



Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 03:56 PM EST

PDB ID : 7LQI
EMDB ID : EMD-23487
Title : Cryo-EM of KFE8 thicker nanotube
Authors : Wang, F.; Gnewou, O.M.; Egelman, E.H.; Conticello, V.P.
Deposited on : 2021-02-13
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

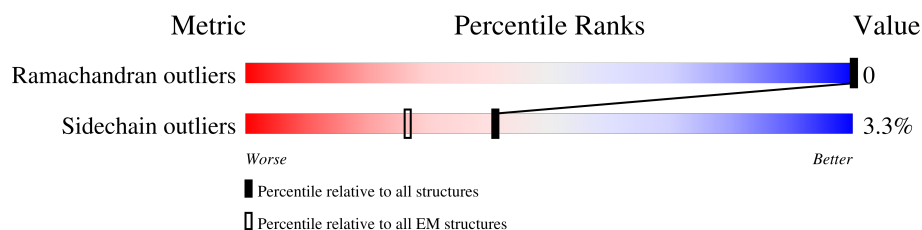
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (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 3.50 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	8	<div> <div>38%</div> <div>88%</div> <div>12%</div> </div>
1	1	8	<div> <div>38%</div> <div>88%</div> <div>12%</div> </div>
1	1A	8	<div> <div>75%</div> <div>75%</div> <div>25%</div> </div>
1	2A	8	<div> <div>50%</div> <div>75%</div> <div>25%</div> </div>
1	3A	8	<div> <div>62%</div> <div>75%</div> <div>25%</div> </div>
1	4A	8	<div> <div>75%</div> <div>75%</div> <div>25%</div> </div>
1	5	8	<div> <div>38%</div> <div>88%</div> <div>12%</div> </div>
1	5A	8	<div> <div>62%</div> <div>75%</div> <div>25%</div> </div>
1	6	8	<div> <div>38%</div> <div>75%</div> <div>25%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	6A	8	<div> <div>75%</div> <div>88%</div> <div>12%</div> </div>
1	7	8	<div> <div>38%</div> <div>88%</div> <div>12%</div> </div>
1	7A	8	<div> <div>62%</div> <div>75%</div> <div>25%</div> </div>
1	8	8	<div> <div>38%</div> <div>88%</div> <div>12%</div> </div>
1	8A	8	<div> <div>62%</div> <div>75%</div> <div>25%</div> </div>
1	9A	8	<div> <div>62%</div> <div>75%</div> <div>25%</div> </div>
1	A	8	<div> <div>38%</div> <div>75%</div> <div>25%</div> </div>
1	B	8	<div> <div>38%</div> <div>75%</div> <div>25%</div> </div>
1	C	8	<div> <div>38%</div> <div>75%</div> <div>25%</div> </div>
1	CA	8	<div> <div>38%</div> <div>88%</div> <div>12%</div> </div>
1	D	8	<div> <div>38%</div> <div>75%</div> <div>25%</div> </div>
1	DA	8	<div> <div>25%</div> <div>75%</div> <div>25%</div> </div>
1	E	8	<div> <div>50%</div> <div>75%</div> <div>25%</div> </div>
1	EA	8	<div> <div>38%</div> <div>88%</div> <div>12%</div> </div>
1	F	8	<div> <div>38%</div> <div>75%</div> <div>25%</div> </div>
1	FA	8	<div> <div>38%</div> <div>88%</div> <div>12%</div> </div>
1	G	8	<div> <div>38%</div> <div>75%</div> <div>25%</div> </div>
1	GB	8	<div> <div>62%</div> <div>75%</div> <div>25%</div> </div>
1	H	8	<div> <div>50%</div> <div>75%</div> <div>25%</div> </div>
1	HB	8	<div> <div>50%</div> <div>75%</div> <div>25%</div> </div>
1	I	8	<div> <div>38%</div> <div>75%</div> <div>25%</div> </div>
1	IB	8	<div> <div>50%</div> <div>75%</div> <div>25%</div> </div>
1	J	8	<div> <div>12%</div> <div>75%</div> <div>25%</div> </div>
1	JA	8	<div> <div>50%</div> <div>88%</div> <div>12%</div> </div>
1	JB	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	K	8	<div> <div>38%</div> <div>88%</div> <div>12%</div> </div>
1	KA	8	<div> <div>38%</div> <div>75%</div> <div>25%</div> </div>
1	KB	8	<div> <div>62%</div> <div>75%</div> <div>25%</div> </div>
1	L	8	<div> <div>38%</div> <div>62%</div> <div>38%</div> </div>
1	LA	8	<div> <div>50%</div> <div>88%</div> <div>12%</div> </div>
1	LB	8	<div> <div>62%</div> <div>75%</div> <div>25%</div> </div>
1	M	8	<div> <div>38%</div> <div>88%</div> <div>12%</div> </div>
1	MA	8	<div> <div>38%</div> <div>88%</div> <div>12%</div> </div>
1	MB	8	<div> <div>62%</div> <div>75%</div> <div>25%</div> </div>
1	N	8	<div> <div>38%</div> <div>88%</div> <div>12%</div> </div>
1	NB	8	<div> <div>62%</div> <div>75%</div> <div>25%</div> </div>
1	OB	8	<div> <div>50%</div> <div>75%</div> <div>25%</div> </div>
1	QA	8	<div> <div>12%</div> <div>88%</div> <div>12%</div> </div>
1	R	8	<div> <div>38%</div> <div>88%</div> <div>12%</div> </div>
1	RA	8	<div> <div>12%</div> <div>75%</div> <div>25%</div> </div>
1	S	8	<div> <div>25%</div> <div>75%</div> <div>25%</div> </div>
1	SA	8	<div> <div>25%</div> <div>75%</div> <div>25%</div> </div>
1	T	8	<div> <div>38%</div> <div>88%</div> <div>12%</div> </div>
1	TA	8	<div> <div>12%</div> <div>88%</div> <div>12%</div> </div>
1	U	8	<div> <div>38%</div> <div>88%</div> <div>12%</div> </div>
1	VB	8	<div> <div>62%</div> <div>75%</div> <div>25%</div> </div>
1	WB	8	<div> <div>62%</div> <div>75%</div> <div>25%</div> </div>
1	XA	8	<div> <div>62%</div> <div>75%</div> <div>25%</div> </div>
1	XB	8	<div> <div>62%</div> <div>75%</div> <div>25%</div> </div>
1	Y	8	<div> <div>38%</div> <div>88%</div> <div>12%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	YA	8	<div> <div>50%</div> <div>75%</div> <div>25%</div> </div>
1	YB	8	<div> <div>62%</div> <div>75%</div> <div>25%</div> </div>
1	Z	8	<div> <div>38%</div> <div>75%</div> <div>25%</div> </div>
1	ZA	8	<div> <div>62%</div> <div>75%</div> <div>25%</div> </div>
1	ZB	8	<div> <div>62%</div> <div>75%</div> <div>25%</div> </div>
1	a	8	<div> <div>50%</div> <div>75%</div> <div>25%</div> </div>
1	aA	8	<div> <div>50%</div> <div>75%</div> <div>25%</div> </div>
1	aB	8	<div> <div>62%</div> <div>75%</div> <div>25%</div> </div>
1	b	8	<div> <div>50%</div> <div>75%</div> <div>25%</div> </div>
1	bA	8	<div> <div>62%</div> <div>75%</div> <div>25%</div> </div>
1	bB	8	<div> <div>62%</div> <div>75%</div> <div>25%</div> </div>
1	c	8	<div> <div>50%</div> <div>75%</div> <div>25%</div> </div>
1	cA	8	<div> <div>75%</div> <div>75%</div> <div>25%</div> </div>
1	cB	8	<div> <div>62%</div> <div>75%</div> <div>25%</div> </div>
1	d	8	<div> <div>62%</div> <div>75%</div> <div>25%</div> </div>
1	dA	8	<div> <div>62%</div> <div>75%</div> <div>25%</div> </div>
1	dB	8	<div> <div>62%</div> <div>75%</div> <div>25%</div> </div>
1	e	8	<div> <div>62%</div> <div>75%</div> <div>25%</div> </div>
1	eA	8	<div> <div>62%</div> <div>75%</div> <div>25%</div> </div>
1	f	8	<div> <div>38%</div> <div>88%</div> <div>12%</div> </div>
1	fA	8	<div> <div>62%</div> <div>75%</div> <div>25%</div> </div>
1	g	8	<div> <div>38%</div> <div>88%</div> <div>12%</div> </div>
1	k	8	<div> <div>38%</div> <div>88%</div> <div>12%</div> </div>
1	l	8	<div> <div>38%</div> <div>75%</div> <div>25%</div> </div>
1	m	8	<div> <div>38%</div> <div>88%</div> <div>12%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	mA	8	
1	n	8	
1	nA	8	
1	oA	8	
1	pA	8	
1	qA	8	
1	r	8	
1	rA	8	
1	s	8	
1	sA	8	
1	t	8	
1	tA	8	
1	u	8	
1	uA	8	
1	y	8	
1	z	8	

