	1.34
1	mA	1201	5CR	CAL-N	3.19	1.45	1.34
1	bA	201	5CR	CAL-N	3.19	1.45	1.34
1	fA	1201	5CR	CAL-N	3.19	1.45	1.34
1	3A	201	5CR	CAL-N	3.18	1.45	1.34
1	7A	1201	5CR	CAL-N	3.18	1.45	1.34
1	VA	301	5CR	CAL-N	3.18	1.45	1.34
1	ZA	1301	5CR	CAL-N	3.18	1.45	1.34
1	oA	101	5CR	CAL-N	3.18	1.45	1.34
1	sA	1101	5CR	CAL-N	3.18	1.45	1.34
1	4A	301	5CR	CAL-N	3.18	1.45	1.34
1	8A	1301	5CR	CAL-N	3.18	1.45	1.34
1	BB	301	5CR	CAL-N	3.18	1.45	1.34
1	FB	1301	5CR	CAL-N	3.18	1.45	1.34
1	PB	301	5CR	CAL-N	3.18	1.45	1.34
1	TB	1301	5CR	CAL-N	3.18	1.45	1.34
1	AB	201	5CR	CAL-N	3.18	1.45	1.34
1	EB	1201	5CR	CAL-N	3.18	1.45	1.34
1	xA	301	5CR	CAL-N	3.17	1.45	1.34
1	1A	1301	5CR	CAL-N	3.17	1.45	1.34
1	jA	301	5CR	CAL-N	3.16	1.45	1.34
1	nA	1301	5CR	CAL-N	3.16	1.45	1.34
1	TA	101	5CR	CAL-N	3.16	1.45	1.34
1	XA	1101	5CR	CAL-N	3.16	1.45	1.34
1	2A	101	5CR	CAL-N	3.16	1.45	1.34
1	6A	1101	5CR	CAL-N	3.16	1.45	1.34

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	aA	101	5CR	CAL-N	3.16	1.45	1.34
1	eA	1101	5CR	CAL-N	3.16	1.45	1.34
1	cA	301	5CR	CAL-N	3.15	1.45	1.34
1	gA	1301	5CR	CAL-N	3.15	1.45	1.34
1	vA	101	5CR	CAL-N	3.15	1.45	1.34
1	zA	1101	5CR	CAL-N	3.15	1.45	1.34
1	R	201	5CR	CAL-N	3.15	1.45	1.34
1	V	1201	5CR	CAL-N	3.15	1.45	1.34
1	Y	201	5CR	CAL-N	3.15	1.45	1.34
1	l	1201	5CR	CAL-N	3.15	1.45	1.34
1	NA	201	5CR	CAL-N	3.14	1.45	1.34
1	RA	1201	5CR	CAL-N	3.14	1.45	1.34
1	v	201	5CR	CAL-N	3.14	1.45	1.34
1	z	1201	5CR	CAL-N	3.14	1.45	1.34
1	9	201	5CR	CAL-N	3.13	1.45	1.34
1	DA	1201	5CR	CAL-N	3.13	1.45	1.34
1	GA	201	5CR	CAL-N	3.13	1.45	1.34
1	KA	1201	5CR	CAL-N	3.13	1.45	1.34
1	o	201	5CR	CAL-N	3.13	1.45	1.34
1	s	1201	5CR	CAL-N	3.13	1.45	1.34
1	2	201	5CR	CAL-N	3.12	1.45	1.34
1	6	1201	5CR	CAL-N	3.12	1.45	1.34
1	K	201	5CR	CAL-N	3.11	1.45	1.34
1	O	1201	5CR	CAL-N	3.11	1.45	1.34
1	E	1	5CR	CAL-N	3.10	1.45	1.34
1	x	1001	5CR	CAL-N	3.10	1.45	1.34
1	D	1	5CR	CAL-N	3.10	1.45	1.34
1	q	1001	5CR	CAL-N	3.10	1.45	1.34
1	F	1	5CR	CAL-N	3.09	1.45	1.34
1	4	1001	5CR	CAL-N	3.09	1.45	1.34
1	A	1	5CR	CAL-N	3.09	1.45	1.34
1	M	1001	5CR	CAL-N	3.09	1.45	1.34
1	C	1	5CR	CAL-N	3.09	1.45	1.34
1	j	1001	5CR	CAL-N	3.09	1.45	1.34
1	H	1	5CR	CAL-N	3.08	1.44	1.34
1	IA	1001	5CR	CAL-N	3.08	1.44	1.34
1	I	1	5CR	CAL-N	3.08	1.44	1.34
1	PA	1001	5CR	CAL-N	3.08	1.44	1.34
1	B	1	5CR	CAL-N	3.08	1.44	1.34
1	T	1001	5CR	CAL-N	3.08	1.44	1.34
1	w	301	5CR	CAL-N	3.08	1.44	1.34
1	0	1301	5CR	CAL-N	3.08	1.44	1.34

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Z	301	5CR	CAL-N	3.07	1.44	1.34
1	m	1301	5CR	CAL-N	3.07	1.44	1.34
1	p	301	5CR	CAL-N	3.07	1.44	1.34
1	t	1301	5CR	CAL-N	3.07	1.44	1.34
1	G	1	5CR	CAL-N	3.06	1.44	1.34
1	BA	1001	5CR	CAL-N	3.06	1.44	1.34
1	L	301	5CR	CAL-N	3.05	1.44	1.34
1	P	1301	5CR	CAL-N	3.05	1.44	1.34
1	S	301	5CR	CAL-N	3.05	1.44	1.34
1	W	1301	5CR	CAL-N	3.05	1.44	1.34
1	AA	301	5CR	CAL-N	3.04	1.44	1.34
1	EA	1301	5CR	CAL-N	3.04	1.44	1.34
1	OA	301	5CR	CAL-N	3.04	1.44	1.34
1	SA	1301	5CR	CAL-N	3.04	1.44	1.34
1	3	301	5CR	CAL-N	3.03	1.44	1.34
1	7	1301	5CR	CAL-N	3.03	1.44	1.34
1	HA	301	5CR	CAL-N	3.02	1.44	1.34
1	LA	1301	5CR	CAL-N	3.02	1.44	1.34
1	GA	208	GMA	C-N2	2.18	1.38	1.32
1	KA	1208	GMA	C-N2	2.18	1.38	1.32
1	9	208	GMA	C-N2	2.16	1.38	1.32
1	DA	1208	GMA	C-N2	2.16	1.38	1.32
1	Y	208	GMA	C-N2	2.16	1.38	1.32
1	l	1208	GMA	C-N2	2.16	1.38	1.32
1	Z	308	GMA	C-N2	2.15	1.38	1.32
1	m	1308	GMA	C-N2	2.15	1.38	1.32
1	S	308	GMA	C-N2	2.15	1.38	1.32
1	W	1308	GMA	C-N2	2.15	1.38	1.32
1	2	208	GMA	C-N2	2.15	1.38	1.32
1	6	1208	GMA	C-N2	2.15	1.38	1.32
1	v	208	GMA	C-N2	2.15	1.38	1.32
1	z	1208	GMA	C-N2	2.15	1.38	1.32
1	o	208	GMA	C-N2	2.15	1.38	1.32
1	s	1208	GMA	C-N2	2.15	1.38	1.32
1	R	208	GMA	C-N2	2.15	1.38	1.32
1	V	1208	GMA	C-N2	2.15	1.38	1.32
1	NA	208	GMA	C-N2	2.14	1.38	1.32
1	RA	1208	GMA	C-N2	2.14	1.38	1.32
1	f	8	GMA	C-N2	2.14	1.38	1.32
1	5A	1008	GMA	C-N2	2.14	1.38	1.32
1	iA	208	GMA	C-N2	2.14	1.38	1.32
1	mA	1208	GMA	C-N2	2.14	1.38	1.32

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	UA	208	GMA	C-N2	2.13	1.38	1.32
1	YA	1208	GMA	C-N2	2.13	1.38	1.32
1	e	8	GMA	C-N2	2.13	1.38	1.32
1	yA	1008	GMA	C-N2	2.13	1.38	1.32
1	OA	308	GMA	C-N2	2.13	1.38	1.32
1	SA	1308	GMA	C-N2	2.13	1.38	1.32
1	3	308	GMA	C-N2	2.13	1.38	1.32
1	7	1308	GMA	C-N2	2.13	1.38	1.32
1	p	308	GMA	C-N2	2.12	1.38	1.32
1	t	1308	GMA	C-N2	2.12	1.38	1.32
1	PB	308	GMA	C-N2	2.12	1.38	1.32
1	TB	1308	GMA	C-N2	2.12	1.38	1.32
1	AA	308	GMA	C-N2	2.12	1.38	1.32
1	EA	1308	GMA	C-N2	2.12	1.38	1.32
1	VA	308	GMA	C-N2	2.12	1.38	1.32
1	ZA	1308	GMA	C-N2	2.12	1.38	1.32
1	wA	208	GMA	C-N2	2.12	1.38	1.32
1	0A	1208	GMA	C-N2	2.12	1.38	1.32
1	BB	308	GMA	C-N2	2.12	1.38	1.32
1	FB	1308	GMA	C-N2	2.12	1.38	1.32
1	jA	308	GMA	C-N2	2.12	1.38	1.32
1	nA	1308	GMA	C-N2	2.12	1.38	1.32
1	K	208	GMA	C-N2	2.11	1.38	1.32
1	O	1208	GMA	C-N2	2.11	1.38	1.32
1	HA	308	GMA	C-N2	2.11	1.38	1.32
1	LA	1308	GMA	C-N2	2.11	1.38	1.32
1	HB	208	GMA	C-N2	2.11	1.38	1.32
1	LB	1208	GMA	C-N2	2.11	1.38	1.32
1	IB	308	GMA	C-N2	2.11	1.38	1.32
1	MB	1308	GMA	C-N2	2.11	1.38	1.32
1	AB	208	GMA	C-N2	2.11	1.38	1.32
1	EB	1208	GMA	C-N2	2.11	1.38	1.32
1	c	8	GMA	C-N2	2.10	1.38	1.32
1	kA	1008	GMA	C-N2	2.10	1.38	1.32
1	a	8	GMA	C-N2	2.10	1.38	1.32
1	WA	1008	GMA	C-N2	2.10	1.38	1.32
1	i	8	GMA	C-N2	2.10	1.38	1.32
1	QB	1008	GMA	C-N2	2.10	1.38	1.32
1	cA	308	GMA	C-N2	2.10	1.38	1.32
1	gA	1308	GMA	C-N2	2.10	1.38	1.32
1	L	308	GMA	C-N2	2.10	1.38	1.32
1	P	1308	GMA	C-N2	2.10	1.38	1.32

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	3	301	5CR	OAB-CAL	-2.10	1.18	1.23
1	7	1301	5CR	OAB-CAL	-2.10	1.18	1.23
1	3A	208	GMA	C-N2	2.10	1.38	1.32
1	7A	1208	GMA	C-N2	2.10	1.38	1.32
1	w	308	GMA	C-N2	2.10	1.38	1.32
1	0	1308	GMA	C-N2	2.10	1.38	1.32
1	h	8	GMA	C-N2	2.10	1.38	1.32
1	JB	1008	GMA	C-N2	2.10	1.38	1.32
1	OB	208	GMA	C-N2	2.10	1.38	1.32
1	SB	1208	GMA	C-N2	2.10	1.38	1.32
1	I	8	GMA	C-N2	2.09	1.38	1.32
1	PA	1008	GMA	C-N2	2.09	1.38	1.32
1	xA	308	GMA	C-N2	2.09	1.38	1.32
1	1A	1308	GMA	C-N2	2.09	1.38	1.32
1	b	8	GMA	C-N2	2.09	1.38	1.32
1	dA	1008	GMA	C-N2	2.09	1.38	1.32
1	w	301	5CR	OAB-CAL	-2.09	1.18	1.23
1	0	1301	5CR	OAB-CAL	-2.09	1.18	1.23
1	g	8	GMA	C-N2	2.09	1.38	1.32
1	CB	1008	GMA	C-N2	2.09	1.38	1.32
1	d	8	GMA	C-N2	2.08	1.38	1.32
1	rA	1008	GMA	C-N2	2.08	1.38	1.32
1	4A	308	GMA	C-N2	2.08	1.38	1.32
1	8A	1308	GMA	C-N2	2.08	1.38	1.32
1	pA	208	GMA	C-N2	2.08	1.38	1.32
1	tA	1208	GMA	C-N2	2.08	1.38	1.32
1	qA	308	GMA	C-N2	2.07	1.38	1.32
1	uA	1308	GMA	C-N2	2.07	1.38	1.32
1	vA	108	GMA	C-N2	2.07	1.38	1.32
1	zA	1108	GMA	C-N2	2.07	1.38	1.32
1	Z	301	5CR	OAB-CAL	-2.07	1.18	1.23
1	m	1301	5CR	OAB-CAL	-2.07	1.18	1.23
1	OA	301	5CR	OAB-CAL	-2.06	1.18	1.23
1	SA	1301	5CR	OAB-CAL	-2.06	1.18	1.23
1	bA	208	GMA	C-N2	2.06	1.38	1.32
1	fA	1208	GMA	C-N2	2.06	1.38	1.32
1	2A	108	GMA	C-N2	2.05	1.38	1.32
1	6A	1108	GMA	C-N2	2.05	1.38	1.32
1	p	301	5CR	OAB-CAL	-2.05	1.18	1.23
1	t	1301	5CR	OAB-CAL	-2.05	1.18	1.23
1	L	301	5CR	OAB-CAL	-2.05	1.18	1.23
1	P	1301	5CR	OAB-CAL	-2.05	1.18	1.23