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 8400 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	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	B	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	C	8	Total	C	N	O	0	0
			84	60	11	13		
1	Y	8	Total	C	N	O	0	0
			84	60	11	13		
1	Z	8	Total	C	N	O	0	0
			84	60	11	13		
1	f	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	D	8	Total	C	N	O	0	0
			84	60	11	13		
1	k	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	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	E	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	F	8	Total	C	N	O	0	0
			84	60	11	13		
1	y	8	Total	C	N	O	0	0
			84	60	11	13		
1	z	8	Total	C	N	O	0	0
			84	60	11	13		
1	0	8	Total	C	N	O	0	0
			84	60	11	13		
1	1	8	Total	C	N	O	0	0
			84	60	11	13		
1	G	8	Total	C	N	O	0	0
			84	60	11	13		
1	5	8	Total	C	N	O	0	0
			84	60	11	13		
1	6	8	Total	C	N	O	0	0
			84	60	11	13		
1	7	8	Total	C	N	O	0	0
			84	60	11	13		
1	8	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	CA	8	Total	C	N	O	0	0
			84	60	11	13		
1	DA	8	Total	C	N	O	0	0
			84	60	11	13		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
1	EA	8	Total	C	N	O	0	0
			84	60	11	13		
1	FA	8	Total	C	N	O	0	0
			84	60	11	13		
1	I	8	Total	C	N	O	0	0
			84	60	11	13		
1	JA	8	Total	C	N	O	0	0
			84	60	11	13		
1	KA	8	Total	C	N	O	0	0
			84	60	11	13		
1	LA	8	Total	C	N	O	0	0
			84	60	11	13		
1	MA	8	Total	C	N	O	0	0
			84	60	11	13		
1	J	8	Total	C	N	O	0	0
			84	60	11	13		
1	QA	8	Total	C	N	O	0	0
			84	60	11	13		
1	RA	8	Total	C	N	O	0	0
			84	60	11	13		
1	SA	8	Total	C	N	O	0	0
			84	60	11	13		
1	TA	8	Total	C	N	O	0	0
			84	60	11	13		
1	a	8	Total	C	N	O	0	0
			84	60	11	13		
1	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	aA	8	Total	C	N	O	0	0
			84	60	11	13		
1	bA	8	Total	C	N	O	0	0
			84	60	11	13		
1	cA	8	Total	C	N	O	0	0
			84	60	11	13		
1	dA	8	Total	C	N	O	0	0
			84	60	11	13		
1	eA	8	Total	C	N	O	0	0
			84	60	11	13		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
1	fA	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	mA	8	Total	C	N	O	0	0
			84	60	11	13		
1	nA	8	Total	C	N	O	0	0
			84	60	11	13		
1	oA	8	Total	C	N	O	0	0
			84	60	11	13		
1	pA	8	Total	C	N	O	0	0
			84	60	11	13		
1	qA	8	Total	C	N	O	0	0
			84	60	11	13		
1	rA	8	Total	C	N	O	0	0
			84	60	11	13		
1	sA	8	Total	C	N	O	0	0
			84	60	11	13		
1	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	c	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	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	9A	8	Total	C	N	O	0	0
			84	60	11	13		

Continued on next page...

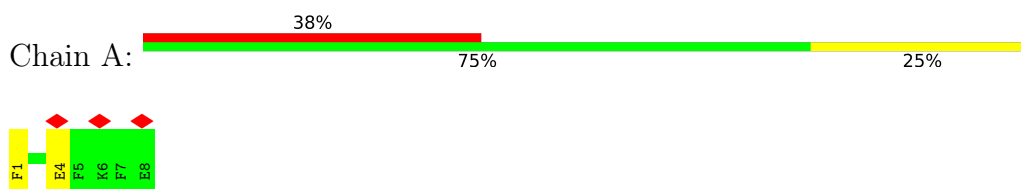
Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
1	d	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	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	e	8	Total	C	N	O	0	0
			84	60	11	13		
1	VB	8	Total	C	N	O	0	0
			84	60	11	13		
1	WB	8	Total	C	N	O	0	0
			84	60	11	13		
1	XB	8	Total	C	N	O	0	0
			84	60	11	13		
1	YB	8	Total	C	N	O	0	0
			84	60	11	13		
1	ZB	8	Total	C	N	O	0	0
			84	60	11	13		
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		

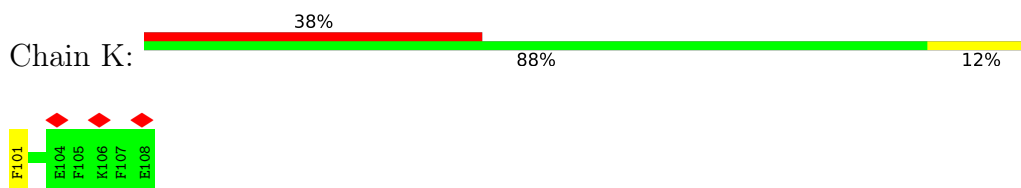
3 Residue-property plots [i](#)

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.

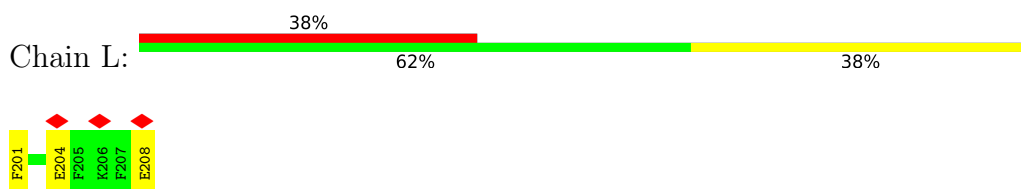
- Molecule 1: KFE8 peptide



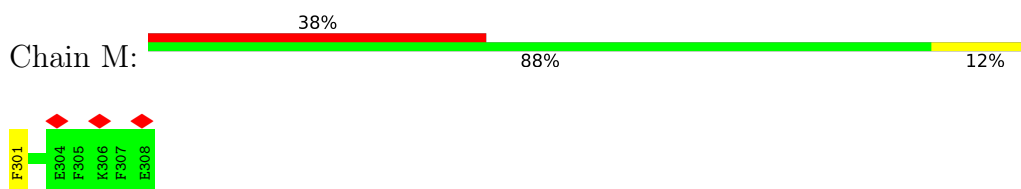
- Molecule 1: KFE8 peptide



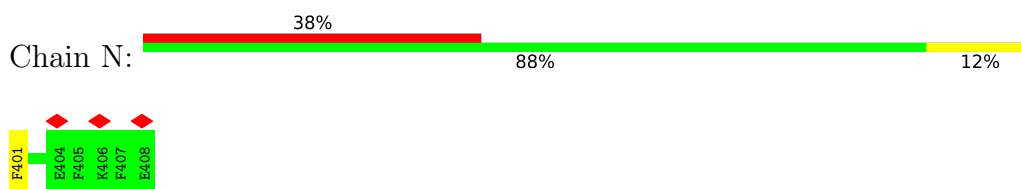
- Molecule 1: KFE8 peptide



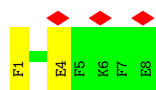
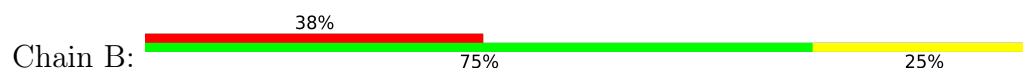
- Molecule 1: KFE8 peptide



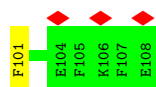
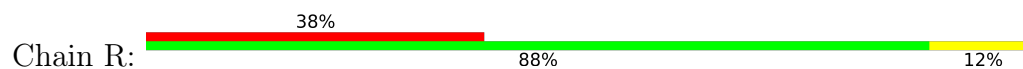
- Molecule 1: KFE8 peptide



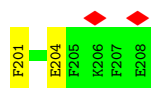
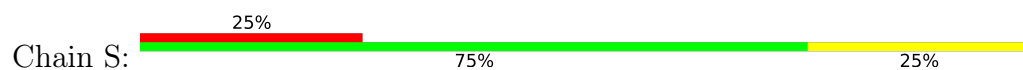
● Molecule 1: KFE8 peptide



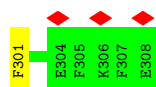
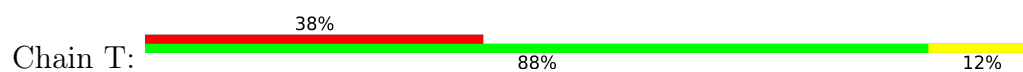
● Molecule 1: KFE8 peptide



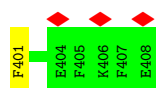
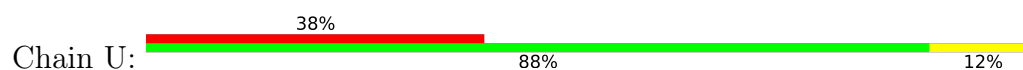
● Molecule 1: KFE8 peptide



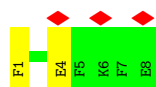
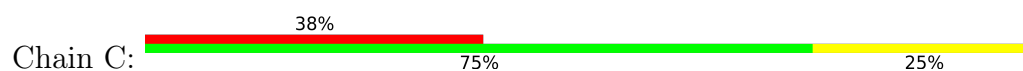
● Molecule 1: KFE8 peptide



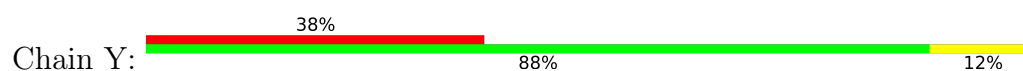
● Molecule 1: KFE8 peptide

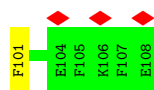


● Molecule 1: KFE8 peptide

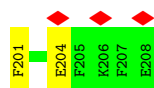
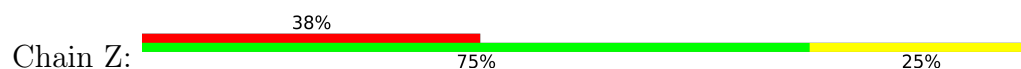


● Molecule 1: KFE8 peptide

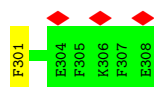
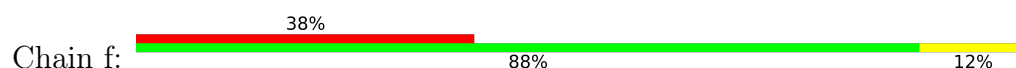




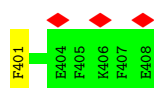
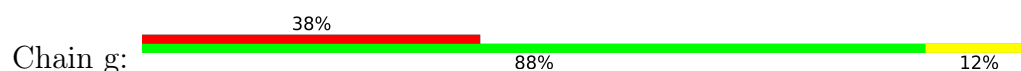
- Molecule 1: KFE8 peptide



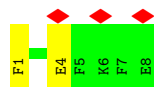
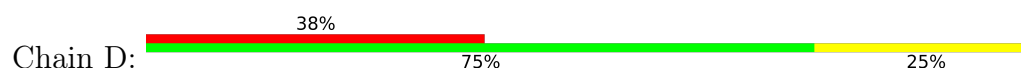
- Molecule 1: KFE8 peptide



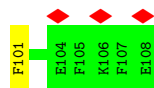
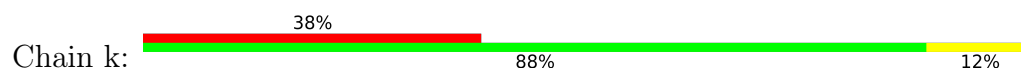
- Molecule 1: KFE8 peptide



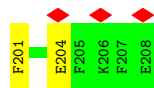
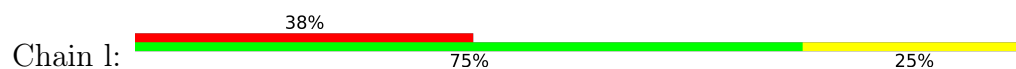
- Molecule 1: KFE8 peptide



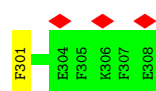
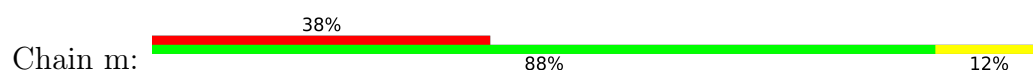
- Molecule 1: KFE8 peptide



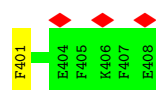
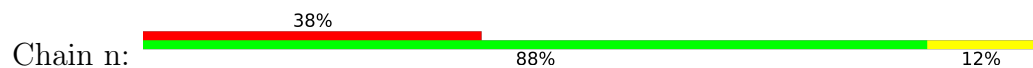
- Molecule 1: KFE8 peptide



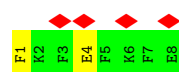
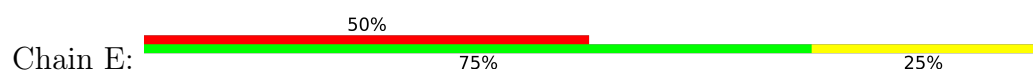
- Molecule 1: KFE8 peptide



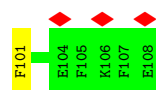
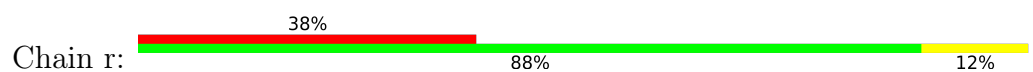
- Molecule 1: KFE8 peptide



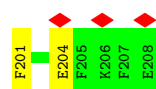
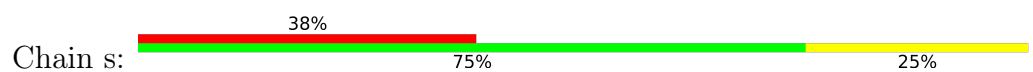
- Molecule 1: KFE8 peptide



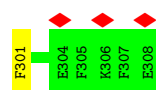
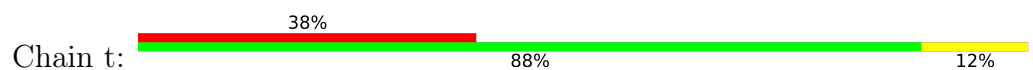
- Molecule 1: KFE8 peptide



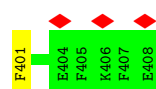
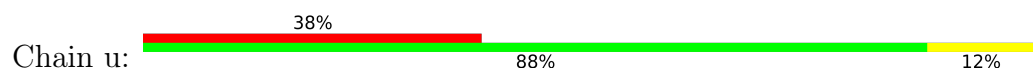
- Molecule 1: KFE8 peptide



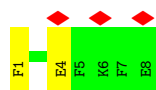
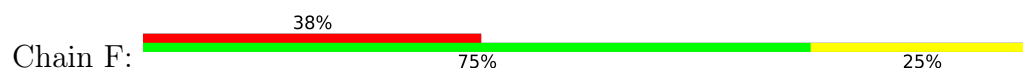
- Molecule 1: KFE8 peptide



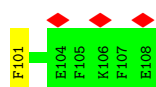
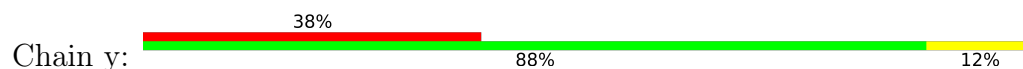
- Molecule 1: KFE8 peptide



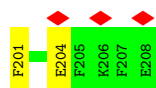
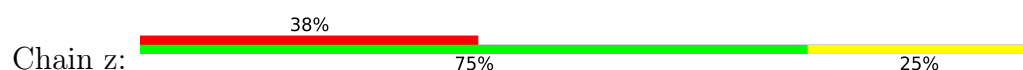
• Molecule 1: KFE8 peptide



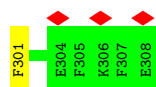
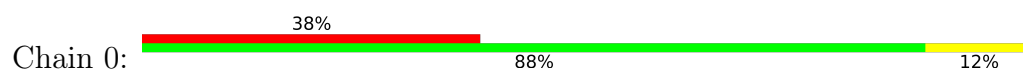
• Molecule 1: KFE8 peptide



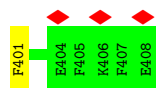
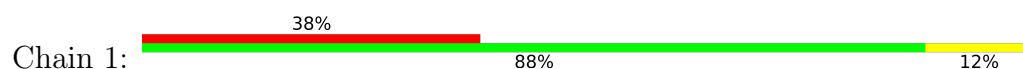
• Molecule 1: KFE8 peptide



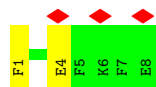
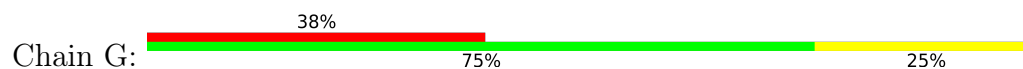
• Molecule 1: KFE8 peptide



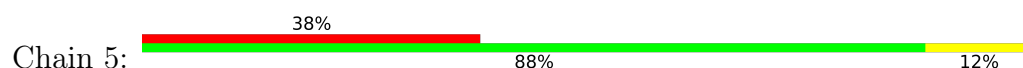
• Molecule 1: KFE8 peptide

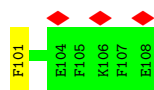


• Molecule 1: KFE8 peptide

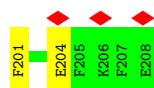
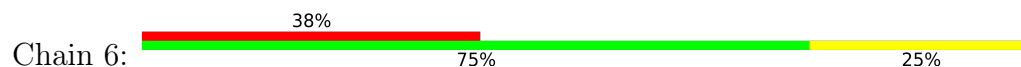


• Molecule 1: KFE8 peptide

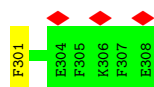
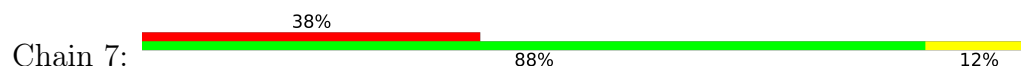




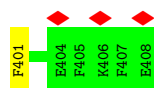
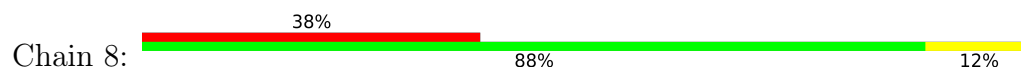
- Molecule 1: KFE8 peptide



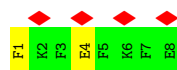
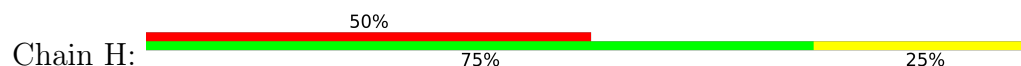
- Molecule 1: KFE8 peptide



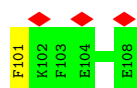
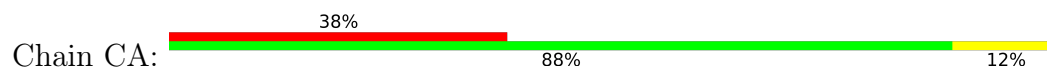
- Molecule 1: KFE8 peptide



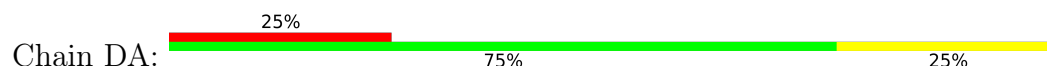
- Molecule 1: KFE8 peptide



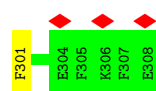
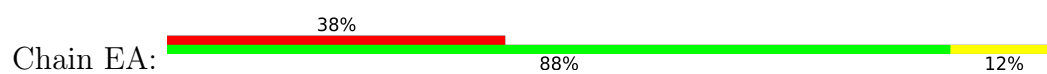
- Molecule 1: KFE8 peptide



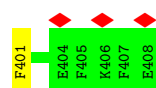
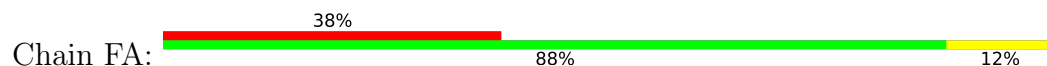
- Molecule 1: KFE8 peptide