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	8	GMA	C-N2	2.05	1.38	1.32
1	T	1008	GMA	C-N2	2.05	1.38	1.32
1	9A	108	GMA	C-N2	2.05	1.38	1.32
1	DB	1108	GMA	C-N2	2.05	1.38	1.32
1	J	108	GMA	C-N2	2.04	1.38	1.32
1	N	1108	GMA	C-N2	2.04	1.38	1.32
1	MA	108	GMA	C-N2	2.04	1.38	1.32
1	QA	1108	GMA	C-N2	2.04	1.38	1.32
1	HA	301	5CR	OAB-CAL	-2.04	1.18	1.23
1	LA	1301	5CR	OAB-CAL	-2.04	1.18	1.23
1	n	108	GMA	C-N2	2.04	1.38	1.32
1	r	1108	GMA	C-N2	2.04	1.38	1.32
1	g	1	5CR	OAB-CAL	-2.03	1.18	1.23
1	CB	1001	5CR	OAB-CAL	-2.03	1.18	1.23
1	AA	301	5CR	OAB-CAL	-2.03	1.18	1.23
1	EA	1301	5CR	OAB-CAL	-2.03	1.18	1.23
1	hA	108	GMA	C-N2	2.03	1.38	1.32
1	lA	1108	GMA	C-N2	2.03	1.38	1.32
1	F	8	GMA	C-N2	2.03	1.38	1.32
1	4	1008	GMA	C-N2	2.03	1.38	1.32
1	TA	108	GMA	C-N2	2.03	1.38	1.32
1	XA	1108	GMA	C-N2	2.03	1.38	1.32
1	B	1	5CR	OAB-CAL	-2.03	1.18	1.23
1	T	1001	5CR	OAB-CAL	-2.03	1.18	1.23
1	S	301	5CR	OAB-CAL	-2.03	1.18	1.23
1	W	1301	5CR	OAB-CAL	-2.03	1.18	1.23
1	aA	108	GMA	C-N2	2.03	1.38	1.32
1	eA	1108	GMA	C-N2	2.03	1.38	1.32
1	e	1	5CR	OAB-CAL	-2.02	1.18	1.23
1	yA	1001	5CR	OAB-CAL	-2.02	1.18	1.23
1	f	1	5CR	OAB-CAL	-2.02	1.18	1.23
1	5A	1001	5CR	OAB-CAL	-2.02	1.18	1.23
1	FA	108	GMA	C-N2	2.02	1.38	1.32
1	JA	1108	GMA	C-N2	2.02	1.38	1.32
1	GB	108	GMA	C-N2	2.02	1.38	1.32
1	KB	1108	GMA	C-N2	2.02	1.38	1.32
1	a	1	5CR	OAB-CAL	-2.02	1.18	1.23
1	WA	1001	5CR	OAB-CAL	-2.02	1.18	1.23
1	oA	108	GMA	C-N2	2.02	1.38	1.32
1	sA	1108	GMA	C-N2	2.02	1.38	1.32
1	b	1	5CR	OAB-CAL	-2.02	1.18	1.23
1	dA	1001	5CR	OAB-CAL	-2.02	1.18	1.23

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	1	5CR	OAB-CAL	-2.02	1.18	1.23
1	PA	1001	5CR	OAB-CAL	-2.02	1.18	1.23
1	A	8	GMA	C-N2	2.01	1.38	1.32
1	M	1008	GMA	C-N2	2.01	1.38	1.32
1	E	8	GMA	C-N2	2.01	1.38	1.32
1	x	1008	GMA	C-N2	2.01	1.38	1.32
1	Q	108	GMA	C-N2	2.01	1.38	1.32
1	U	1108	GMA	C-N2	2.01	1.38	1.32
1	D	1	5CR	OAB-CAL	-2.01	1.18	1.23
1	q	1001	5CR	OAB-CAL	-2.01	1.18	1.23
1	Y	201	5CR	OAB-CAL	-2.01	1.18	1.23
1	l	1201	5CR	OAB-CAL	-2.01	1.18	1.23
1	C	8	GMA	C-N2	2.01	1.38	1.32
1	j	1008	GMA	C-N2	2.01	1.38	1.32
1	2	201	5CR	OAB-CAL	-2.01	1.18	1.23
1	6	1201	5CR	OAB-CAL	-2.01	1.18	1.23
1	NB	108	GMA	C-N2	2.01	1.38	1.32
1	RB	1108	GMA	C-N2	2.01	1.38	1.32
1	C	1	5CR	OAB-CAL	-2.00	1.18	1.23
1	j	1001	5CR	OAB-CAL	-2.00	1.18	1.23
1	H	1	5CR	OAB-CAL	-2.00	1.18	1.23
1	IA	1001	5CR	OAB-CAL	-2.00	1.18	1.23
1	d	1	5CR	OAB-CAL	-2.00	1.18	1.23
1	rA	1001	5CR	OAB-CAL	-2.00	1.18	1.23
1	D	8	GMA	C-N2	2.00	1.38	1.32
1	q	1008	GMA	C-N2	2.00	1.38	1.32
1	E	1	5CR	OAB-CAL	-2.00	1.18	1.23
1	x	1001	5CR	OAB-CAL	-2.00	1.18	1.23

All (368) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	f	1	5CR	CAA-CAL-N	5.13	124.79	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
1	i	1	5CR	CAA-CAL-N	5.13	124.79	116.10
1	QB	1001	5CR	CAA-CAL-N	5.13	124.79	116.10
1	b	1	5CR	CAA-CAL-N	5.12	124.78	116.10
1	dA	1001	5CR	CAA-CAL-N	5.12	124.78	116.10
1	g	1	5CR	CAA-CAL-N	5.12	124.78	116.10
1	CB	1001	5CR	CAA-CAL-N	5.12	124.78	116.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	h	1	5CR	CAA-CAL-N	5.12	124.77	116.10
1	JB	1001	5CR	CAA-CAL-N	5.12	124.77	116.10
1	d	1	5CR	CAA-CAL-N	5.11	124.76	116.10
1	rA	1001	5CR	CAA-CAL-N	5.11	124.76	116.10
1	c	1	5CR	CAA-CAL-N	5.11	124.75	116.10
1	kA	1001	5CR	CAA-CAL-N	5.11	124.75	116.10
1	e	1	5CR	CAA-CAL-N	5.10	124.73	116.10
1	yA	1001	5CR	CAA-CAL-N	5.10	124.73	116.10
1	G	1	5CR	CG-CB-CA	-4.78	106.79	113.63
1	BA	1001	5CR	CG-CB-CA	-4.78	106.79	113.63
1	A	1	5CR	CG-CB-CA	-4.77	106.81	113.63
1	M	1001	5CR	CG-CB-CA	-4.77	106.81	113.63
1	I	1	5CR	CG-CB-CA	-4.76	106.82	113.63
1	PA	1001	5CR	CG-CB-CA	-4.76	106.82	113.63
1	B	1	5CR	CG-CB-CA	-4.75	106.83	113.63
1	T	1001	5CR	CG-CB-CA	-4.75	106.83	113.63
1	D	1	5CR	CG-CB-CA	-4.75	106.84	113.63
1	q	1001	5CR	CG-CB-CA	-4.75	106.84	113.63
1	E	1	5CR	CG-CB-CA	-4.73	106.86	113.63
1	x	1001	5CR	CG-CB-CA	-4.73	106.86	113.63
1	C	1	5CR	CG-CB-CA	-4.72	106.88	113.63
1	j	1001	5CR	CG-CB-CA	-4.72	106.88	113.63
1	H	1	5CR	CG-CB-CA	-4.72	106.88	113.63
1	IA	1001	5CR	CG-CB-CA	-4.72	106.88	113.63
1	F	1	5CR	CG-CB-CA	-4.71	106.88	113.63
1	4	1001	5CR	CG-CB-CA	-4.71	106.88	113.63
1	Q	101	5CR	CG-CB-CA	-4.54	107.14	113.63
1	U	1101	5CR	CG-CB-CA	-4.54	107.14	113.63
1	MA	101	5CR	CG-CB-CA	-4.52	107.16	113.63
1	QA	1101	5CR	CG-CB-CA	-4.52	107.16	113.63
1	8	101	5CR	CG-CB-CA	-4.51	107.17	113.63
1	CA	1101	5CR	CG-CB-CA	-4.51	107.17	113.63
1	u	101	5CR	CG-CB-CA	-4.51	107.18	113.63
1	y	1101	5CR	CG-CB-CA	-4.51	107.18	113.63
1	l	101	5CR	CG-CB-CA	-4.51	107.18	113.63
1	5	1101	5CR	CG-CB-CA	-4.51	107.18	113.63
1	X	101	5CR	CG-CB-CA	-4.49	107.20	113.63
1	k	1101	5CR	CG-CB-CA	-4.49	107.20	113.63
1	J	101	5CR	CG-CB-CA	-4.49	107.21	113.63
1	N	1101	5CR	CG-CB-CA	-4.49	107.21	113.63
1	n	101	5CR	CG-CB-CA	-4.49	107.21	113.63
1	r	1101	5CR	CG-CB-CA	-4.49	107.21	113.63

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	FA	101	5CR	CG-CB-CA	-4.48	107.22	113.63
1	JA	1101	5CR	CG-CB-CA	-4.48	107.22	113.63
1	R	201	5CR	CAA-CAL-N	2.95	121.09	116.10
1	V	1201	5CR	CAA-CAL-N	2.95	121.09	116.10
1	9	201	5CR	CAA-CAL-N	2.94	121.08	116.10
1	DA	1201	5CR	CAA-CAL-N	2.94	121.08	116.10
1	wA	201	5CR	CG-CB-CA	-2.94	109.42	113.63
1	0A	1201	5CR	CG-CB-CA	-2.94	109.42	113.63
1	NA	201	5CR	CAA-CAL-N	2.94	121.08	116.10
1	RA	1201	5CR	CAA-CAL-N	2.94	121.08	116.10
1	UA	201	5CR	CG-CB-CA	-2.93	109.43	113.63
1	YA	1201	5CR	CG-CB-CA	-2.93	109.43	113.63
1	o	201	5CR	CAA-CAL-N	2.93	121.07	116.10
1	s	1201	5CR	CAA-CAL-N	2.93	121.07	116.10
1	Y	201	5CR	CAA-CAL-N	2.93	121.06	116.10
1	l	1201	5CR	CAA-CAL-N	2.93	121.06	116.10
1	GA	201	5CR	CAA-CAL-N	2.93	121.06	116.10
1	KA	1201	5CR	CAA-CAL-N	2.93	121.06	116.10
1	iA	201	5CR	CG-CB-CA	-2.93	109.44	113.63
1	mA	1201	5CR	CG-CB-CA	-2.93	109.44	113.63
1	K	201	5CR	CAA-CAL-N	2.92	121.04	116.10
1	O	1201	5CR	CAA-CAL-N	2.92	121.04	116.10
1	v	201	5CR	CAA-CAL-N	2.92	121.04	116.10
1	z	1201	5CR	CAA-CAL-N	2.92	121.04	116.10
1	OB	201	5CR	CG-CB-CA	-2.91	109.46	113.63
1	SB	1201	5CR	CG-CB-CA	-2.91	109.46	113.63
1	2	201	5CR	CAA-CAL-N	2.91	121.03	116.10
1	6	1201	5CR	CAA-CAL-N	2.91	121.03	116.10
1	bA	201	5CR	CG-CB-CA	-2.91	109.47	113.63
1	fA	1201	5CR	CG-CB-CA	-2.91	109.47	113.63
1	HB	201	5CR	CG-CB-CA	-2.90	109.48	113.63
1	LB	1201	5CR	CG-CB-CA	-2.90	109.48	113.63
1	AB	201	5CR	CG-CB-CA	-2.90	109.48	113.63
1	EB	1201	5CR	CG-CB-CA	-2.90	109.48	113.63
1	3A	201	5CR	CG-CB-CA	-2.89	109.50	113.63
1	7A	1201	5CR	CG-CB-CA	-2.89	109.50	113.63
1	pA	201	5CR	CG-CB-CA	-2.89	109.50	113.63
1	tA	1201	5CR	CG-CB-CA	-2.89	109.50	113.63
1	D	1	5CR	CA-N-CAL	-2.73	118.11	123.15
1	q	1001	5CR	CA-N-CAL	-2.73	118.11	123.15
1	I	1	5CR	CA-N-CAL	-2.73	118.12	123.15
1	PA	1001	5CR	CA-N-CAL	-2.73	118.12	123.15

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	5CR	CA-N-CAL	-2.72	118.13	123.15
1	M	1001	5CR	CA-N-CAL	-2.72	118.13	123.15
1	G	1	5CR	CA-N-CAL	-2.72	118.14	123.15
1	BA	1001	5CR	CA-N-CAL	-2.72	118.14	123.15
1	H	1	5CR	CA-N-CAL	-2.72	118.14	123.15
1	IA	1001	5CR	CA-N-CAL	-2.72	118.14	123.15
1	F	1	5CR	CA-N-CAL	-2.72	118.14	123.15
1	4	1001	5CR	CA-N-CAL	-2.72	118.14	123.15
1	B	1	5CR	CA-N-CAL	-2.71	118.14	123.15
1	T	1001	5CR	CA-N-CAL	-2.71	118.14	123.15
1	GB	101	5CR	CA-N-CAL	-2.71	118.15	123.15
1	KB	1101	5CR	CA-N-CAL	-2.71	118.15	123.15
1	C	1	5CR	CA-N-CAL	-2.71	118.16	123.15
1	j	1001	5CR	CA-N-CAL	-2.71	118.16	123.15
1	aA	101	5CR	CA-N-CAL	-2.70	118.17	123.15
1	eA	1101	5CR	CA-N-CAL	-2.70	118.17	123.15
1	NB	101	5CR	CA-N-CAL	-2.69	118.19	123.15
1	RB	1101	5CR	CA-N-CAL	-2.69	118.19	123.15
1	E	1	5CR	CA-N-CAL	-2.69	118.19	123.15
1	x	1001	5CR	CA-N-CAL	-2.69	118.19	123.15
1	hA	101	5CR	CA-N-CAL	-2.69	118.19	123.15
1	lA	1101	5CR	CA-N-CAL	-2.69	118.19	123.15
1	oA	101	5CR	CA-N-CAL	-2.69	118.19	123.15
1	sA	1101	5CR	CA-N-CAL	-2.69	118.19	123.15
1	2A	101	5CR	CA-N-CAL	-2.68	118.20	123.15
1	6A	1101	5CR	CA-N-CAL	-2.68	118.20	123.15
1	9A	101	5CR	CA-N-CAL	-2.68	118.21	123.15
1	DB	1101	5CR	CA-N-CAL	-2.68	118.21	123.15
1	vA	101	5CR	CA-N-CAL	-2.68	118.21	123.15
1	zA	1101	5CR	CA-N-CAL	-2.68	118.21	123.15
1	TA	101	5CR	CA-N-CAL	-2.67	118.23	123.15
1	XA	1101	5CR	CA-N-CAL	-2.67	118.23	123.15
1	F	1	5CR	CAA-CAL-N	2.64	120.57	116.10
1	4	1001	5CR	CAA-CAL-N	2.64	120.57	116.10
1	A	1	5CR	CAA-CAL-N	2.63	120.55	116.10
1	M	1001	5CR	CAA-CAL-N	2.63	120.55	116.10
1	B	1	5CR	CAA-CAL-N	2.63	120.54	116.10
1	T	1001	5CR	CAA-CAL-N	2.63	120.54	116.10
1	I	1	5CR	CAA-CAL-N	2.62	120.54	116.10
1	PA	1001	5CR	CAA-CAL-N	2.62	120.54	116.10
1	C	1	5CR	CAA-CAL-N	2.61	120.52	116.10
1	j	1001	5CR	CAA-CAL-N	2.61	120.52	116.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	1	5CR	CAA-CAL-N	2.61	120.52	116.10
1	x	1001	5CR	CAA-CAL-N	2.61	120.52	116.10
1	G	1	5CR	CAA-CAL-N	2.61	120.52	116.10
1	BA	1001	5CR	CAA-CAL-N	2.61	120.52	116.10
1	H	1	5CR	CAA-CAL-N	2.60	120.49	116.10
1	IA	1001	5CR	CAA-CAL-N	2.60	120.49	116.10
1	D	1	5CR	CAA-CAL-N	2.59	120.48	116.10
1	q	1001	5CR	CAA-CAL-N	2.59	120.48	116.10
1	TA	101	5CR	CAA-CAL-N	2.52	120.37	116.10
1	XA	1101	5CR	CAA-CAL-N	2.52	120.37	116.10
1	hA	101	5CR	CAA-CAL-N	2.52	120.37	116.10
1	lA	1101	5CR	CAA-CAL-N	2.52	120.37	116.10
1	NB	101	5CR	CAA-CAL-N	2.52	120.36	116.10
1	RB	1101	5CR	CAA-CAL-N	2.52	120.36	116.10
1	vA	101	5CR	CAA-CAL-N	2.51	120.35	116.10
1	zA	1101	5CR	CAA-CAL-N	2.51	120.35	116.10
1	oA	101	5CR	CAA-CAL-N	2.50	120.33	116.10
1	sA	1101	5CR	CAA-CAL-N	2.50	120.33	116.10
1	aA	101	5CR	CAA-CAL-N	2.50	120.32	116.10
1	eA	1101	5CR	CAA-CAL-N	2.50	120.32	116.10
1	9A	101	5CR	CAA-CAL-N	2.49	120.32	116.10
1	DB	1101	5CR	CAA-CAL-N	2.49	120.32	116.10
1	2A	101	5CR	CAA-CAL-N	2.49	120.31	116.10
1	6A	1101	5CR	CAA-CAL-N	2.49	120.31	116.10
1	GB	101	5CR	CAA-CAL-N	2.45	120.25	116.10
1	KB	1101	5CR	CAA-CAL-N	2.45	120.25	116.10
1	a	1	5CR	OAB-CAL-N	-2.43	117.48	121.95
1	WA	1001	5CR	OAB-CAL-N	-2.43	117.48	121.95
1	d	1	5CR	OAB-CAL-N	-2.43	117.49	121.95
1	rA	1001	5CR	OAB-CAL-N	-2.43	117.49	121.95
1	o	201	5CR	CG-CB-CA	-2.42	110.17	113.63
1	s	1201	5CR	CG-CB-CA	-2.42	110.17	113.63
1	i	1	5CR	OAB-CAL-N	-2.40	117.54	121.95
1	QB	1001	5CR	OAB-CAL-N	-2.40	117.54	121.95
1	e	1	5CR	OAB-CAL-N	-2.39	117.55	121.95
1	yA	1001	5CR	OAB-CAL-N	-2.39	117.55	121.95
1	b	1	5CR	OAB-CAL-CAA	-2.39	117.62	122.06
1	dA	1001	5CR	OAB-CAL-CAA	-2.39	117.62	122.06
1	f	1	5CR	OAB-CAL-N	-2.39	117.56	121.95
1	5A	1001	5CR	OAB-CAL-N	-2.39	117.56	121.95
1	g	1	5CR	OAB-CAL-CAA	-2.39	117.62	122.06
1	CB	1001	5CR	OAB-CAL-CAA	-2.39	117.62	122.06