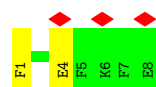
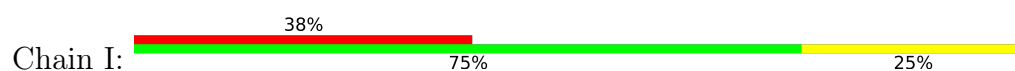
- Molecule 1: KFE8 peptide



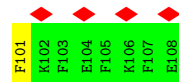
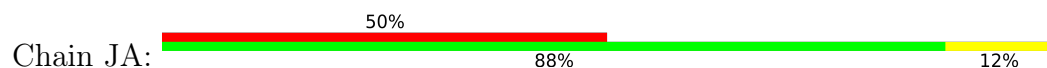
- Molecule 1: KFE8 peptide



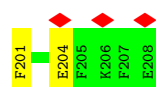
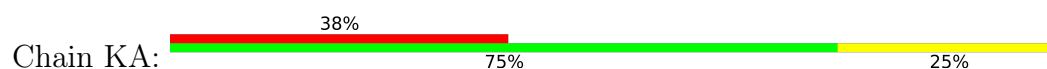
- Molecule 1: KFE8 peptide



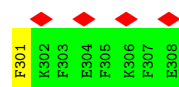
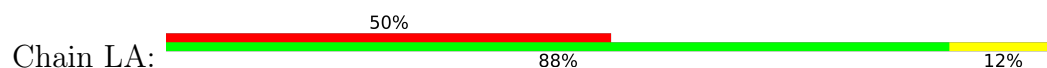
- Molecule 1: KFE8 peptide



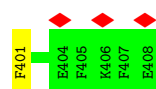
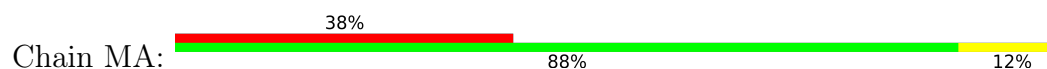
- Molecule 1: KFE8 peptide



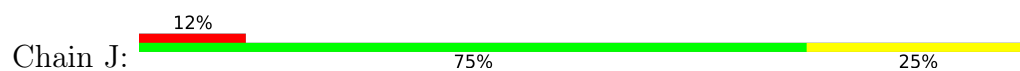
- Molecule 1: KFE8 peptide



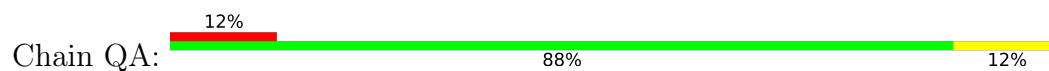
- Molecule 1: KFE8 peptide



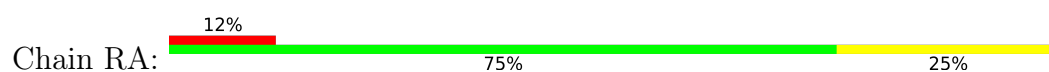
- Molecule 1: KFE8 peptide



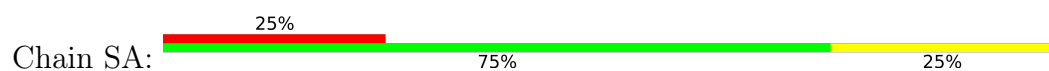
- Molecule 1: KFE8 peptide



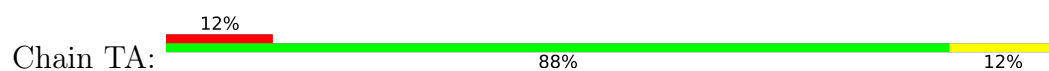
- Molecule 1: KFE8 peptide



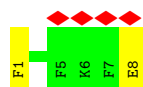
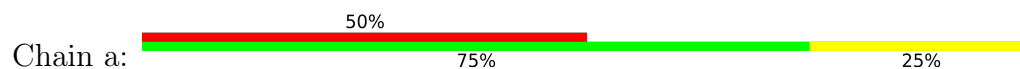
- Molecule 1: KFE8 peptide



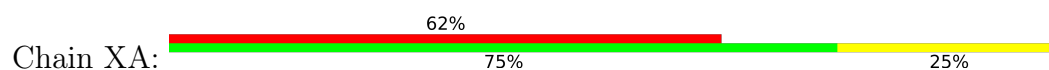
- Molecule 1: KFE8 peptide

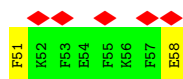


- Molecule 1: KFE8 peptide

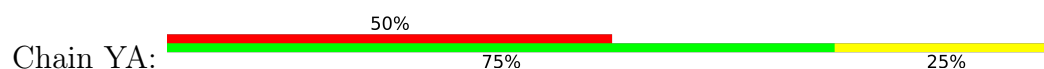


- Molecule 1: KFE8 peptide

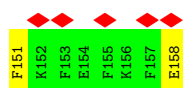
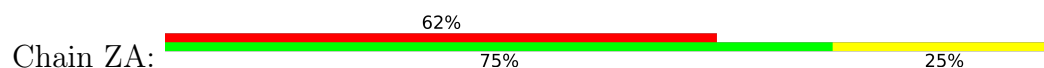




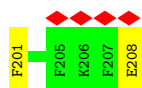
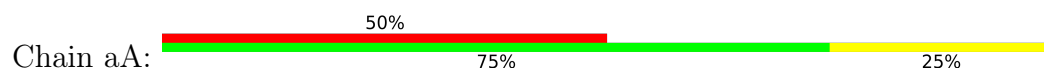
- Molecule 1: KFE8 peptide



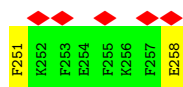
- Molecule 1: KFE8 peptide



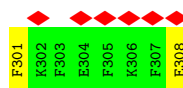
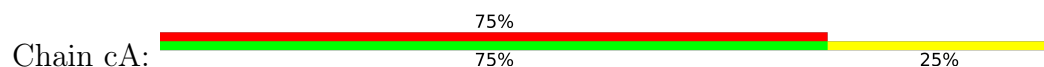
- Molecule 1: KFE8 peptide



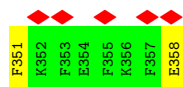
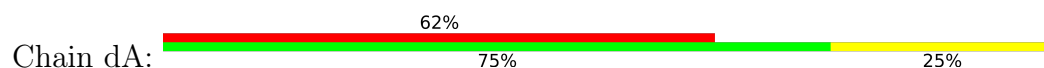
- Molecule 1: KFE8 peptide



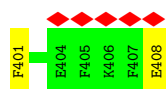
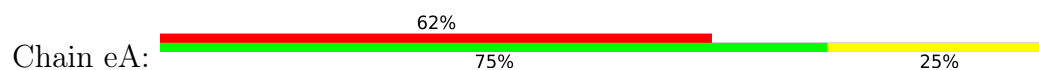
- Molecule 1: KFE8 peptide



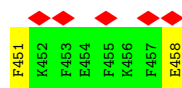
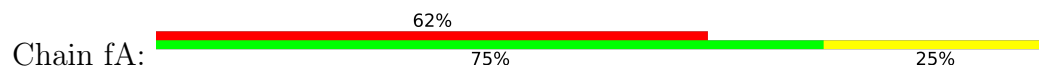
- Molecule 1: KFE8 peptide



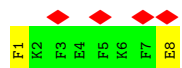
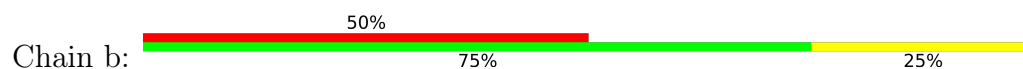
- Molecule 1: KFE8 peptide



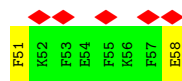
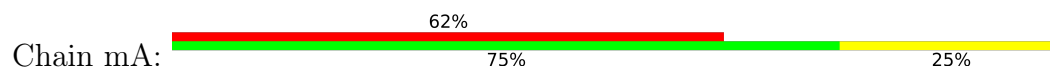
- Molecule 1: KFE8 peptide



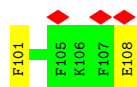
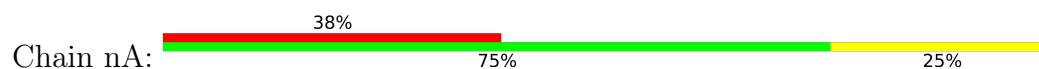
- Molecule 1: KFE8 peptide



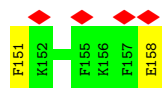
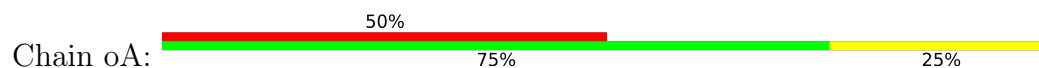
- Molecule 1: KFE8 peptide



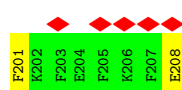
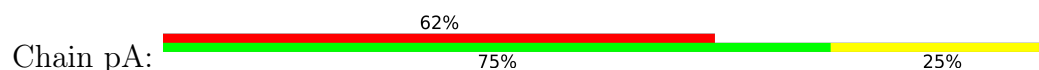
- Molecule 1: KFE8 peptide



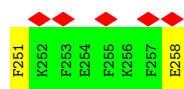
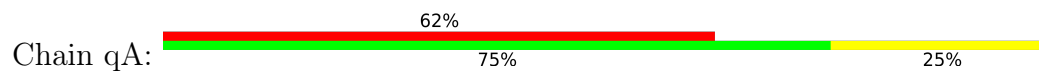
- Molecule 1: KFE8 peptide



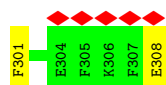
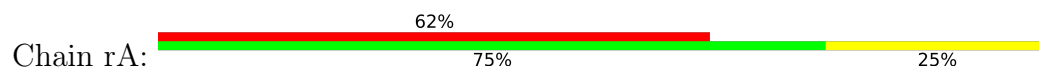
- Molecule 1: KFE8 peptide



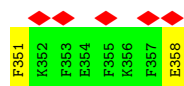
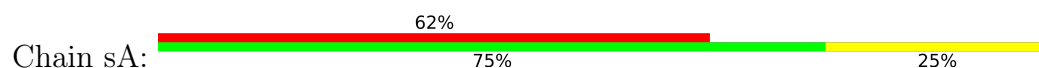
- Molecule 1: KFE8 peptide



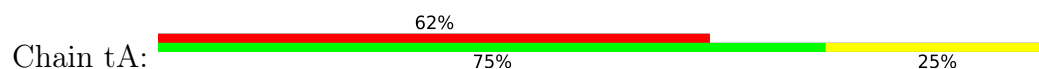
- Molecule 1: KFE8 peptide



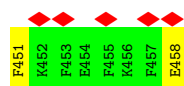
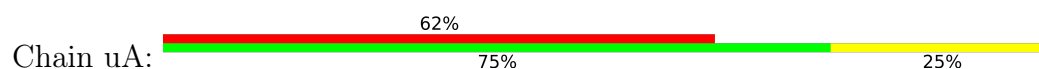
- Molecule 1: KFE8 peptide



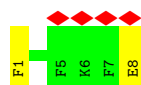
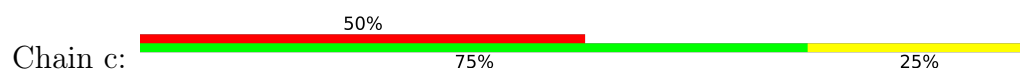
- Molecule 1: KFE8 peptide



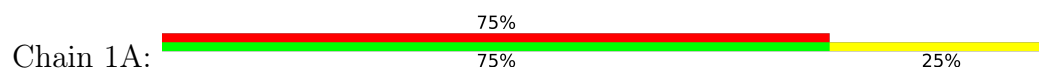
- Molecule 1: KFE8 peptide

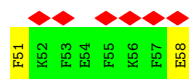


- Molecule 1: KFE8 peptide

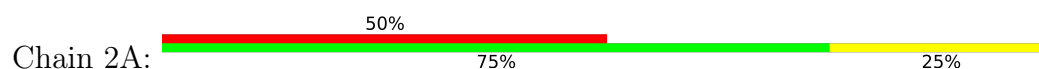


- Molecule 1: KFE8 peptide

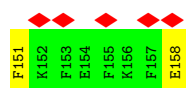
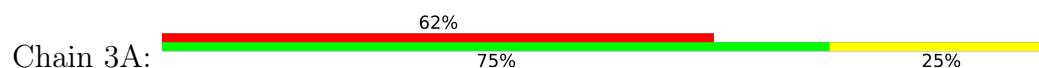




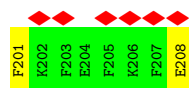
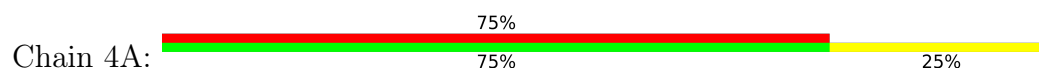
- Molecule 1: KFE8 peptide



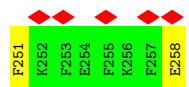
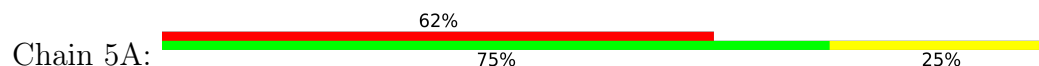
- Molecule 1: KFE8 peptide



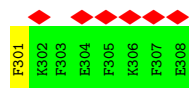
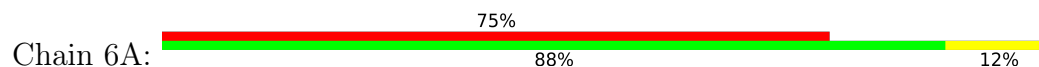
- Molecule 1: KFE8 peptide



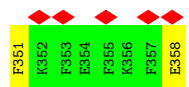
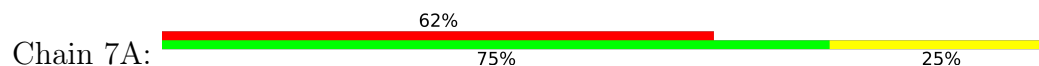
- Molecule 1: KFE8 peptide



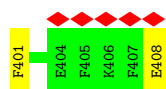
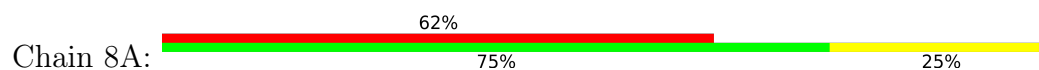
- Molecule 1: KFE8 peptide



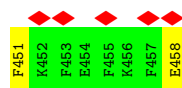
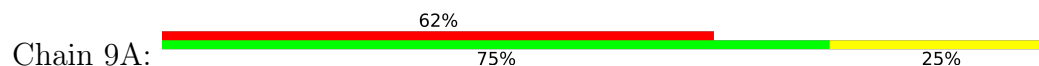
- Molecule 1: KFE8 peptide



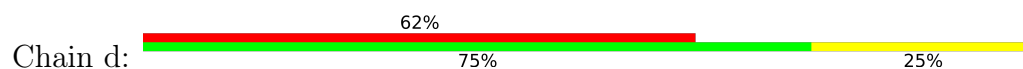
- Molecule 1: KFE8 peptide



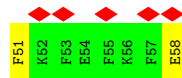
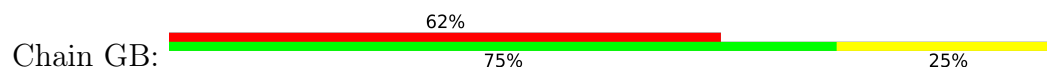
- Molecule 1: KFE8 peptide



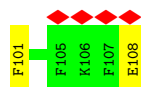
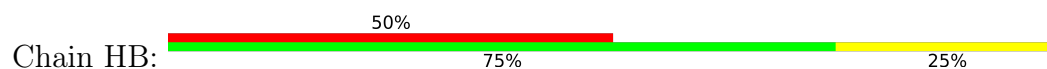
- Molecule 1: KFE8 peptide



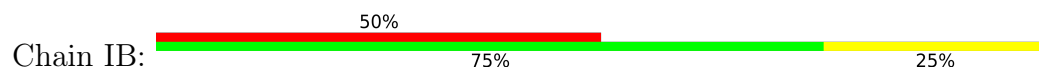
- Molecule 1: KFE8 peptide



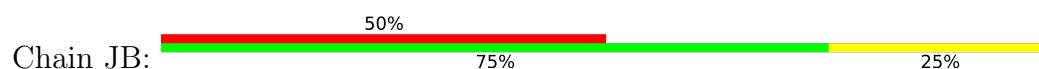
- Molecule 1: KFE8 peptide



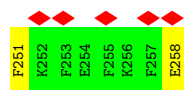
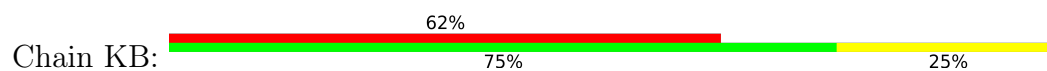
- Molecule 1: KFE8 peptide



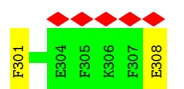
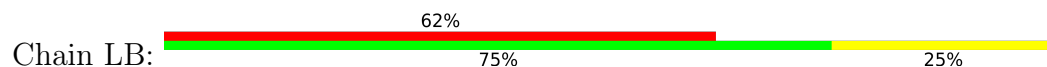
- Molecule 1: KFE8 peptide



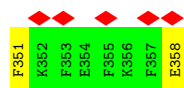
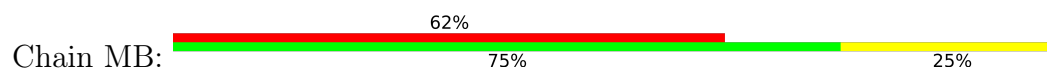
- Molecule 1: KFE8 peptide



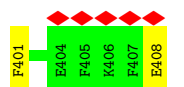
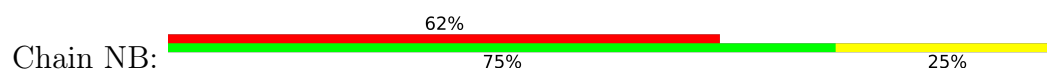
- Molecule 1: KFE8 peptide



- Molecule 1: KFE8 peptide



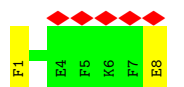
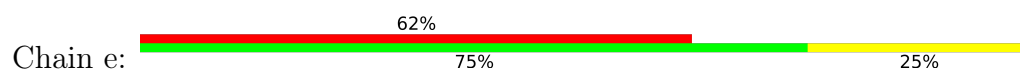
- Molecule 1: KFE8 peptide



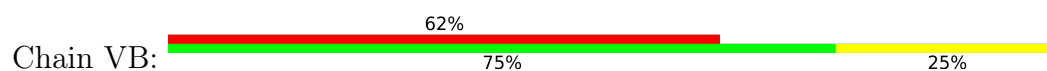
- Molecule 1: KFE8 peptide

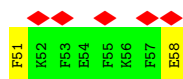


- Molecule 1: KFE8 peptide

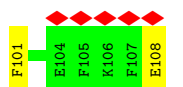
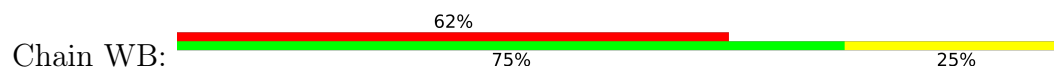