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	c	1	5CR	OAB-CAL-CAA	-2.38	117.64	122.06
1	kA	1001	5CR	OAB-CAL-CAA	-2.38	117.64	122.06
1	h	1	5CR	OAB-CAL-N	-2.38	117.58	121.95
1	JB	1001	5CR	OAB-CAL-N	-2.38	117.58	121.95
1	h	1	5CR	OAB-CAL-CAA	-2.38	117.64	122.06
1	JB	1001	5CR	OAB-CAL-CAA	-2.38	117.64	122.06
1	f	1	5CR	OAB-CAL-CAA	-2.37	117.65	122.06
1	5A	1001	5CR	OAB-CAL-CAA	-2.37	117.65	122.06
1	2	201	5CR	CG-CB-CA	-2.37	110.24	113.63
1	6	1201	5CR	CG-CB-CA	-2.37	110.24	113.63
1	R	201	5CR	CG-CB-CA	-2.37	110.24	113.63
1	V	1201	5CR	CG-CB-CA	-2.37	110.24	113.63
1	g	1	5CR	OAB-CAL-N	-2.37	117.60	121.95
1	CB	1001	5CR	OAB-CAL-N	-2.37	117.60	121.95
1	b	1	5CR	OAB-CAL-N	-2.37	117.60	121.95
1	dA	1001	5CR	OAB-CAL-N	-2.37	117.60	121.95
1	Y	201	5CR	CG-CB-CA	-2.36	110.25	113.63
1	l	1201	5CR	CG-CB-CA	-2.36	110.25	113.63
1	i	1	5CR	OAB-CAL-CAA	-2.36	117.67	122.06
1	QB	1001	5CR	OAB-CAL-CAA	-2.36	117.67	122.06
1	c	1	5CR	OAB-CAL-N	-2.36	117.61	121.95
1	kA	1001	5CR	OAB-CAL-N	-2.36	117.61	121.95
1	v	201	5CR	CG-CB-CA	-2.36	110.26	113.63
1	z	1201	5CR	CG-CB-CA	-2.36	110.26	113.63
1	K	201	5CR	CG-CB-CA	-2.35	110.27	113.63
1	O	1201	5CR	CG-CB-CA	-2.35	110.27	113.63
1	NA	201	5CR	CG-CB-CA	-2.35	110.27	113.63
1	RA	1201	5CR	CG-CB-CA	-2.35	110.27	113.63
1	e	1	5CR	OAB-CAL-CAA	-2.34	117.72	122.06
1	yA	1001	5CR	OAB-CAL-CAA	-2.34	117.72	122.06
1	a	1	5CR	OAB-CAL-CAA	-2.33	117.73	122.06
1	WA	1001	5CR	OAB-CAL-CAA	-2.33	117.73	122.06
1	GA	201	5CR	CG-CB-CA	-2.33	110.30	113.63
1	KA	1201	5CR	CG-CB-CA	-2.33	110.30	113.63
1	9	201	5CR	CG-CB-CA	-2.32	110.31	113.63
1	DA	1201	5CR	CG-CB-CA	-2.32	110.31	113.63
1	d	1	5CR	OAB-CAL-CAA	-2.32	117.75	122.06
1	rA	1001	5CR	OAB-CAL-CAA	-2.32	117.75	122.06
1	p	301	5CR	CA-N-CAL	-2.27	118.97	123.15
1	t	1301	5CR	CA-N-CAL	-2.27	118.97	123.15
1	L	301	5CR	CA-N-CAL	-2.26	118.98	123.15
1	P	1301	5CR	CA-N-CAL	-2.26	118.98	123.15

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	OA	301	5CR	CA-N-CAL	-2.26	118.98	123.15
1	SA	1301	5CR	CA-N-CAL	-2.26	118.98	123.15
1	3	301	5CR	CAA-CAL-N	2.25	119.91	116.10
1	7	1301	5CR	CAA-CAL-N	2.25	119.91	116.10
1	3	301	5CR	CA-N-CAL	-2.25	119.00	123.15
1	7	1301	5CR	CA-N-CAL	-2.25	119.00	123.15
1	AA	301	5CR	CA-N-CAL	-2.25	119.00	123.15
1	EA	1301	5CR	CA-N-CAL	-2.25	119.00	123.15
1	Z	301	5CR	CA-N-CAL	-2.24	119.01	123.15
1	m	1301	5CR	CA-N-CAL	-2.24	119.01	123.15
1	HA	301	5CR	CA-N-CAL	-2.24	119.01	123.15
1	LA	1301	5CR	CA-N-CAL	-2.24	119.01	123.15
1	BB	301	5CR	CAA-CAL-N	2.24	119.89	116.10
1	FB	1301	5CR	CAA-CAL-N	2.24	119.89	116.10
1	S	301	5CR	CAA-CAL-N	2.24	119.88	116.10
1	W	1301	5CR	CAA-CAL-N	2.24	119.88	116.10
1	IB	301	5CR	CAA-CAL-N	2.24	119.88	116.10
1	MB	1301	5CR	CAA-CAL-N	2.24	119.88	116.10
1	PB	301	5CR	CAA-CAL-N	2.23	119.88	116.10
1	TB	1301	5CR	CAA-CAL-N	2.23	119.88	116.10
1	HA	301	5CR	CAA-CAL-N	2.23	119.88	116.10
1	LA	1301	5CR	CAA-CAL-N	2.23	119.88	116.10
1	w	301	5CR	CA-N-CAL	-2.23	119.04	123.15
1	0	1301	5CR	CA-N-CAL	-2.23	119.04	123.15
1	cA	301	5CR	CAA-CAL-N	2.23	119.87	116.10
1	gA	1301	5CR	CAA-CAL-N	2.23	119.87	116.10
1	AA	301	5CR	CAA-CAL-N	2.22	119.86	116.10
1	EA	1301	5CR	CAA-CAL-N	2.22	119.86	116.10
1	S	301	5CR	CA-N-CAL	-2.22	119.05	123.15
1	W	1301	5CR	CA-N-CAL	-2.22	119.05	123.15
1	xA	301	5CR	CAA-CAL-N	2.22	119.86	116.10
1	1A	1301	5CR	CAA-CAL-N	2.22	119.86	116.10
1	Z	301	5CR	CAA-CAL-N	2.22	119.86	116.10
1	m	1301	5CR	CAA-CAL-N	2.22	119.86	116.10
1	L	301	5CR	CAA-CAL-N	2.22	119.85	116.10
1	P	1301	5CR	CAA-CAL-N	2.22	119.85	116.10
1	jA	301	5CR	CAA-CAL-N	2.21	119.84	116.10
1	nA	1301	5CR	CAA-CAL-N	2.21	119.84	116.10
1	3	301	5CR	O-C-CA	-2.21	118.98	124.78
1	7	1301	5CR	O-C-CA	-2.21	118.98	124.78
1	w	301	5CR	O-C-CA	-2.21	118.99	124.78
1	0	1301	5CR	O-C-CA	-2.21	118.99	124.78

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	OA	301	5CR	CAA-CAL-N	2.21	119.83	116.10
1	SA	1301	5CR	CAA-CAL-N	2.21	119.83	116.10
1	w	301	5CR	CAA-CAL-N	2.20	119.83	116.10
1	0	1301	5CR	CAA-CAL-N	2.20	119.83	116.10
1	qA	301	5CR	CAA-CAL-N	2.20	119.83	116.10
1	uA	1301	5CR	CAA-CAL-N	2.20	119.83	116.10
1	p	301	5CR	O-C-CA	-2.20	119.01	124.78
1	t	1301	5CR	O-C-CA	-2.20	119.01	124.78
1	p	301	5CR	CAA-CAL-N	2.20	119.82	116.10
1	t	1301	5CR	CAA-CAL-N	2.20	119.82	116.10
1	Z	301	5CR	O-C-CA	-2.20	119.01	124.78
1	m	1301	5CR	O-C-CA	-2.20	119.01	124.78
1	VA	301	5CR	CAA-CAL-N	2.20	119.82	116.10
1	ZA	1301	5CR	CAA-CAL-N	2.20	119.82	116.10
1	4A	301	5CR	CAA-CAL-N	2.19	119.81	116.10
1	8A	1301	5CR	CAA-CAL-N	2.19	119.81	116.10
1	OA	301	5CR	O-C-CA	-2.19	119.05	124.78
1	SA	1301	5CR	O-C-CA	-2.19	119.05	124.78
1	AA	301	5CR	O-C-CA	-2.19	119.05	124.78
1	EA	1301	5CR	O-C-CA	-2.19	119.05	124.78
1	HA	301	5CR	O-C-CA	-2.19	119.05	124.78
1	LA	1301	5CR	O-C-CA	-2.19	119.05	124.78
1	L	301	5CR	O-C-CA	-2.16	119.11	124.78
1	P	1301	5CR	O-C-CA	-2.16	119.11	124.78
1	S	301	5CR	O-C-CA	-2.16	119.12	124.78
1	W	1301	5CR	O-C-CA	-2.16	119.12	124.78
1	e	1	5CR	CA-N-CAL	2.12	127.06	123.15
1	yA	1001	5CR	CA-N-CAL	2.12	127.06	123.15
1	X	101	5CR	CAA-CAL-N	2.12	119.69	116.10
1	k	1101	5CR	CAA-CAL-N	2.12	119.69	116.10
1	J	101	5CR	CAA-CAL-N	2.12	119.69	116.10
1	N	1101	5CR	CAA-CAL-N	2.12	119.69	116.10
1	c	1	5CR	CA-N-CAL	2.12	127.05	123.15
1	kA	1001	5CR	CA-N-CAL	2.12	127.05	123.15
1	b	1	5CR	CA-N-CAL	2.11	127.05	123.15
1	dA	1001	5CR	CA-N-CAL	2.11	127.05	123.15
1	n	101	5CR	CAA-CAL-N	2.11	119.67	116.10
1	r	1101	5CR	CAA-CAL-N	2.11	119.67	116.10
1	f	1	5CR	CA-N-CAL	2.11	127.04	123.15
1	5A	1001	5CR	CA-N-CAL	2.11	127.04	123.15
1	g	1	5CR	CA-N-CAL	2.10	127.03	123.15
1	CB	1001	5CR	CA-N-CAL	2.10	127.03	123.15