- Molecule 1: KFE8 peptide

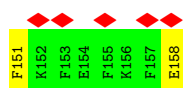
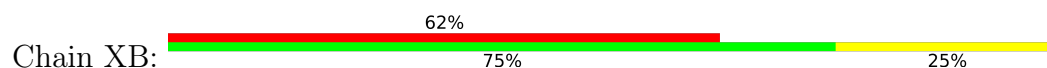




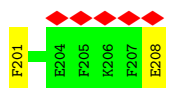
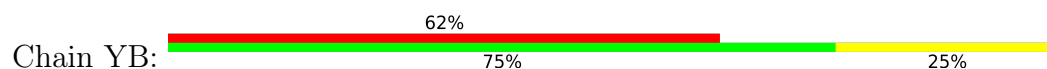
- Molecule 1: KFE8 peptide



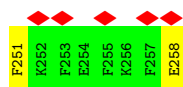
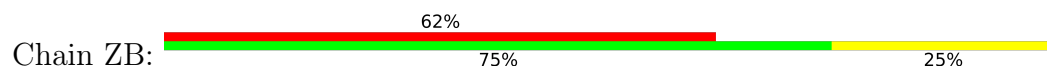
- Molecule 1: KFE8 peptide



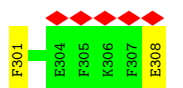
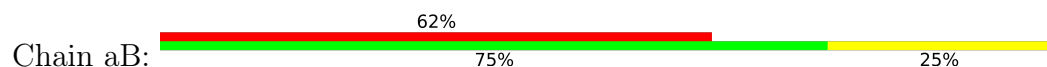
- Molecule 1: KFE8 peptide



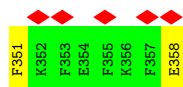
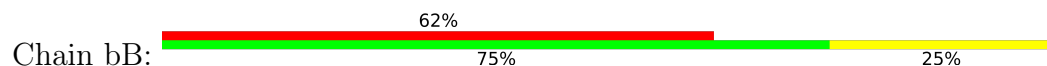
- Molecule 1: KFE8 peptide



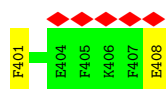
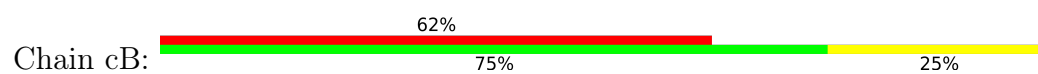
- Molecule 1: KFE8 peptide



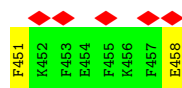
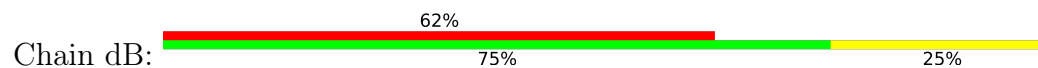
- Molecule 1: KFE8 peptide



- Molecule 1: KFE8 peptide



- Molecule 1: KFE8 peptide



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-6.4°, rise=3.95 Å, axial sym=C5	Depositor
Number of segments used	50655	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	0.001	Depositor
Minimum map value	-0.001	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.000	Depositor
Recommended contour level	0.000542	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	0.56	0/62	0.36	0/79
1	1	0.53	0/62	0.34	0/79
1	1A	0.33	0/62	0.48	0/79
1	2A	0.47	0/62	0.47	0/79
1	3A	0.33	0/62	0.50	0/79
1	4A	0.46	0/62	0.52	0/79
1	5	0.59	0/62	0.35	0/79
1	5A	0.33	0/62	0.47	0/79
1	6	0.55	0/62	0.37	0/79
1	6A	0.45	0/62	0.44	0/79
1	7	0.55	0/62	0.36	0/79
1	7A	0.31	0/62	0.48	0/79
1	8	0.53	0/62	0.35	0/79
1	8A	0.47	0/62	0.44	0/79
1	9A	0.32	0/62	0.48	0/79
1	A	0.58	0/62	0.51	0/79
1	B	0.57	0/62	0.51	0/79
1	C	0.58	0/62	0.51	0/79
1	CA	0.59	0/62	0.36	0/79
1	D	0.57	0/62	0.51	0/79
1	DA	0.56	0/62	0.37	0/79
1	E	0.57	0/62	0.51	0/79
1	EA	0.56	0/62	0.36	0/79
1	F	0.58	0/62	0.51	0/79
1	FA	0.53	0/62	0.35	0/79
1	G	0.58	0/62	0.50	0/79
1	GB	0.33	0/62	0.48	0/79
1	H	0.57	0/62	0.51	0/79
1	HB	0.47	0/62	0.47	0/79
1	I	0.57	0/62	0.51	0/79
1	IB	0.33	0/62	0.50	0/79
1	J	0.58	0/62	0.51	0/79

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	JA	0.59	0/62	0.36	0/79
1	JB	0.46	0/62	0.52	0/79
1	K	0.58	0/62	0.36	0/79
1	KA	0.56	0/62	0.38	0/79
1	KB	0.33	0/62	0.47	0/79
1	L	0.56	0/62	0.37	0/79
1	LA	0.56	0/62	0.35	0/79
1	LB	0.45	0/62	0.44	0/79
1	M	0.56	0/62	0.35	0/79
1	MA	0.53	0/62	0.35	0/79
1	MB	0.31	0/62	0.48	0/79
1	N	0.53	0/62	0.34	0/79
1	NB	0.46	0/62	0.44	0/79
1	OB	0.32	0/62	0.48	0/79
1	QA	0.59	0/62	0.36	0/79
1	R	0.59	0/62	0.36	0/79
1	RA	0.56	0/62	0.38	0/79
1	S	0.56	0/62	0.37	0/79
1	SA	0.56	0/62	0.36	0/79
1	T	0.56	0/62	0.36	0/79
1	TA	0.53	0/62	0.35	0/79
1	U	0.53	0/62	0.35	0/79
1	VB	0.33	0/62	0.48	0/79
1	WB	0.47	0/62	0.46	0/79
1	XA	0.33	0/62	0.48	0/79
1	XB	0.33	0/62	0.50	0/79
1	Y	0.59	0/62	0.35	0/79
1	YA	0.48	0/62	0.46	0/79
1	YB	0.46	0/62	0.51	0/79
1	Z	0.56	0/62	0.38	0/79
1	ZA	0.33	0/62	0.49	0/79
1	ZB	0.32	0/62	0.47	0/79
1	a	0.47	0/62	0.46	0/79
1	aA	0.46	0/62	0.52	0/79
1	aB	0.45	0/62	0.44	0/79
1	b	0.47	0/62	0.47	0/79
1	bA	0.32	0/62	0.47	0/79
1	bB	0.31	0/62	0.48	0/79
1	c	0.47	0/62	0.46	0/79
1	cA	0.45	0/62	0.44	0/79
1	cB	0.46	0/62	0.44	0/79
1	d	0.47	0/62	0.47	0/79
1	dA	0.30	0/62	0.48	0/79

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	dB	0.32	0/62	0.48	0/79
1	e	0.47	0/62	0.47	0/79
1	eA	0.46	0/62	0.44	0/79
1	f	0.56	0/62	0.36	0/79
1	fA	0.32	0/62	0.48	0/79
1	g	0.53	0/62	0.34	0/79
1	k	0.59	0/62	0.35	0/79
1	l	0.56	0/62	0.38	0/79
1	m	0.56	0/62	0.36	0/79
1	mA	0.33	0/62	0.48	0/79
1	n	0.53	0/62	0.34	0/79
1	nA	0.47	0/62	0.46	0/79
1	oA	0.33	0/62	0.49	0/79
1	pA	0.46	0/62	0.52	0/79
1	qA	0.33	0/62	0.47	0/79
1	r	0.59	0/62	0.36	0/79
1	rA	0.45	0/62	0.44	0/79
1	s	0.55	0/62	0.38	0/79
1	sA	0.30	0/62	0.49	0/79
1	t	0.56	0/62	0.36	0/79
1	tA	0.46	0/62	0.44	0/79
1	u	0.53	0/62	0.35	0/79
1	uA	0.32	0/62	0.48	0/79
1	y	0.58	0/62	0.36	0/79
1	z	0.56	0/62	0.37	0/79
All	All	0.49	0/6200	0.44	0/7900

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles

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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	6/8 (75%)	6 (100%)	0	0	100	100
1	GB	6/8 (75%)	6 (100%)	0	0	100	100
1	H	6/8 (75%)	6 (100%)	0	0	100	100
1	HB	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	I	6/8 (75%)	6 (100%)	0	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%)	6 (100%)	0	0	100	100
1	KA	6/8 (75%)	6 (100%)	0	0	100	100
1	KB	6/8 (75%)	6 (100%)	0	0	100	100
1	L	6/8 (75%)	6 (100%)	0	0	100	100
1	LA	6/8 (75%)	6 (100%)	0	0	100	100
1	LB	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	M	6/8 (75%)	6 (100%)	0	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	NB	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	OB	6/8 (75%)	6 (100%)	0	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%)	6 (100%)	0	0	100	100
1	SA	6/8 (75%)	6 (100%)	0	0	100	100
1	T	6/8 (75%)	6 (100%)	0	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	VB	6/8 (75%)	6 (100%)	0	0	100	100
1	WB	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	XA	6/8 (75%)	6 (100%)	0	0	100	100
1	XB	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%)	5 (83%)	1 (17%)	0	100	100
1	YB	6/8 (75%)	6 (100%)	0	0	100	100
1	Z	6/8 (75%)	6 (100%)	0	0	100	100
1	ZA	6/8 (75%)	6 (100%)	0	0	100	100
1	ZB	6/8 (75%)	6 (100%)	0	0	100	100
1	a	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	aA	6/8 (75%)	6 (100%)	0	0	100	100
1	aB	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	b	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	bA	6/8 (75%)	6 (100%)	0	0	100	100
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%)	5 (83%)	1 (17%)	0	100	100
1	cB	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	d	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	dA	6/8 (75%)	6 (100%)	0	0	100	100
1	dB	6/8 (75%)	6 (100%)	0	0	100	100
1	e	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	eA	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
1	f	6/8 (75%)	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	k	6/8 (75%)	6 (100%)	0	0	100	100
1	l	6/8 (75%)	6 (100%)	0	0	100	100
1	m	6/8 (75%)	6 (100%)	0	0	100	100
1	mA	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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	oA	6/8 (75%)	6 (100%)	0	0	100	100
1	pA	6/8 (75%)	6 (100%)	0	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%)	5 (83%)	1 (17%)	0	100	100
1	s	6/8 (75%)	6 (100%)	0	0	100	100
1	sA	6/8 (75%)	6 (100%)	0	0	100	100
1	t	6/8 (75%)	6 (100%)	0	0	100	100
1	tA	6/8 (75%)	5 (83%)	1 (17%)	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	y	6/8 (75%)	6 (100%)	0	0	100	100
1	z	6/8 (75%)	6 (100%)	0	0	100	100
All	All	600/800 (75%)	580 (97%)	20 (3%)	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%)	6 (100%)	0	100	100
1	1	6/6 (100%)	6 (100%)	0	100	100
1	1A	6/6 (100%)	6 (100%)	0	100	100
1	2A	6/6 (100%)	6 (100%)	0	100	100
1	3A	6/6 (100%)	6 (100%)	0	100	100
1	4A	6/6 (100%)	6 (100%)	0	100	100
1	5	6/6 (100%)	6 (100%)	0	100	100
1	5A	6/6 (100%)	6 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	6	6/6 (100%)	5 (83%)	1 (17%)	2	12
1	6A	6/6 (100%)	6 (100%)	0	100	100
1	7	6/6 (100%)	6 (100%)	0	100	100
1	7A	6/6 (100%)	6 (100%)	0	100	100
1	8	6/6 (100%)	6 (100%)	0	100	100
1	8A	6/6 (100%)	6 (100%)	0	100	100
1	9A	6/6 (100%)	6 (100%)	0	100	100
1	A	6/6 (100%)	5 (83%)	1 (17%)	2	12
1	B	6/6 (100%)	5 (83%)	1 (17%)	2	12
1	C	6/6 (100%)	5 (83%)	1 (17%)	2	12
1	CA	6/6 (100%)	6 (100%)	0	100	100
1	D	6/6 (100%)	5 (83%)	1 (17%)	2	12
1	DA	6/6 (100%)	5 (83%)	1 (17%)	2	12
1	E	6/6 (100%)	5 (83%)	1 (17%)	2	12
1	EA	6/6 (100%)	6 (100%)	0	100	100
1	F	6/6 (100%)	5 (83%)	1 (17%)	2	12
1	FA	6/6 (100%)	6 (100%)	0	100	100
1	G	6/6 (100%)	5 (83%)	1 (17%)	2	12
1	GB	6/6 (100%)	6 (100%)	0	100	100
1	H	6/6 (100%)	5 (83%)	1 (17%)	2	12
1	HB	6/6 (100%)	6 (100%)	0	100	100
1	I	6/6 (100%)	5 (83%)	1 (17%)	2	12
1	IB	6/6 (100%)	6 (100%)	0	100	100
1	J	6/6 (100%)	5 (83%)	1 (17%)	2	12
1	JA	6/6 (100%)	6 (100%)	0	100	100
1	JB	6/6 (100%)	6 (100%)	0	100	100
1	K	6/6 (100%)	6 (100%)	0	100	100
1	KA	6/6 (100%)	5 (83%)	1 (17%)	2	12
1	KB	6/6 (100%)	6 (100%)	0	100	100
1	L	6/6 (100%)	5 (83%)	1 (17%)	2	12
1	LA	6/6 (100%)	6 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	LB	6/6 (100%)	6 (100%)	0	100	100
1	M	6/6 (100%)	6 (100%)	0	100	100
1	MA	6/6 (100%)	6 (100%)	0	100	100
1	MB	6/6 (100%)	6 (100%)	0	100	100
1	N	6/6 (100%)	6 (100%)	0	100	100
1	NB	6/6 (100%)	6 (100%)	0	100	100
1	OB	6/6 (100%)	6 (100%)	0	100	100
1	QA	6/6 (100%)	6 (100%)	0	100	100
1	R	6/6 (100%)	6 (100%)	0	100	100
1	RA	6/6 (100%)	5 (83%)	1 (17%)	2	12
1	S	6/6 (100%)	5 (83%)	1 (17%)	2	12
1	SA	6/6 (100%)	6 (100%)	0	100	100
1	T	6/6 (100%)	6 (100%)	0	100	100
1	TA	6/6 (100%)	6 (100%)	0	100	100
1	U	6/6 (100%)	6 (100%)	0	100	100
1	VB	6/6 (100%)	6 (100%)	0	100	100
1	WB	6/6 (100%)	6 (100%)	0	100	100
1	XA	6/6 (100%)	6 (100%)	0	100	100
1	XB	6/6 (100%)	6 (100%)	0	100	100
1	Y	6/6 (100%)	6 (100%)	0	100	100
1	YA	6/6 (100%)	6 (100%)	0	100	100
1	YB	6/6 (100%)	6 (100%)	0	100	100
1	Z	6/6 (100%)	5 (83%)	1 (17%)	2	12
1	ZA	6/6 (100%)	6 (100%)	0	100	100
1	ZB	6/6 (100%)	6 (100%)	0	100	100
1	a	6/6 (100%)	6 (100%)	0	100	100
1	aA	6/6 (100%)	6 (100%)	0	100	100
1	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%)	6 (100%)	0	100	100
1	cB	6/6 (100%)	6 (100%)	0	100	100
1	d	6/6 (100%)	6 (100%)	0	100	100
1	dA	6/6 (100%)	6 (100%)	0	100	100
1	dB	6/6 (100%)	6 (100%)	0	100	100
1	e	6/6 (100%)	6 (100%)	0	100	100
1	eA	6/6 (100%)	6 (100%)	0	100	100
1	f	6/6 (100%)	6 (100%)	0	100	100
1	fA	6/6 (100%)	6 (100%)	0	100	100
1	g	6/6 (100%)	6 (100%)	0	100	100
1	k	6/6 (100%)	6 (100%)	0	100	100
1	l	6/6 (100%)	5 (83%)	1 (17%)	2	12
1	m	6/6 (100%)	6 (100%)	0	100	100
1	mA	6/6 (100%)	6 (100%)	0	100	100
1	n	6/6 (100%)	6 (100%)	0	100	100
1	nA	6/6 (100%)	6 (100%)	0	100	100
1	oA	6/6 (100%)	6 (100%)	0	100	100
1	pA	6/6 (100%)	6 (100%)	0	100	100
1	qA	6/6 (100%)	6 (100%)	0	100	100
1	r	6/6 (100%)	6 (100%)	0	100	100
1	rA	6/6 (100%)	6 (100%)	0	100	100
1	s	6/6 (100%)	5 (83%)	1 (17%)	2	12
1	sA	6/6 (100%)	6 (100%)	0	100	100
1	t	6/6 (100%)	6 (100%)	0	100	100
1	tA	6/6 (100%)	6 (100%)	0	100	100
1	u	6/6 (100%)	6 (100%)	0	100	100
1	uA	6/6 (100%)	6 (100%)	0	100	100
1	y	6/6 (100%)	6 (100%)	0	100	100
1	z	6/6 (100%)	5 (83%)	1 (17%)	2	12
All	All	600/600 (100%)	580 (97%)	20 (3%)	41	68

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	L	204	GLU
1	B	4	GLU
1	S	204	GLU
1	C	4	GLU
1	Z	204	GLU
1	D	4	GLU
1	l	204	GLU
1	E	4	GLU
1	s	204	GLU
1	F	4	GLU
1	z	204	GLU
1	G	4	GLU
1	6	204	GLU
1	H	4	GLU
1	DA	204	GLU
1	I	4	GLU
1	KA	204	GLU
1	J	4	GLU
1	RA	204	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 ⓘ