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	u	101	5CR	CAA-CAL-N	2.10	119.66	116.10
1	y	1101	5CR	CAA-CAL-N	2.10	119.66	116.10
1	i	1	5CR	CA-N-CAL	2.10	127.02	123.15
1	QB	1001	5CR	CA-N-CAL	2.10	127.02	123.15
1	a	1	5CR	CA-N-CAL	2.10	127.01	123.15
1	WA	1001	5CR	CA-N-CAL	2.10	127.01	123.15
1	d	1	5CR	CA-N-CAL	2.09	127.01	123.15
1	rA	1001	5CR	CA-N-CAL	2.09	127.01	123.15
1	Q	101	5CR	CAA-CAL-N	2.09	119.64	116.10
1	U	1101	5CR	CAA-CAL-N	2.09	119.64	116.10
1	h	1	5CR	CA-N-CAL	2.09	127.00	123.15
1	JB	1001	5CR	CA-N-CAL	2.09	127.00	123.15
1	8	101	5CR	CAA-CAL-N	2.08	119.63	116.10
1	CA	1101	5CR	CAA-CAL-N	2.08	119.63	116.10
1	GA	208	GMA	O-C-CA	2.08	123.35	120.30
1	KA	1208	GMA	O-C-CA	2.08	123.35	120.30
1	FA	101	5CR	CAA-CAL-N	2.08	119.62	116.10
1	JA	1101	5CR	CAA-CAL-N	2.08	119.62	116.10
1	1	101	5CR	CAA-CAL-N	2.08	119.62	116.10
1	5	1101	5CR	CAA-CAL-N	2.08	119.62	116.10
1	MA	101	5CR	CAA-CAL-N	2.06	119.59	116.10
1	QA	1101	5CR	CAA-CAL-N	2.06	119.59	116.10
1	9	208	GMA	O-C-CA	2.06	123.32	120.30
1	DA	1208	GMA	O-C-CA	2.06	123.32	120.30
1	NA	208	GMA	O-C-CA	2.05	123.30	120.30
1	RA	1208	GMA	O-C-CA	2.05	123.30	120.30
1	NA	208	GMA	O-C-N2	-2.04	119.46	123.00
1	RA	1208	GMA	O-C-N2	-2.04	119.46	123.00
1	o	208	GMA	O-C-CA	2.04	123.28	120.30
1	s	1208	GMA	O-C-CA	2.04	123.28	120.30
1	Y	208	GMA	O-C-CA	2.03	123.28	120.30
1	l	1208	GMA	O-C-CA	2.03	123.28	120.30
1	FA	108	GMA	O-C-CA	2.02	123.26	120.30
1	JA	1108	GMA	O-C-CA	2.02	123.26	120.30
1	1	108	GMA	O-C-CA	2.02	123.26	120.30
1	5	1108	GMA	O-C-CA	2.02	123.26	120.30
1	9	208	GMA	O-C-N2	-2.02	119.48	123.00
1	DA	1208	GMA	O-C-N2	-2.02	119.48	123.00
1	Y	208	GMA	O-C-N2	-2.02	119.49	123.00
1	l	1208	GMA	O-C-N2	-2.02	119.49	123.00
1	Q	108	GMA	O-C-CA	2.02	123.26	120.30
1	U	1108	GMA	O-C-CA	2.02	123.26	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	n	108	GMA	O-C-CA	2.02	123.26	120.30
1	r	1108	GMA	O-C-CA	2.02	123.26	120.30
1	2	208	GMA	O-C-CA	2.02	123.25	120.30
1	6	1208	GMA	O-C-CA	2.02	123.25	120.30
1	F	8	GMA	O-C-CA	2.02	123.25	120.30
1	4	1008	GMA	O-C-CA	2.02	123.25	120.30
1	R	208	GMA	O-C-CA	2.01	123.25	120.30
1	V	1208	GMA	O-C-CA	2.01	123.25	120.30
1	J	108	GMA	O-C-CA	2.01	123.25	120.30
1	N	1108	GMA	O-C-CA	2.01	123.25	120.30
1	v	208	GMA	O-C-CA	2.01	123.25	120.30
1	z	1208	GMA	O-C-CA	2.01	123.25	120.30
1	MA	108	GMA	O-C-CA	2.01	123.25	120.30
1	QA	1108	GMA	O-C-CA	2.01	123.25	120.30
1	I	8	GMA	O-C-CA	2.01	123.25	120.30
1	PA	1008	GMA	O-C-CA	2.01	123.25	120.30
1	GA	208	GMA	O-C-N2	-2.01	119.51	123.00
1	KA	1208	GMA	O-C-N2	-2.01	119.51	123.00
1	B	8	GMA	O-C-CA	2.00	123.24	120.30
1	T	1008	GMA	O-C-CA	2.00	123.24	120.30
1	GA	201	5CR	O-C-CA	-2.00	119.53	124.78
1	KA	1201	5CR	O-C-CA	-2.00	119.53	124.78

There are no chirality outliers.

All (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
1	N	1101	5CR	C-CA-N-CAL
1	N	1101	5CR	N-CA-CB-CG
1	O	1201	5CR	N-CA-CB-CG
1	P	1301	5CR	N-CA-CB-CG
1	P	1301	5CR	C-CA-CB-CG
1	Q	101	5CR	C-CA-N-CAL
1	Q	101	5CR	N-CA-CB-CG
1	R	201	5CR	N-CA-CB-CG
1	S	301	5CR	N-CA-CB-CG
1	S	301	5CR	C-CA-CB-CG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
1	U	1101	5CR	C-CA-N-CAL
1	U	1101	5CR	N-CA-CB-CG
1	V	1201	5CR	N-CA-CB-CG
1	W	1301	5CR	N-CA-CB-CG
1	W	1301	5CR	C-CA-CB-CG
1	X	101	5CR	C-CA-N-CAL
1	X	101	5CR	N-CA-CB-CG
1	Y	201	5CR	N-CA-CB-CG
1	Z	301	5CR	N-CA-CB-CG
1	Z	301	5CR	C-CA-CB-CG
1	k	1101	5CR	C-CA-N-CAL
1	k	1101	5CR	N-CA-CB-CG
1	l	1201	5CR	N-CA-CB-CG
1	m	1301	5CR	N-CA-CB-CG
1	m	1301	5CR	C-CA-CB-CG
1	n	101	5CR	C-CA-N-CAL
1	n	101	5CR	N-CA-CB-CG
1	o	201	5CR	N-CA-CB-CG
1	p	301	5CR	N-CA-CB-CG
1	p	301	5CR	C-CA-CB-CG
1	r	1101	5CR	C-CA-N-CAL
1	r	1101	5CR	N-CA-CB-CG
1	s	1201	5CR	N-CA-CB-CG
1	t	1301	5CR	N-CA-CB-CG
1	t	1301	5CR	C-CA-CB-CG
1	u	101	5CR	C-CA-N-CAL
1	u	101	5CR	N-CA-CB-CG
1	v	201	5CR	N-CA-CB-CG
1	w	301	5CR	N-CA-CB-CG
1	w	301	5CR	C-CA-CB-CG
1	y	1101	5CR	C-CA-N-CAL
1	y	1101	5CR	N-CA-CB-CG
1	z	1201	5CR	N-CA-CB-CG
1	0	1301	5CR	N-CA-CB-CG
1	0	1301	5CR	C-CA-CB-CG
1	1	101	5CR	C-CA-N-CAL
1	1	101	5CR	N-CA-CB-CG
1	2	201	5CR	N-CA-CB-CG
1	3	301	5CR	N-CA-CB-CG
1	3	301	5CR	C-CA-CB-CG
1	5	1101	5CR	C-CA-N-CAL
1	5	1101	5CR	N-CA-CB-CG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
1	6	1201	5CR	N-CA-CB-CG
1	7	1301	5CR	N-CA-CB-CG
1	7	1301	5CR	C-CA-CB-CG
1	8	101	5CR	C-CA-N-CAL
1	8	101	5CR	N-CA-CB-CG
1	9	201	5CR	N-CA-CB-CG
1	AA	301	5CR	N-CA-CB-CG
1	AA	301	5CR	C-CA-CB-CG
1	CA	1101	5CR	C-CA-N-CAL
1	CA	1101	5CR	N-CA-CB-CG
1	DA	1201	5CR	N-CA-CB-CG
1	EA	1301	5CR	N-CA-CB-CG
1	EA	1301	5CR	C-CA-CB-CG
1	FA	101	5CR	C-CA-N-CAL
1	FA	101	5CR	N-CA-CB-CG
1	GA	201	5CR	N-CA-CB-CG
1	HA	301	5CR	N-CA-CB-CG
1	HA	301	5CR	C-CA-CB-CG
1	JA	1101	5CR	C-CA-N-CAL
1	JA	1101	5CR	N-CA-CB-CG
1	KA	1201	5CR	N-CA-CB-CG
1	LA	1301	5CR	N-CA-CB-CG
1	LA	1301	5CR	C-CA-CB-CG
1	MA	101	5CR	C-CA-N-CAL
1	MA	101	5CR	N-CA-CB-CG
1	NA	201	5CR	N-CA-CB-CG
1	OA	301	5CR	N-CA-CB-CG
1	OA	301	5CR	C-CA-CB-CG
1	QA	1101	5CR	C-CA-N-CAL
1	QA	1101	5CR	N-CA-CB-CG
1	RA	1201	5CR	N-CA-CB-CG
1	SA	1301	5CR	N-CA-CB-CG
1	SA	1301	5CR	C-CA-CB-CG
1	a	1	5CR	C-CA-CB-CG
1	UA	201	5CR	C-CA-N-CAL
1	WA	1001	5CR	C-CA-CB-CG
1	YA	1201	5CR	C-CA-N-CAL
1	b	1	5CR	C-CA-CB-CG
1	bA	201	5CR	C-CA-N-CAL
1	dA	1001	5CR	C-CA-CB-CG
1	fA	1201	5CR	C-CA-N-CAL
1	c	1	5CR	C-CA-CB-CG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
1	iA	201	5CR	C-CA-N-CAL
1	kA	1001	5CR	C-CA-CB-CG
1	mA	1201	5CR	C-CA-N-CAL
1	d	1	5CR	C-CA-CB-CG
1	pA	201	5CR	C-CA-N-CAL
1	rA	1001	5CR	C-CA-CB-CG
1	tA	1201	5CR	C-CA-N-CAL
1	e	1	5CR	C-CA-CB-CG
1	wA	201	5CR	C-CA-N-CAL
1	yA	1001	5CR	C-CA-CB-CG
1	0A	1201	5CR	C-CA-N-CAL
1	f	1	5CR	C-CA-CB-CG
1	3A	201	5CR	C-CA-N-CAL
1	5A	1001	5CR	C-CA-CB-CG
1	7A	1201	5CR	C-CA-N-CAL
1	g	1	5CR	C-CA-CB-CG
1	AB	201	5CR	C-CA-N-CAL
1	CB	1001	5CR	C-CA-CB-CG
1	EB	1201	5CR	C-CA-N-CAL
1	h	1	5CR	C-CA-CB-CG
1	HB	201	5CR	C-CA-N-CAL
1	JB	1001	5CR	C-CA-CB-CG
1	LB	1201	5CR	C-CA-N-CAL
1	i	1	5CR	C-CA-CB-CG
1	OB	201	5CR	C-CA-N-CAL
1	QB	1001	5CR	C-CA-CB-CG
1	SB	1201	5CR	C-CA-N-CAL
1	A	8	GMA	N2-C-CA-N
1	M	1008	GMA	N2-C-CA-N
1	B	8	GMA	N2-C-CA-N
1	T	1008	GMA	N2-C-CA-N
1	C	8	GMA	N2-C-CA-N
1	j	1008	GMA	N2-C-CA-N
1	D	8	GMA	N2-C-CA-N
1	q	1008	GMA	N2-C-CA-N
1	E	8	GMA	N2-C-CA-N
1	x	1008	GMA	N2-C-CA-N
1	F	8	GMA	N2-C-CA-N
1	4	1008	GMA	N2-C-CA-N
1	G	8	GMA	N2-C-CA-N
1	BA	1008	GMA	N2-C-CA-N
1	H	8	GMA	N2-C-CA-N

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
1	IA	1008	GMA	N2-C-CA-N
1	I	8	GMA	N2-C-CA-N
1	PA	1008	GMA	N2-C-CA-N
1	a	8	GMA	N-CA-CB-CG
1	a	8	GMA	C-CA-CB-CG
1	UA	208	GMA	N-CA-CB-CG
1	UA	208	GMA	C-CA-CB-CG
1	WA	1008	GMA	N-CA-CB-CG
1	WA	1008	GMA	C-CA-CB-CG
1	YA	1208	GMA	N-CA-CB-CG
1	YA	1208	GMA	C-CA-CB-CG
1	b	8	GMA	N-CA-CB-CG
1	b	8	GMA	C-CA-CB-CG
1	bA	208	GMA	N-CA-CB-CG
1	bA	208	GMA	C-CA-CB-CG
1	dA	1008	GMA	N-CA-CB-CG
1	dA	1008	GMA	C-CA-CB-CG
1	fA	1208	GMA	N-CA-CB-CG
1	fA	1208	GMA	C-CA-CB-CG
1	c	8	GMA	N-CA-CB-CG
1	c	8	GMA	C-CA-CB-CG
1	iA	208	GMA	N-CA-CB-CG
1	iA	208	GMA	C-CA-CB-CG
1	kA	1008	GMA	N-CA-CB-CG
1	kA	1008	GMA	C-CA-CB-CG
1	mA	1208	GMA	N-CA-CB-CG
1	mA	1208	GMA	C-CA-CB-CG
1	d	8	GMA	N-CA-CB-CG
1	d	8	GMA	C-CA-CB-CG
1	pA	208	GMA	N-CA-CB-CG
1	pA	208	GMA	C-CA-CB-CG
1	rA	1008	GMA	N-CA-CB-CG
1	rA	1008	GMA	C-CA-CB-CG
1	tA	1208	GMA	N-CA-CB-CG
1	tA	1208	GMA	C-CA-CB-CG
1	e	8	GMA	N-CA-CB-CG
1	e	8	GMA	C-CA-CB-CG
1	wA	208	GMA	N-CA-CB-CG
1	wA	208	GMA	C-CA-CB-CG
1	yA	1008	GMA	N-CA-CB-CG
1	yA	1008	GMA	C-CA-CB-CG
1	0A	1208	GMA	N-CA-CB-CG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
1	0A	1208	GMA	C-CA-CB-CG
1	f	8	GMA	N-CA-CB-CG
1	f	8	GMA	C-CA-CB-CG
1	3A	208	GMA	N-CA-CB-CG
1	3A	208	GMA	C-CA-CB-CG
1	5A	1008	GMA	N-CA-CB-CG
1	5A	1008	GMA	C-CA-CB-CG
1	7A	1208	GMA	N-CA-CB-CG
1	7A	1208	GMA	C-CA-CB-CG
1	g	8	GMA	N-CA-CB-CG
1	g	8	GMA	C-CA-CB-CG
1	AB	208	GMA	N-CA-CB-CG
1	AB	208	GMA	C-CA-CB-CG
1	CB	1008	GMA	N-CA-CB-CG
1	CB	1008	GMA	C-CA-CB-CG
1	EB	1208	GMA	N-CA-CB-CG
1	EB	1208	GMA	C-CA-CB-CG
1	h	8	GMA	N-CA-CB-CG
1	h	8	GMA	C-CA-CB-CG
1	HB	208	GMA	N-CA-CB-CG
1	HB	208	GMA	C-CA-CB-CG
1	JB	1008	GMA	N-CA-CB-CG
1	JB	1008	GMA	C-CA-CB-CG
1	LB	1208	GMA	N-CA-CB-CG
1	LB	1208	GMA	C-CA-CB-CG
1	i	8	GMA	N-CA-CB-CG
1	i	8	GMA	C-CA-CB-CG
1	OB	208	GMA	N-CA-CB-CG
1	OB	208	GMA	C-CA-CB-CG
1	QB	1008	GMA	N-CA-CB-CG
1	QB	1008	GMA	C-CA-CB-CG
1	SB	1208	GMA	N-CA-CB-CG
1	SB	1208	GMA	C-CA-CB-CG
1	K	201	5CR	CAA-CAL-N-CA
1	K	201	5CR	OAB-CAL-N-CA
1	O	1201	5CR	CAA-CAL-N-CA
1	O	1201	5CR	OAB-CAL-N-CA
1	R	201	5CR	CAA-CAL-N-CA
1	R	201	5CR	OAB-CAL-N-CA
1	V	1201	5CR	CAA-CAL-N-CA
1	V	1201	5CR	OAB-CAL-N-CA
1	Y	201	5CR	CAA-CAL-N-CA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
1	Y	201	5CR	OAB-CAL-N-CA
1	l	1201	5CR	CAA-CAL-N-CA
1	l	1201	5CR	OAB-CAL-N-CA
1	o	201	5CR	CAA-CAL-N-CA
1	o	201	5CR	OAB-CAL-N-CA
1	s	1201	5CR	CAA-CAL-N-CA
1	s	1201	5CR	OAB-CAL-N-CA
1	v	201	5CR	CAA-CAL-N-CA
1	v	201	5CR	OAB-CAL-N-CA
1	z	1201	5CR	CAA-CAL-N-CA
1	z	1201	5CR	OAB-CAL-N-CA
1	2	201	5CR	CAA-CAL-N-CA
1	2	201	5CR	OAB-CAL-N-CA
1	6	1201	5CR	CAA-CAL-N-CA
1	6	1201	5CR	OAB-CAL-N-CA
1	9	201	5CR	CAA-CAL-N-CA
1	9	201	5CR	OAB-CAL-N-CA
1	DA	1201	5CR	CAA-CAL-N-CA
1	DA	1201	5CR	OAB-CAL-N-CA
1	GA	201	5CR	CAA-CAL-N-CA
1	GA	201	5CR	OAB-CAL-N-CA
1	KA	1201	5CR	CAA-CAL-N-CA
1	KA	1201	5CR	OAB-CAL-N-CA
1	NA	201	5CR	CAA-CAL-N-CA
1	NA	201	5CR	OAB-CAL-N-CA
1	RA	1201	5CR	CAA-CAL-N-CA
1	RA	1201	5CR	OAB-CAL-N-CA
1	a	1	5CR	CAA-CAL-N-CA
1	a	1	5CR	OAB-CAL-N-CA
1	WA	1001	5CR	CAA-CAL-N-CA
1	WA	1001	5CR	OAB-CAL-N-CA
1	b	1	5CR	CAA-CAL-N-CA
1	b	1	5CR	OAB-CAL-N-CA
1	dA	1001	5CR	CAA-CAL-N-CA
1	dA	1001	5CR	OAB-CAL-N-CA
1	c	1	5CR	CAA-CAL-N-CA
1	c	1	5CR	OAB-CAL-N-CA
1	kA	1001	5CR	CAA-CAL-N-CA
1	kA	1001	5CR	OAB-CAL-N-CA
1	d	1	5CR	CAA-CAL-N-CA
1	d	1	5CR	OAB-CAL-N-CA
1	rA	1001	5CR	CAA-CAL-N-CA

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
1	rA	1001	5CR	OAB-CAL-N-CA
1	e	1	5CR	CAA-CAL-N-CA
1	e	1	5CR	OAB-CAL-N-CA
1	yA	1001	5CR	CAA-CAL-N-CA
1	yA	1001	5CR	OAB-CAL-N-CA
1	f	1	5CR	CAA-CAL-N-CA
1	f	1	5CR	OAB-CAL-N-CA
1	5A	1001	5CR	CAA-CAL-N-CA
1	5A	1001	5CR	OAB-CAL-N-CA
1	g	1	5CR	CAA-CAL-N-CA
1	g	1	5CR	OAB-CAL-N-CA
1	CB	1001	5CR	CAA-CAL-N-CA
1	CB	1001	5CR	OAB-CAL-N-CA
1	h	1	5CR	CAA-CAL-N-CA
1	h	1	5CR	OAB-CAL-N-CA
1	JB	1001	5CR	CAA-CAL-N-CA
1	JB	1001	5CR	OAB-CAL-N-CA
1	i	1	5CR	CAA-CAL-N-CA
1	i	1	5CR	OAB-CAL-N-CA
1	QB	1001	5CR	CAA-CAL-N-CA
1	QB	1001	5CR	OAB-CAL-N-CA
1	K	208	GMA	CA-CB-CG-CD
1	L	308	GMA	CA-CB-CG-CD
1	O	1208	GMA	CA-CB-CG-CD
1	P	1308	GMA	CA-CB-CG-CD
1	R	208	GMA	CA-CB-CG-CD
1	S	308	GMA	CA-CB-CG-CD
1	V	1208	GMA	CA-CB-CG-CD
1	W	1308	GMA	CA-CB-CG-CD
1	Y	208	GMA	CA-CB-CG-CD
1	Z	308	GMA	CA-CB-CG-CD
1	l	1208	GMA	CA-CB-CG-CD
1	m	1308	GMA	CA-CB-CG-CD
1	o	208	GMA	CA-CB-CG-CD
1	p	308	GMA	CA-CB-CG-CD
1	s	1208	GMA	CA-CB-CG-CD
1	t	1308	GMA	CA-CB-CG-CD
1	v	208	GMA	CA-CB-CG-CD
1	w	308	GMA	CA-CB-CG-CD
1	z	1208	GMA	CA-CB-CG-CD
1	0	1308	GMA	CA-CB-CG-CD
1	2	208	GMA	CA-CB-CG-CD

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
1	3	308	GMA	CA-CB-CG-CD
1	6	1208	GMA	CA-CB-CG-CD
1	7	1308	GMA	CA-CB-CG-CD
1	9	208	GMA	CA-CB-CG-CD
1	AA	308	GMA	CA-CB-CG-CD
1	DA	1208	GMA	CA-CB-CG-CD
1	EA	1308	GMA	CA-CB-CG-CD
1	GA	208	GMA	CA-CB-CG-CD
1	HA	308	GMA	CA-CB-CG-CD
1	KA	1208	GMA	CA-CB-CG-CD
1	LA	1308	GMA	CA-CB-CG-CD
1	NA	208	GMA	CA-CB-CG-CD
1	OA	308	GMA	CA-CB-CG-CD
1	RA	1208	GMA	CA-CB-CG-CD
1	SA	1308	GMA	CA-CB-CG-CD
1	a	8	GMA	O-C-CA-N
1	WA	1008	GMA	O-C-CA-N
1	b	8	GMA	O-C-CA-N
1	dA	1008	GMA	O-C-CA-N
1	c	8	GMA	O-C-CA-N
1	kA	1008	GMA	O-C-CA-N
1	d	8	GMA	O-C-CA-N
1	rA	1008	GMA	O-C-CA-N
1	e	8	GMA	O-C-CA-N
1	yA	1008	GMA	O-C-CA-N
1	f	8	GMA	O-C-CA-N
1	5A	1008	GMA	O-C-CA-N
1	g	8	GMA	O-C-CA-N
1	CB	1008	GMA	O-C-CA-N
1	h	8	GMA	O-C-CA-N
1	JB	1008	GMA	O-C-CA-N
1	i	8	GMA	O-C-CA-N
1	QB	1008	GMA	O-C-CA-N
1	cA	301	5CR	CA-CB-CG-CD2
1	gA	1301	5CR	CA-CB-CG-CD2
1	qA	301	5CR	CA-CB-CG-CD2
1	uA	1301	5CR	CA-CB-CG-CD2
1	xA	301	5CR	CA-CB-CG-CD2
1	1A	1301	5CR	CA-CB-CG-CD2
1	BB	301	5CR	CA-CB-CG-CD2
1	FB	1301	5CR	CA-CB-CG-CD2
1	cA	301	5CR	CA-CB-CG-CD1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
1	gA	1301	5CR	CA-CB-CG-CD1
1	jA	301	5CR	CA-CB-CG-CD2
1	nA	1301	5CR	CA-CB-CG-CD2
1	4A	301	5CR	CA-CB-CG-CD1
1	8A	1301	5CR	CA-CB-CG-CD1
1	BB	301	5CR	CA-CB-CG-CD1
1	FB	1301	5CR	CA-CB-CG-CD1
1	IB	301	5CR	CA-CB-CG-CD1
1	MB	1301	5CR	CA-CB-CG-CD1
1	PB	301	5CR	CA-CB-CG-CD2
1	TB	1301	5CR	CA-CB-CG-CD2
1	VA	301	5CR	CA-CB-CG-CD1
1	VA	301	5CR	CA-CB-CG-CD2
1	ZA	1301	5CR	CA-CB-CG-CD1
1	ZA	1301	5CR	CA-CB-CG-CD2
1	jA	301	5CR	CA-CB-CG-CD1
1	nA	1301	5CR	CA-CB-CG-CD1
1	qA	301	5CR	CA-CB-CG-CD1
1	uA	1301	5CR	CA-CB-CG-CD1
1	xA	301	5CR	CA-CB-CG-CD1
1	1A	1301	5CR	CA-CB-CG-CD1
1	4A	301	5CR	CA-CB-CG-CD2
1	8A	1301	5CR	CA-CB-CG-CD2
1	IB	301	5CR	CA-CB-CG-CD2
1	MB	1301	5CR	CA-CB-CG-CD2
1	PB	301	5CR	CA-CB-CG-CD1
1	TB	1301	5CR	CA-CB-CG-CD1
1	L	301	5CR	C-CA-N-CAL
1	P	1301	5CR	C-CA-N-CAL
1	S	301	5CR	C-CA-N-CAL
1	W	1301	5CR	C-CA-N-CAL
1	Z	301	5CR	C-CA-N-CAL
1	m	1301	5CR	C-CA-N-CAL
1	p	301	5CR	C-CA-N-CAL
1	t	1301	5CR	C-CA-N-CAL
1	w	301	5CR	C-CA-N-CAL
1	0	1301	5CR	C-CA-N-CAL
1	3	301	5CR	C-CA-N-CAL
1	7	1301	5CR	C-CA-N-CAL
1	AA	301	5CR	C-CA-N-CAL
1	EA	1301	5CR	C-CA-N-CAL
1	HA	301	5CR	C-CA-N-CAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
1	LA	1301	5CR	C-CA-N-CAL
1	OA	301	5CR	C-CA-N-CAL
1	SA	1301	5CR	C-CA-N-CAL
1	a	1	5CR	CB-CA-N-CAL
1	VA	301	5CR	CB-CA-N-CAL
1	WA	1001	5CR	CB-CA-N-CAL
1	ZA	1301	5CR	CB-CA-N-CAL
1	b	1	5CR	CB-CA-N-CAL
1	cA	301	5CR	CB-CA-N-CAL
1	dA	1001	5CR	CB-CA-N-CAL
1	gA	1301	5CR	CB-CA-N-CAL
1	c	1	5CR	CB-CA-N-CAL
1	jA	301	5CR	CB-CA-N-CAL
1	kA	1001	5CR	CB-CA-N-CAL
1	nA	1301	5CR	CB-CA-N-CAL
1	d	1	5CR	CB-CA-N-CAL
1	qA	301	5CR	CB-CA-N-CAL
1	rA	1001	5CR	CB-CA-N-CAL
1	uA	1301	5CR	CB-CA-N-CAL
1	e	1	5CR	CB-CA-N-CAL
1	xA	301	5CR	CB-CA-N-CAL
1	yA	1001	5CR	CB-CA-N-CAL
1	lA	1301	5CR	CB-CA-N-CAL
1	f	1	5CR	CB-CA-N-CAL
1	4A	301	5CR	CB-CA-N-CAL
1	5A	1001	5CR	CB-CA-N-CAL
1	8A	1301	5CR	CB-CA-N-CAL
1	g	1	5CR	CB-CA-N-CAL
1	BB	301	5CR	CB-CA-N-CAL
1	CB	1001	5CR	CB-CA-N-CAL
1	FB	1301	5CR	CB-CA-N-CAL
1	IB	301	5CR	CB-CA-N-CAL
1	MB	1301	5CR	CB-CA-N-CAL
1	i	1	5CR	CB-CA-N-CAL
1	PB	301	5CR	CB-CA-N-CAL
1	QB	1001	5CR	CB-CA-N-CAL
1	TB	1301	5CR	CB-CA-N-CAL
1	J	108	GMA	N-CA-CB-CG
1	N	1108	GMA	N-CA-CB-CG
1	Q	108	GMA	N-CA-CB-CG
1	U	1108	GMA	N-CA-CB-CG
1	X	108	GMA	N-CA-CB-CG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
1	k	1108	GMA	N-CA-CB-CG
1	n	108	GMA	N-CA-CB-CG
1	r	1108	GMA	N-CA-CB-CG
1	u	108	GMA	N-CA-CB-CG
1	y	1108	GMA	N-CA-CB-CG
1	1	108	GMA	N-CA-CB-CG
1	5	1108	GMA	N-CA-CB-CG
1	8	108	GMA	N-CA-CB-CG
1	CA	1108	GMA	N-CA-CB-CG
1	FA	108	GMA	N-CA-CB-CG
1	JA	1108	GMA	N-CA-CB-CG
1	MA	108	GMA	N-CA-CB-CG
1	QA	1108	GMA	N-CA-CB-CG
1	a	8	GMA	O-C-CA-CB
1	a	8	GMA	N2-C-CA-CB
1	WA	1008	GMA	O-C-CA-CB
1	WA	1008	GMA	N2-C-CA-CB
1	b	8	GMA	O-C-CA-CB
1	b	8	GMA	N2-C-CA-CB
1	dA	1008	GMA	O-C-CA-CB
1	dA	1008	GMA	N2-C-CA-CB
1	c	8	GMA	O-C-CA-CB
1	c	8	GMA	N2-C-CA-CB
1	kA	1008	GMA	O-C-CA-CB
1	kA	1008	GMA	N2-C-CA-CB
1	d	8	GMA	O-C-CA-CB
1	d	8	GMA	N2-C-CA-CB
1	rA	1008	GMA	O-C-CA-CB
1	rA	1008	GMA	N2-C-CA-CB
1	e	8	GMA	O-C-CA-CB
1	e	8	GMA	N2-C-CA-CB
1	yA	1008	GMA	O-C-CA-CB
1	yA	1008	GMA	N2-C-CA-CB
1	f	8	GMA	O-C-CA-CB
1	f	8	GMA	N2-C-CA-CB
1	5A	1008	GMA	O-C-CA-CB
1	5A	1008	GMA	N2-C-CA-CB
1	g	8	GMA	O-C-CA-CB
1	g	8	GMA	N2-C-CA-CB
1	CB	1008	GMA	O-C-CA-CB
1	CB	1008	GMA	N2-C-CA-CB
1	h	8	GMA	O-C-CA-CB

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
1	h	8	GMA	N2-C-CA-CB
1	JB	1008	GMA	O-C-CA-CB
1	JB	1008	GMA	N2-C-CA-CB
1	i	8	GMA	O-C-CA-CB
1	i	8	GMA	N2-C-CA-CB
1	QB	1008	GMA	O-C-CA-CB
1	QB	1008	GMA	N2-C-CA-CB
1	a	8	GMA	CA-CB-CG-CD
1	WA	1008	GMA	CA-CB-CG-CD
1	b	8	GMA	CA-CB-CG-CD
1	dA	1008	GMA	CA-CB-CG-CD
1	c	8	GMA	CA-CB-CG-CD
1	kA	1008	GMA	CA-CB-CG-CD
1	d	8	GMA	CA-CB-CG-CD
1	rA	1008	GMA	CA-CB-CG-CD
1	e	8	GMA	CA-CB-CG-CD
1	yA	1008	GMA	CA-CB-CG-CD
1	f	8	GMA	CA-CB-CG-CD
1	5A	1008	GMA	CA-CB-CG-CD
1	g	8	GMA	CA-CB-CG-CD
1	CB	1008	GMA	CA-CB-CG-CD
1	h	8	GMA	CA-CB-CG-CD
1	JB	1008	GMA	CA-CB-CG-CD
1	i	8	GMA	CA-CB-CG-CD
1	QB	1008	GMA	CA-CB-CG-CD
1	J	108	GMA	C-CA-CB-CG
1	N	1108	GMA	C-CA-CB-CG
1	Q	108	GMA	C-CA-CB-CG
1	U	1108	GMA	C-CA-CB-CG
1	X	108	GMA	C-CA-CB-CG
1	k	1108	GMA	C-CA-CB-CG
1	n	108	GMA	C-CA-CB-CG
1	r	1108	GMA	C-CA-CB-CG
1	u	108	GMA	C-CA-CB-CG
1	y	1108	GMA	C-CA-CB-CG
1	1	108	GMA	C-CA-CB-CG
1	5	1108	GMA	C-CA-CB-CG
1	8	108	GMA	C-CA-CB-CG
1	CA	1108	GMA	C-CA-CB-CG
1	FA	108	GMA	C-CA-CB-CG
1	JA	1108	GMA	C-CA-CB-CG
1	MA	108	GMA	C-CA-CB-CG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
1	QA	1108	GMA	C-CA-CB-CG
1	a	8	GMA	OE1-CD-CG-CB
1	WA	1008	GMA	OE1-CD-CG-CB
1	b	8	GMA	OE1-CD-CG-CB
1	dA	1008	GMA	OE1-CD-CG-CB
1	f	8	GMA	OE1-CD-CG-CB
1	5A	1008	GMA	OE1-CD-CG-CB
1	g	8	GMA	OE1-CD-CG-CB
1	CB	1008	GMA	OE1-CD-CG-CB
1	h	8	GMA	OE1-CD-CG-CB
1	JB	1008	GMA	OE1-CD-CG-CB
1	i	8	GMA	OE1-CD-CG-CB
1	QB	1008	GMA	OE1-CD-CG-CB
1	e	8	GMA	OE1-CD-CG-CB
1	yA	1008	GMA	OE1-CD-CG-CB
1	c	8	GMA	OE1-CD-CG-CB
1	kA	1008	GMA	OE1-CD-CG-CB
1	d	8	GMA	OE1-CD-CG-CB
1	rA	1008	GMA	OE1-CD-CG-CB
1	a	8	GMA	OE2-CD-CG-CB
1	WA	1008	GMA	OE2-CD-CG-CB
1	b	8	GMA	OE2-CD-CG-CB
1	dA	1008	GMA	OE2-CD-CG-CB
1	c	8	GMA	OE2-CD-CG-CB
1	kA	1008	GMA	OE2-CD-CG-CB
1	d	8	GMA	OE2-CD-CG-CB
1	rA	1008	GMA	OE2-CD-CG-CB
1	e	8	GMA	OE2-CD-CG-CB
1	yA	1008	GMA	OE2-CD-CG-CB
1	f	8	GMA	OE2-CD-CG-CB
1	5A	1008	GMA	OE2-CD-CG-CB
1	g	8	GMA	OE2-CD-CG-CB
1	CB	1008	GMA	OE2-CD-CG-CB
1	h	8	GMA	OE2-CD-CG-CB
1	JB	1008	GMA	OE2-CD-CG-CB
1	i	8	GMA	OE2-CD-CG-CB
1	QB	1008	GMA	OE2-CD-CG-CB
1	a	1	5CR	N-CA-CB-CG
1	WA	1001	5CR	N-CA-CB-CG
1	b	1	5CR	N-CA-CB-CG
1	dA	1001	5CR	N-CA-CB-CG
1	c	1	5CR	N-CA-CB-CG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
1	kA	1001	5CR	N-CA-CB-CG
1	d	1	5CR	N-CA-CB-CG
1	rA	1001	5CR	N-CA-CB-CG
1	e	1	5CR	N-CA-CB-CG
1	yA	1001	5CR	N-CA-CB-CG
1	f	1	5CR	N-CA-CB-CG
1	5A	1001	5CR	N-CA-CB-CG
1	g	1	5CR	N-CA-CB-CG
1	CB	1001	5CR	N-CA-CB-CG
1	h	1	5CR	N-CA-CB-CG
1	JB	1001	5CR	N-CA-CB-CG
1	i	1	5CR	N-CA-CB-CG
1	QB	1001	5CR	N-CA-CB-CG
1	J	108	GMA	CA-CB-CG-CD
1	N	1108	GMA	CA-CB-CG-CD
1	Q	108	GMA	CA-CB-CG-CD
1	U	1108	GMA	CA-CB-CG-CD
1	X	108	GMA	CA-CB-CG-CD
1	k	1108	GMA	CA-CB-CG-CD
1	n	108	GMA	CA-CB-CG-CD
1	r	1108	GMA	CA-CB-CG-CD
1	u	108	GMA	CA-CB-CG-CD
1	y	1108	GMA	CA-CB-CG-CD
1	l	108	GMA	CA-CB-CG-CD
1	5	1108	GMA	CA-CB-CG-CD
1	8	108	GMA	CA-CB-CG-CD
1	CA	1108	GMA	CA-CB-CG-CD
1	FA	108	GMA	CA-CB-CG-CD
1	JA	1108	GMA	CA-CB-CG-CD
1	MA	108	GMA	CA-CB-CG-CD
1	QA	1108	GMA	CA-CB-CG-CD
1	a	1	5CR	C-CA-N-CAL
1	TA	101	5CR	C-CA-N-CAL
1	VA	301	5CR	C-CA-N-CAL
1	WA	1001	5CR	C-CA-N-CAL
1	XA	1101	5CR	C-CA-N-CAL
1	ZA	1301	5CR	C-CA-N-CAL
1	b	1	5CR	C-CA-N-CAL
1	aA	101	5CR	C-CA-N-CAL
1	cA	301	5CR	C-CA-N-CAL
1	dA	1001	5CR	C-CA-N-CAL
1	eA	1101	5CR	C-CA-N-CAL

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
1	gA	1301	5CR	C-CA-N-CAL
1	c	1	5CR	C-CA-N-CAL
1	hA	101	5CR	C-CA-N-CAL
1	jA	301	5CR	C-CA-N-CAL
1	kA	1001	5CR	C-CA-N-CAL
1	lA	1101	5CR	C-CA-N-CAL
1	nA	1301	5CR	C-CA-N-CAL
1	d	1	5CR	C-CA-N-CAL
1	oA	101	5CR	C-CA-N-CAL
1	qA	301	5CR	C-CA-N-CAL
1	rA	1001	5CR	C-CA-N-CAL
1	sA	1101	5CR	C-CA-N-CAL
1	uA	1301	5CR	C-CA-N-CAL
1	e	1	5CR	C-CA-N-CAL
1	vA	101	5CR	C-CA-N-CAL
1	xA	301	5CR	C-CA-N-CAL
1	yA	1001	5CR	C-CA-N-CAL
1	zA	1101	5CR	C-CA-N-CAL
1	1A	1301	5CR	C-CA-N-CAL
1	f	1	5CR	C-CA-N-CAL
1	2A	101	5CR	C-CA-N-CAL
1	4A	301	5CR	C-CA-N-CAL
1	5A	1001	5CR	C-CA-N-CAL
1	6A	1101	5CR	C-CA-N-CAL
1	8A	1301	5CR	C-CA-N-CAL
1	g	1	5CR	C-CA-N-CAL
1	9A	101	5CR	C-CA-N-CAL
1	BB	301	5CR	C-CA-N-CAL
1	CB	1001	5CR	C-CA-N-CAL
1	DB	1101	5CR	C-CA-N-CAL
1	FB	1301	5CR	C-CA-N-CAL
1	h	1	5CR	C-CA-N-CAL
1	GB	101	5CR	C-CA-N-CAL
1	IB	301	5CR	C-CA-N-CAL
1	JB	1001	5CR	C-CA-N-CAL
1	KB	1101	5CR	C-CA-N-CAL
1	MB	1301	5CR	C-CA-N-CAL
1	i	1	5CR	C-CA-N-CAL
1	NB	101	5CR	C-CA-N-CAL
1	PB	301	5CR	C-CA-N-CAL
1	QB	1001	5CR	C-CA-N-CAL
1	RB	1101	5CR	C-CA-N-CAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
1	TB	1301	5CR	C-CA-N-CAL
1	bA	208	GMA	OE2-CD-CG-CB
1	fA	1208	GMA	OE2-CD-CG-CB
1	pA	208	GMA	OE2-CD-CG-CB
1	tA	1208	GMA	OE2-CD-CG-CB
1	wA	208	GMA	OE2-CD-CG-CB
1	0A	1208	GMA	OE2-CD-CG-CB
1	K	201	5CR	C-CA-CB-CG
1	O	1201	5CR	C-CA-CB-CG
1	R	201	5CR	C-CA-CB-CG
1	V	1201	5CR	C-CA-CB-CG
1	Y	201	5CR	C-CA-CB-CG
1	l	1201	5CR	C-CA-CB-CG
1	o	201	5CR	C-CA-CB-CG
1	s	1201	5CR	C-CA-CB-CG
1	v	201	5CR	C-CA-CB-CG
1	z	1201	5CR	C-CA-CB-CG
1	2	201	5CR	C-CA-CB-CG
1	6	1201	5CR	C-CA-CB-CG
1	9	201	5CR	C-CA-CB-CG
1	DA	1201	5CR	C-CA-CB-CG
1	GA	201	5CR	C-CA-CB-CG
1	KA	1201	5CR	C-CA-CB-CG
1	NA	201	5CR	C-CA-CB-CG
1	RA	1201	5CR	C-CA-CB-CG
1	iA	208	GMA	OE2-CD-CG-CB
1	mA	1208	GMA	OE2-CD-CG-CB
1	HB	208	GMA	OE2-CD-CG-CB
1	LB	1208	GMA	OE2-CD-CG-CB
1	UA	208	GMA	OE2-CD-CG-CB
1	YA	1208	GMA	OE2-CD-CG-CB
1	3A	208	GMA	OE2-CD-CG-CB
1	7A	1208	GMA	OE2-CD-CG-CB
1	UA	208	GMA	OE1-CD-CG-CB
1	YA	1208	GMA	OE1-CD-CG-CB
1	iA	208	GMA	OE1-CD-CG-CB
1	mA	1208	GMA	OE1-CD-CG-CB
1	pA	208	GMA	OE1-CD-CG-CB
1	tA	1208	GMA	OE1-CD-CG-CB
1	3A	208	GMA	OE1-CD-CG-CB
1	7A	1208	GMA	OE1-CD-CG-CB
1	AB	208	GMA	OE1-CD-CG-CB

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
1	AB	208	GMA	OE2-CD-CG-CB
1	EB	1208	GMA	OE1-CD-CG-CB
1	EB	1208	GMA	OE2-CD-CG-CB
1	HB	208	GMA	OE1-CD-CG-CB
1	LB	1208	GMA	OE1-CD-CG-CB
1	OB	208	GMA	OE1-CD-CG-CB
1	OB	208	GMA	OE2-CD-CG-CB
1	SB	1208	GMA	OE1-CD-CG-CB
1	SB	1208	GMA	OE2-CD-CG-CB
1	UA	201	5CR	CB-CA-N-CAL
1	YA	1201	5CR	CB-CA-N-CAL
1	bA	201	5CR	CB-CA-N-CAL
1	fA	1201	5CR	CB-CA-N-CAL
1	iA	201	5CR	CB-CA-N-CAL
1	mA	1201	5CR	CB-CA-N-CAL
1	pA	201	5CR	CB-CA-N-CAL
1	tA	1201	5CR	CB-CA-N-CAL
1	wA	201	5CR	CB-CA-N-CAL
1	0A	1201	5CR	CB-CA-N-CAL
1	3A	201	5CR	CB-CA-N-CAL
1	7A	1201	5CR	CB-CA-N-CAL
1	AB	201	5CR	CB-CA-N-CAL
1	EB	1201	5CR	CB-CA-N-CAL
1	h	1	5CR	CB-CA-N-CAL
1	HB	201	5CR	CB-CA-N-CAL
1	JB	1001	5CR	CB-CA-N-CAL
1	LB	1201	5CR	CB-CA-N-CAL
1	OB	201	5CR	CB-CA-N-CAL
1	SB	1201	5CR	CB-CA-N-CAL
1	bA	208	GMA	OE1-CD-CG-CB
1	fA	1208	GMA	OE1-CD-CG-CB
1	wA	208	GMA	OE1-CD-CG-CB
1	0A	1208	GMA	OE1-CD-CG-CB

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

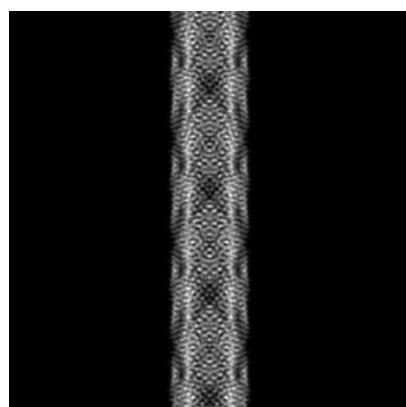
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23485. These allow visual inspection of the internal detail of the map and identification of artifacts.

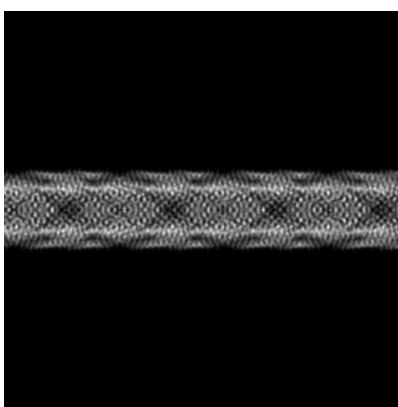
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

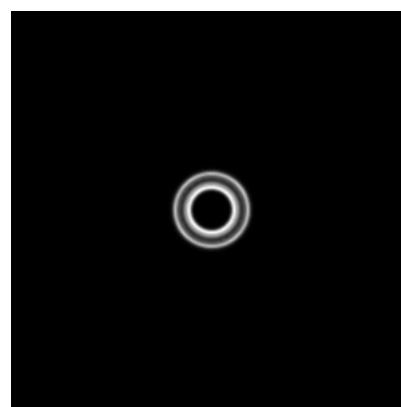
#### 6.1.1 Primary map



X



Y

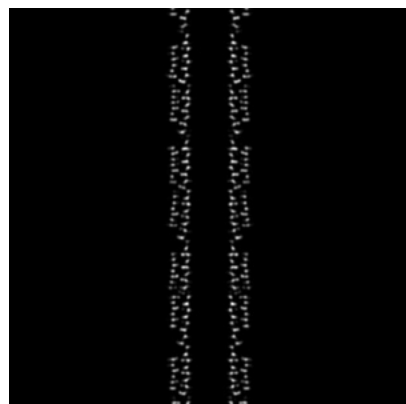


Z

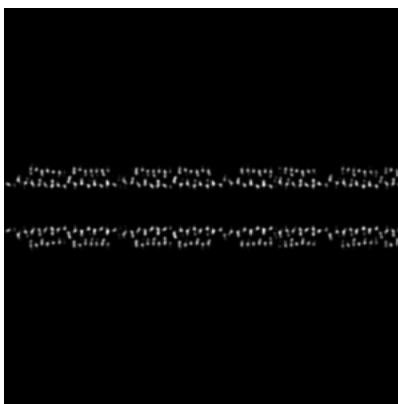
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

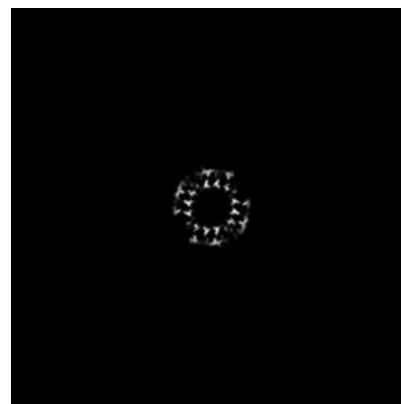
#### 6.2.1 Primary map



X Index: 160



Y Index: 160

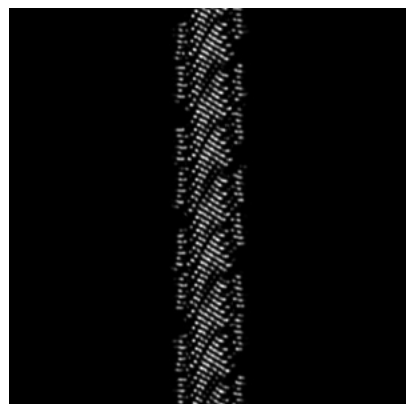


Z Index: 160

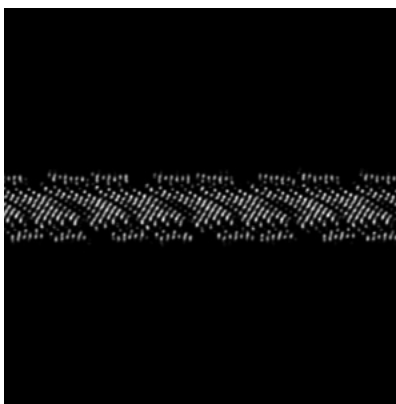
The images above show central slices of the map in three orthogonal directions.

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

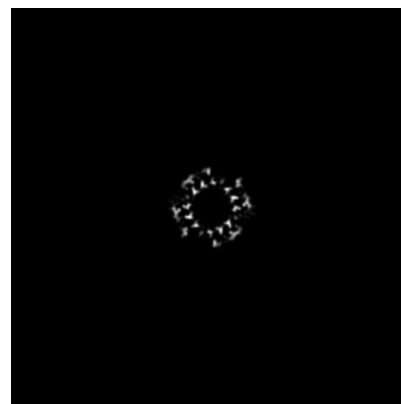
### 6.3.1 Primary map



X Index: 143



Y Index: 143



Z Index: 61

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

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

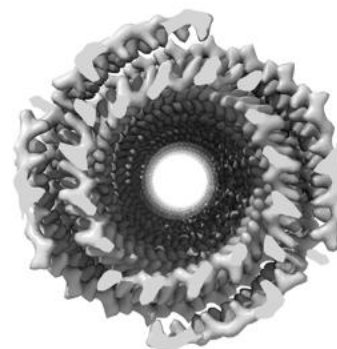
### 6.4.1 Primary map



X



Y



Z

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

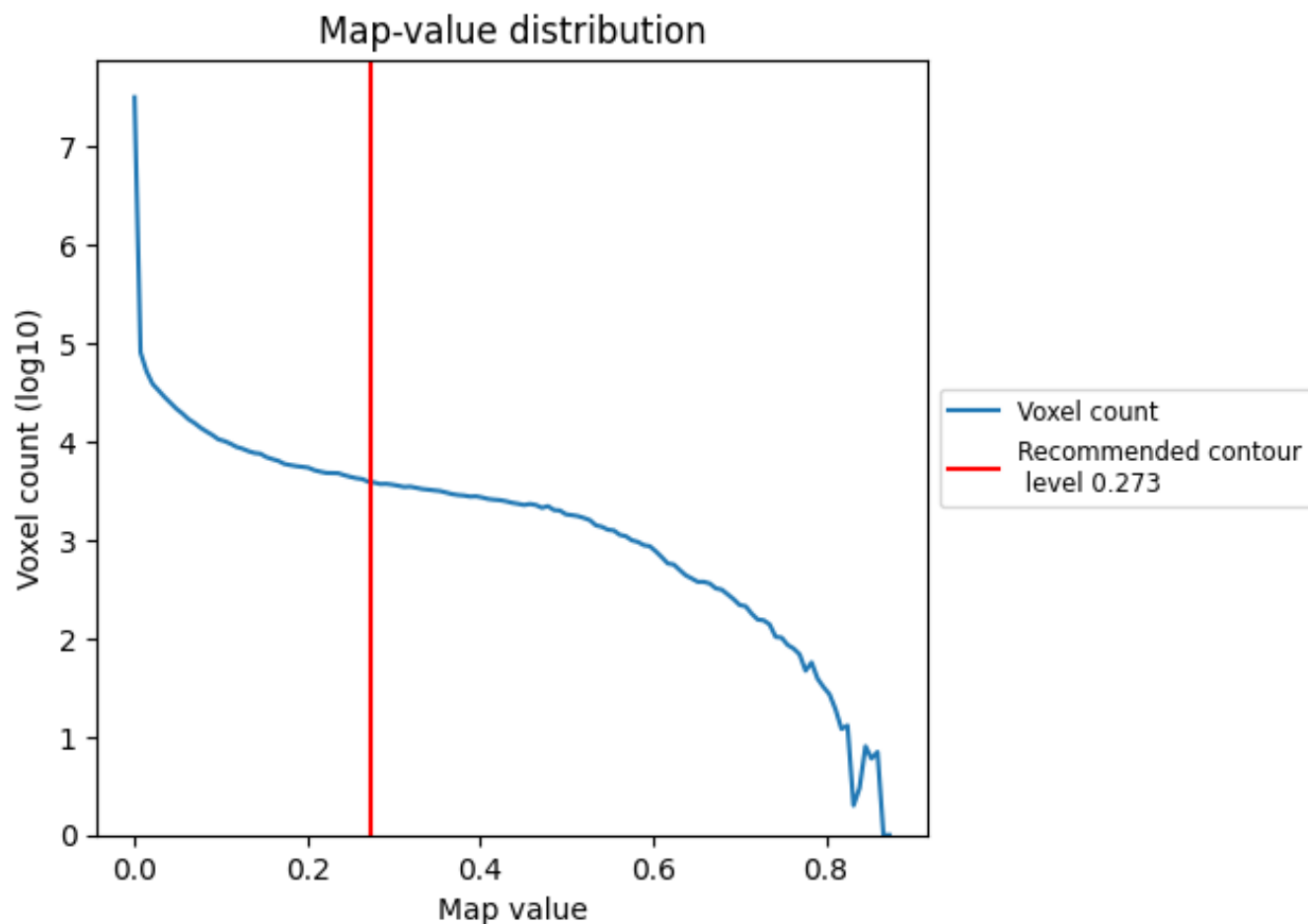
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

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

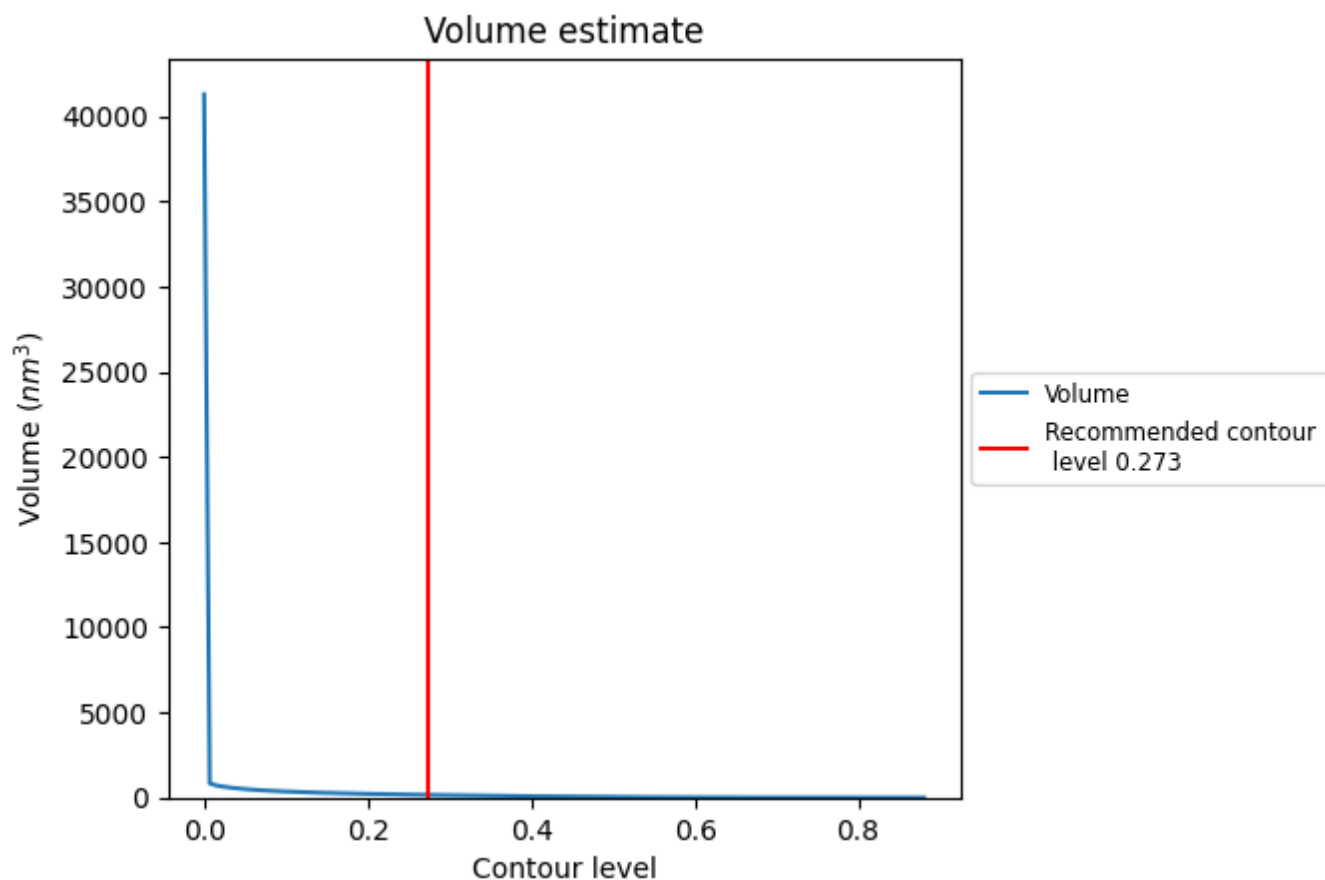
### 7.1 Map-value distribution [i](#)



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



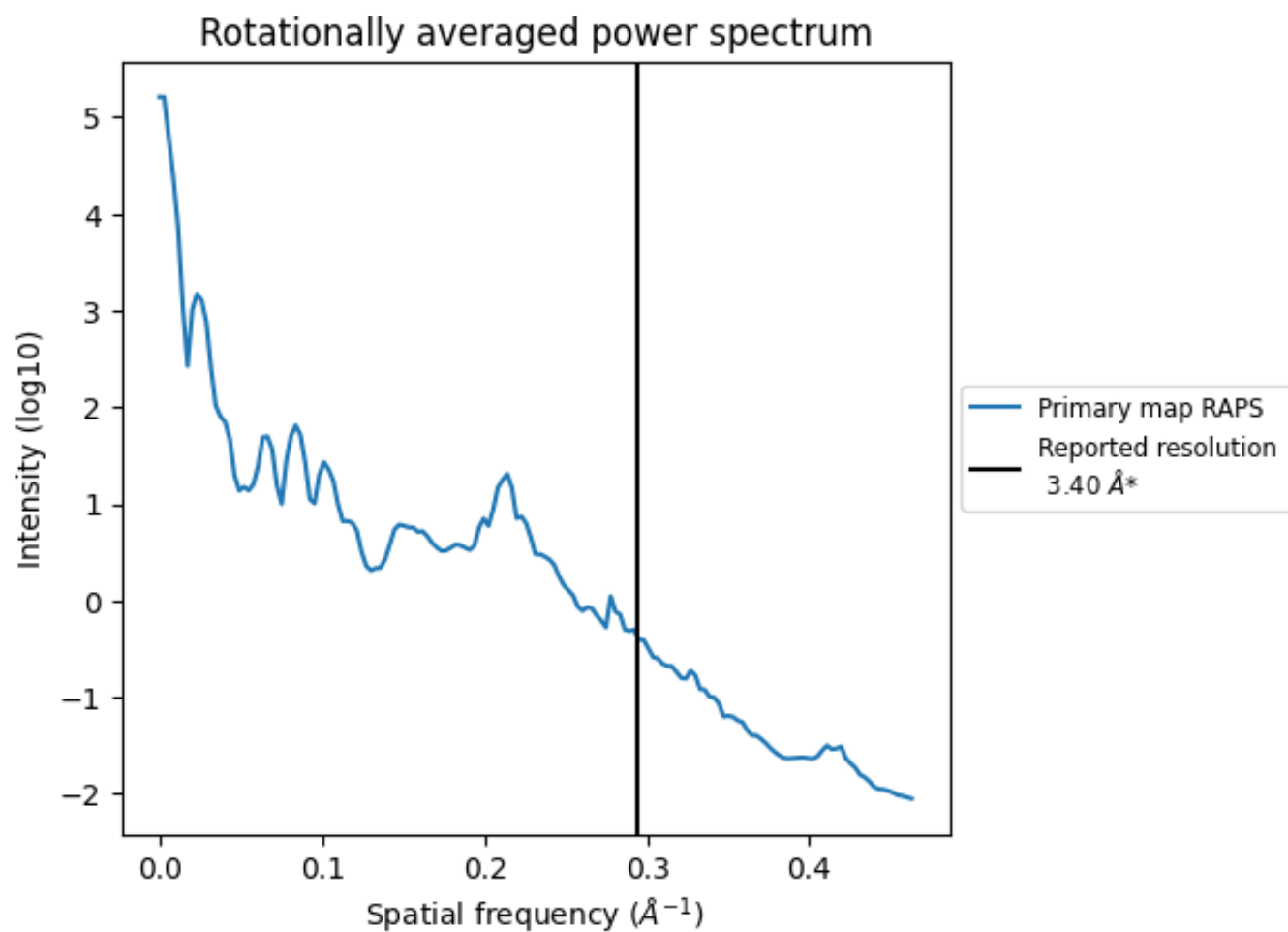
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 154  $\text{nm}^3$ ; this corresponds to an approximate mass of 139 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.294 Å<sup>-1</sup>

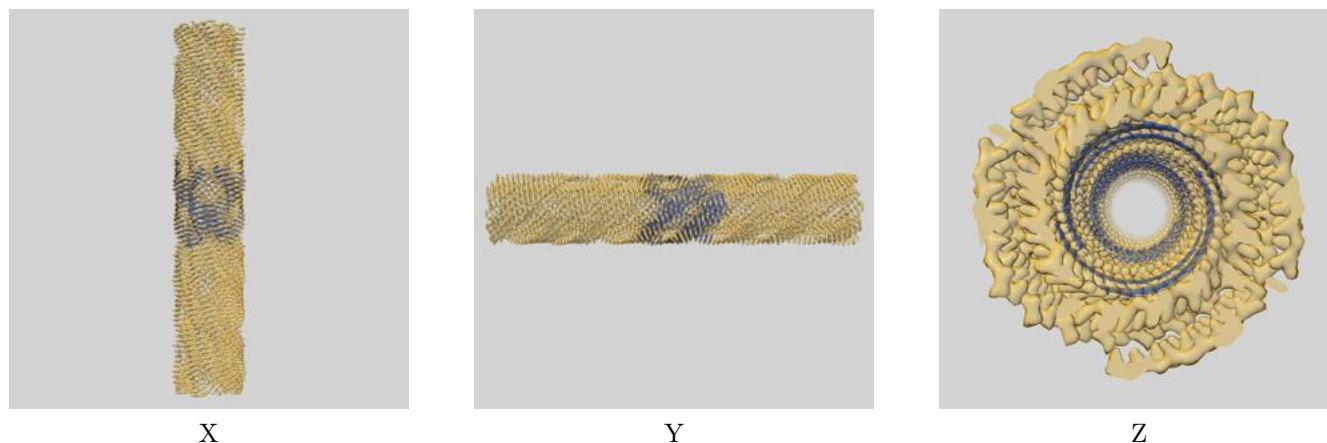
## 8 Fourier-Shell correlation

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

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

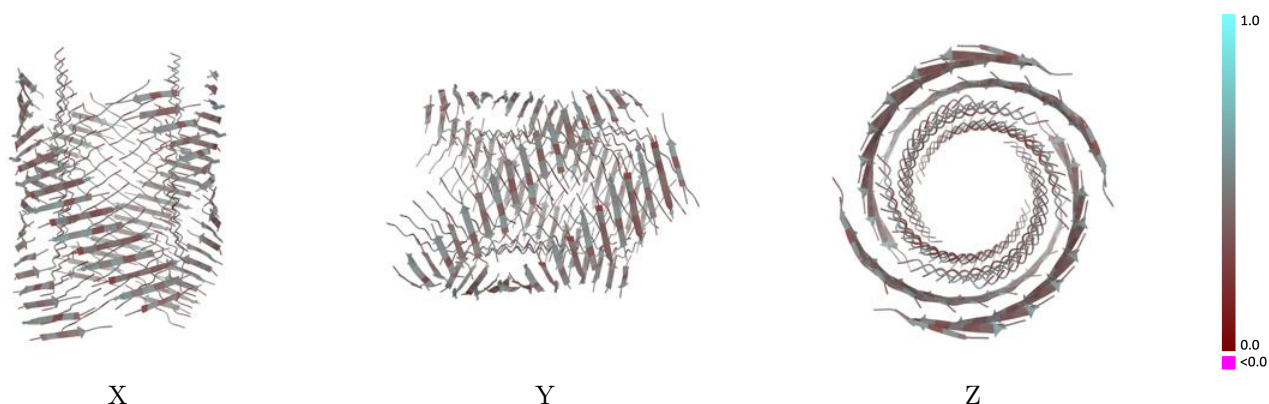
This section contains information regarding the fit between EMDB map EMD-23485 and PDB model 7LQG. Per-residue inclusion information can be found in section 3 on page 17.

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



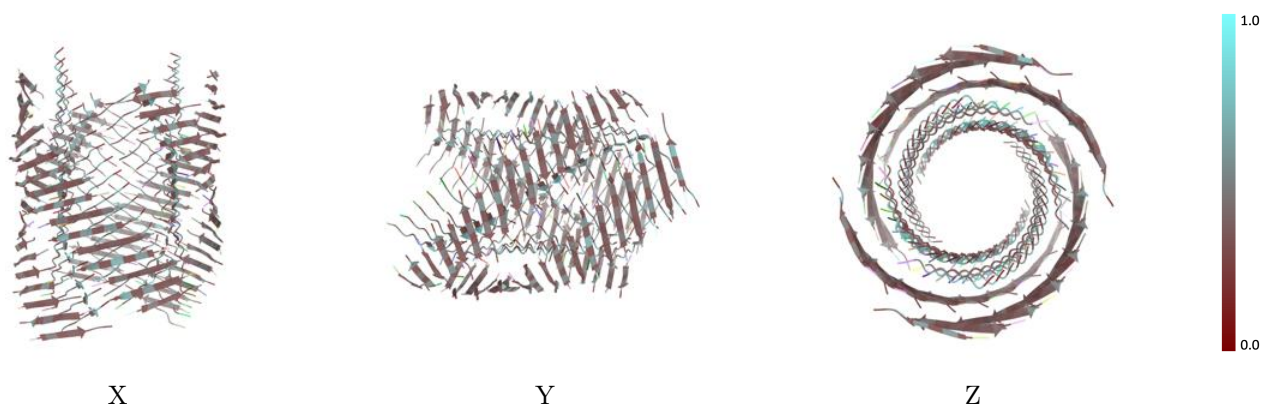
The images above show the 3D surface view of the map at the recommended contour level 0.273 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



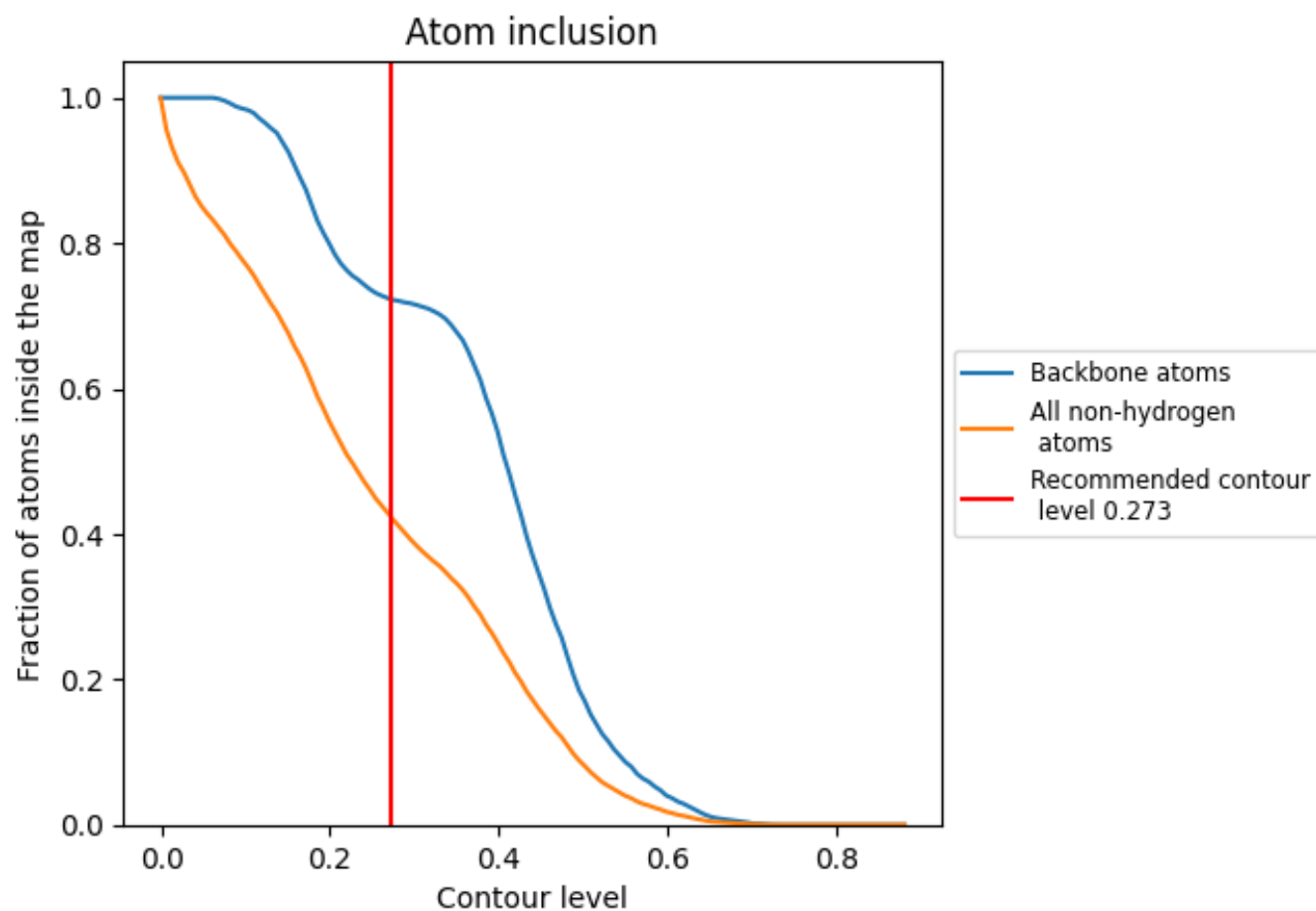
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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, 72% 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	 0.4227	 0.4300
0	 0.4881	 0.4310
0A	 0.4167	 0.4780
1	 0.4405	 0.4150
1A	 0.3690	 0.3900
2	 0.5000	 0.4480
2A	 0.3690	 0.4120
3	 0.5119	 0.4370
3A	 0.4167	 0.4680
4	 0.4286	 0.4370
4A	 0.3690	 0.3820
5	 0.4405	 0.4090
5A	 0.3929	 0.4580
6	 0.5000	 0.4580
6A	 0.3690	 0.4150
7	 0.4881	 0.4320
7A	 0.4048	 0.4600
8	 0.4167	 0.4170
8A	 0.3571	 0.4120
9	 0.5238	 0.4470
9A	 0.3571	 0.4270
A	 0.4286	 0.4140
AA	 0.5119	 0.4380
AB	 0.4286	 0.4540
B	 0.4405	 0.4200
BA	 0.4048	 0.4050
BB	 0.3810	 0.3920
C	 0.4286	 0.4250
CA	 0.4286	 0.4050
CB	 0.3810	 0.4510
D	 0.4167	 0.4170
DA	 0.5119	 0.4410
DB	 0.3571	 0.4210
E	 0.4286	 0.4310
EA	 0.5000	 0.4410



*Continued on next page...*





















































































*Continued from previous page...*

Chain	Atom inclusion	Q-score
EB	 0.4286	 0.4630
F	 0.4286	 0.4320
FA	 0.4167	 0.4070
FB	 0.3690	 0.3910
G	 0.4048	 0.4190
GA	 0.4643	 0.4430
GB	 0.3571	 0.4120
H	 0.4286	 0.4230
HA	 0.5238	 0.4450
HB	 0.4524	 0.4590
I	 0.4405	 0.4340
IA	 0.4286	 0.4270
IB	 0.3810	 0.3830
J	 0.4643	 0.4180
JA	 0.4167	 0.4060
JB	 0.4048	 0.4320
K	 0.4762	 0.4490
KA	 0.4643	 0.4560
KB	 0.3452	 0.4240
L	 0.4881	 0.4400
LA	 0.5119	 0.4410
LB	 0.4405	 0.4440
M	 0.4286	 0.4200
MA	 0.4405	 0.4090
MB	 0.3690	 0.4080
N	 0.4405	 0.4020
NA	 0.4762	 0.4460
NB	 0.3929	 0.4200
O	 0.4762	 0.4440
OA	 0.5238	 0.4310
OB	 0.3929	 0.4610
P	 0.4762	 0.4440
PA	 0.4405	 0.4260
PB	 0.3810	 0.4040
Q	 0.4405	 0.4180
QA	 0.4167	 0.3960
QB	 0.3929	 0.4510
R	 0.4762	 0.4620
RA	 0.4762	 0.4460
RB	 0.3810	 0.4100
S	 0.4881	 0.4410
SA	 0.5357	 0.4470

*Continued on next page...*























































*Continued from previous page...*

Chain	Atom inclusion	Q-score
SB	 0.3810	 0.4710
T	 0.4286	 0.4290
TA	 0.3452	 0.4210
TB	 0.3810	 0.3920
U	 0.4286	 0.4080
UA	 0.3929	 0.4710
V	 0.4881	 0.4500
VA	 0.3810	 0.3900
W	 0.4881	 0.4310
WA	 0.3929	 0.4420
X	 0.4048	 0.4020
XA	 0.3452	 0.4200
Y	 0.4881	 0.4510
YA	 0.3810	 0.4670
Z	 0.4881	 0.4450
ZA	 0.3690	 0.3970
a	 0.3929	 0.4480
aA	 0.3690	 0.4290
b	 0.4048	 0.4580
bA	 0.4286	 0.4720
c	 0.4167	 0.4580
cA	 0.3690	 0.3820
d	 0.3810	 0.4600
dA	 0.3690	 0.4520
e	 0.3810	 0.4480
eA	 0.3690	 0.4340
f	 0.3929	 0.4570
fA	 0.4286	 0.4620
g	 0.3929	 0.4520
gA	 0.3571	 0.3870
h	 0.4048	 0.4440
hA	 0.3929	 0.4180
i	 0.4167	 0.4580
iA	 0.4167	 0.4630
j	 0.4286	 0.4240
jA	 0.4167	 0.3850
k	 0.4048	 0.3900
kA	 0.3810	 0.4530
l	 0.4881	 0.4570
lA	 0.3810	 0.4120
m	 0.4762	 0.4480
mA	 0.4167	 0.4630

*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
n	 0.4286	 0.4030
nA	 0.4167	 0.4010
o	 0.4881	 0.4480
oA	 0.3690	 0.4260
p	 0.5000	 0.4410
pA	 0.3810	 0.4670
q	 0.4167	 0.4170
qA	 0.3690	 0.3790
r	 0.4048	 0.4010
rA	 0.3690	 0.4470
s	 0.5000	 0.4450
sA	 0.3690	 0.4160
t	 0.4881	 0.4330
tA	 0.3810	 0.4650
u	 0.4405	 0.4070
uA	 0.3690	 0.3910
v	 0.4524	 0.4430
vA	 0.3571	 0.4230
w	 0.5000	 0.4290
wA	 0.4405	 0.4690
x	 0.4167	 0.4110
xA	 0.3810	 0.3740
y	 0.4286	 0.4010
yA	 0.3690	 0.4540
z	 0.4524	 0.4490
zA	 0.3333	 0.4240