200 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	1	401	1	13,14,15	1.19	2 (15%)	16,17,19	1.60	3 (18%)
1	GMA	B	8	1	9,9,9	1.17	0	10,11,11	1.15	0
1	GMA	JB	208	1	9,9,9	1.17	1 (11%)	10,11,11	1.26	2 (20%)
1	5CR	g	401	1	13,14,15	1.19	2 (15%)	16,17,19	1.60	3 (18%)
1	GMA	pA	208	1	9,9,9	1.16	0	10,11,11	1.24	1 (10%)
1	GMA	HB	108	1	9,9,9	1.16	1 (11%)	10,11,11	1.24	2 (20%)
1	5CR	F	1	1	13,14,15	1.19	2 (15%)	16,17,19	1.48	3 (18%)
1	5CR	NB	401	1	13,14,15	1.23	1 (7%)	16,17,19	1.05	0
1	5CR	GB	51	1	13,14,15	1.21	2 (15%)	16,17,19	1.23	2 (12%)
1	5CR	8A	401	1	13,14,15	1.23	1 (7%)	16,17,19	1.04	0
1	GMA	dA	358	1	9,9,9	1.14	0	10,11,11	1.22	1 (10%)
1	5CR	S	201	1	13,14,15	1.20	2 (15%)	16,17,19	1.40	3 (18%)
1	5CR	E	1	1	13,14,15	1.19	2 (15%)	16,17,19	1.48	3 (18%)
1	5CR	a	1	1	13,14,15	1.22	1 (7%)	16,17,19	1.02	0
1	5CR	aB	301	1	13,14,15	1.22	1 (7%)	16,17,19	0.95	0
1	GMA	K	108	1	9,9,9	1.15	0	10,11,11	1.15	0
1	5CR	J	1	1	13,14,15	1.20	2 (15%)	16,17,19	1.48	3 (18%)
1	5CR	mA	51	1	13,14,15	1.20	1 (7%)	16,17,19	1.23	2 (12%)
1	GMA	u	408	1	9,9,9	1.16	0	10,11,11	1.09	0
1	5CR	H	1	1	13,14,15	1.19	2 (15%)	16,17,19	1.48	3 (18%)
1	GMA	n	408	1	9,9,9	1.17	0	10,11,11	1.09	0
1	GMA	e	8	1	9,9,9	1.16	1 (11%)	10,11,11	1.23	1 (10%)
1	5CR	qA	251	1	13,14,15	1.19	1 (7%)	16,17,19	1.21	2 (12%)
1	5CR	y	101	1	13,14,15	1.19	2 (15%)	16,17,19	1.40	3 (18%)
1	5CR	KA	201	1	13,14,15	1.20	2 (15%)	16,17,19	1.39	3 (18%)
1	GMA	QA	108	1	9,9,9	1.16	0	10,11,11	1.16	0
1	GMA	fA	458	1	9,9,9	1.16	1 (11%)	10,11,11	1.23	2 (20%)
1	GMA	8	408	1	9,9,9	1.17	0	10,11,11	1.10	0
1	5CR	D	1	1	13,14,15	1.19	2 (15%)	16,17,19	1.47	3 (18%)
1	5CR	MB	351	1	13,14,15	1.20	2 (15%)	16,17,19	1.19	2 (12%)
1	5CR	YB	201	1	13,14,15	1.23	1 (7%)	16,17,19	1.01	1 (6%)
1	GMA	aA	208	1	9,9,9	1.17	1 (11%)	10,11,11	1.24	2 (20%)
1	5CR	OB	451	1	13,14,15	1.20	1 (7%)	16,17,19	1.25	2 (12%)
1	GMA	Z	208	1	9,9,9	1.16	0	10,11,11	1.09	0
1	GMA	C	8	1	9,9,9	1.17	0	10,11,11	1.14	0
1	GMA	z	208	1	9,9,9	1.16	0	10,11,11	1.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	GMA	5A	258	1	9,9,9	1.15	0	10,11,11	1.23	1 (10%)
1	GMA	XA	58	1	9,9,9	1.15	1 (11%)	10,11,11	1.22	1 (10%)
1	GMA	f	308	1	9,9,9	1.15	0	10,11,11	1.06	0
1	GMA	NB	408	1	9,9,9	1.17	0	10,11,11	1.23	1 (10%)
1	GMA	9A	458	1	9,9,9	1.15	0	10,11,11	1.23	2 (20%)
1	5CR	KB	251	1	13,14,15	1.20	1 (7%)	16,17,19	1.21	2 (12%)
1	GMA	oA	158	1	9,9,9	1.15	0	10,11,11	1.24	1 (10%)
1	5CR	uA	451	1	13,14,15	1.20	1 (7%)	16,17,19	1.25	2 (12%)
1	GMA	aB	308	1	9,9,9	1.17	1 (11%)	10,11,11	1.21	0
1	5CR	z	201	1	13,14,15	1.20	2 (15%)	16,17,19	1.40	3 (18%)
1	5CR	HB	101	1	13,14,15	1.22	1 (7%)	16,17,19	1.01	0
1	GMA	RA	208	1	9,9,9	1.16	0	10,11,11	1.08	0
1	GMA	m	308	1	9,9,9	1.14	0	10,11,11	1.05	0
1	5CR	YA	101	1	13,14,15	1.23	1 (7%)	16,17,19	1.01	0
1	5CR	I	1	1	13,14,15	1.20	2 (15%)	16,17,19	1.47	3 (18%)
1	5CR	LA	301	1	13,14,15	1.19	2 (15%)	16,17,19	1.49	3 (18%)
1	5CR	t	301	1	13,14,15	1.19	2 (15%)	16,17,19	1.50	3 (18%)
1	5CR	TA	401	1	13,14,15	1.19	2 (15%)	16,17,19	1.60	3 (18%)
1	GMA	U	408	1	9,9,9	1.17	0	10,11,11	1.09	0
1	GMA	a	8	1	9,9,9	1.17	1 (11%)	10,11,11	1.23	1 (10%)
1	GMA	5	108	1	9,9,9	1.16	0	10,11,11	1.16	0
1	5CR	3A	151	1	13,14,15	1.21	2 (15%)	16,17,19	1.21	2 (12%)
1	GMA	Y	108	1	9,9,9	1.16	0	10,11,11	1.16	0
1	GMA	KB	258	1	9,9,9	1.15	1 (11%)	10,11,11	1.23	2 (20%)
1	GMA	M	308	1	9,9,9	1.15	0	10,11,11	1.05	0
1	GMA	bB	358	1	9,9,9	1.15	1 (11%)	10,11,11	1.22	1 (10%)
1	5CR	u	401	1	13,14,15	1.20	2 (15%)	16,17,19	1.59	3 (18%)
1	5CR	JB	201	1	13,14,15	1.23	1 (7%)	16,17,19	1.00	1 (6%)
1	5CR	5	101	1	13,14,15	1.20	2 (15%)	16,17,19	1.40	3 (18%)
1	5CR	b	1	1	13,14,15	1.22	1 (7%)	16,17,19	1.02	0
1	5CR	9A	451	1	13,14,15	1.20	1 (7%)	16,17,19	1.26	2 (12%)
1	GMA	r	108	1	9,9,9	1.15	0	10,11,11	1.15	0
1	GMA	d	8	1	9,9,9	1.17	1 (11%)	10,11,11	1.22	1 (10%)
1	5CR	nA	101	1	13,14,15	1.22	1 (7%)	16,17,19	1.01	0
1	5CR	LB	301	1	13,14,15	1.22	1 (7%)	16,17,19	0.95	0
1	5CR	5A	251	1	13,14,15	1.20	1 (7%)	16,17,19	1.21	2 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	GMA	CA	108	1	9,9,9	1.16	0	10,11,11	1.15	0
1	GMA	E	8	1	9,9,9	1.17	0	10,11,11	1.15	0
1	GMA	G	8	1	9,9,9	1.17	0	10,11,11	1.15	0
1	GMA	DA	208	1	9,9,9	1.16	0	10,11,11	1.08	0
1	GMA	JA	108	1	9,9,9	1.16	0	10,11,11	1.16	0
1	GMA	3A	158	1	9,9,9	1.15	1 (11%)	10,11,11	1.24	1 (10%)
1	5CR	n	401	1	13,14,15	1.19	2 (15%)	16,17,19	1.60	3 (18%)
1	5CR	dA	351	1	13,14,15	1.21	2 (15%)	16,17,19	1.18	2 (12%)
1	5CR	L	201	1	13,14,15	1.19	2 (15%)	16,17,19	1.40	3 (18%)
1	5CR	IB	151	1	13,14,15	1.21	2 (15%)	16,17,19	1.21	2 (12%)
1	5CR	ZA	151	1	13,14,15	1.21	2 (15%)	16,17,19	1.21	2 (12%)
1	5CR	Z	201	1	13,14,15	1.19	2 (15%)	16,17,19	1.40	3 (18%)
1	5CR	eA	401	1	13,14,15	1.22	1 (7%)	16,17,19	1.04	0
1	GMA	MA	408	1	9,9,9	1.16	0	10,11,11	1.09	0
1	5CR	0	301	1	13,14,15	1.19	2 (15%)	16,17,19	1.49	3 (18%)
1	GMA	N	408	1	9,9,9	1.16	0	10,11,11	1.09	0
1	GMA	4A	208	1	9,9,9	1.17	1 (11%)	10,11,11	1.25	2 (20%)
1	5CR	M	301	1	13,14,15	1.19	2 (15%)	16,17,19	1.49	3 (18%)
1	5CR	l	201	1	13,14,15	1.20	2 (15%)	16,17,19	1.41	3 (18%)
1	5CR	fA	451	1	13,14,15	1.20	1 (7%)	16,17,19	1.25	2 (12%)
1	5CR	f	301	1	13,14,15	1.19	2 (15%)	16,17,19	1.49	3 (18%)
1	GMA	0	308	1	9,9,9	1.15	0	10,11,11	1.06	0
1	GMA	tA	408	1	9,9,9	1.16	0	10,11,11	1.23	1 (10%)
1	5CR	K	101	1	13,14,15	1.20	2 (15%)	16,17,19	1.40	3 (18%)
1	5CR	VB	51	1	13,14,15	1.21	2 (15%)	16,17,19	1.22	2 (12%)
1	GMA	nA	108	1	9,9,9	1.17	0	10,11,11	1.24	1 (10%)
1	5CR	7	301	1	13,14,15	1.20	2 (15%)	16,17,19	1.50	3 (18%)
1	5CR	B	1	1	13,14,15	1.19	2 (15%)	16,17,19	1.48	3 (18%)
1	5CR	R	101	1	13,14,15	1.19	2 (15%)	16,17,19	1.40	3 (18%)
1	GMA	VB	58	1	9,9,9	1.14	0	10,11,11	1.23	1 (10%)
1	5CR	6	201	1	13,14,15	1.20	2 (15%)	16,17,19	1.40	3 (18%)
1	GMA	7	308	1	9,9,9	1.14	0	10,11,11	1.06	0
1	5CR	A	1	1	13,14,15	1.18	2 (15%)	16,17,19	1.48	3 (18%)
1	5CR	G	1	1	13,14,15	1.20	2 (15%)	16,17,19	1.47	3 (18%)
1	GMA	XB	158	1	9,9,9	1.15	0	10,11,11	1.24	2 (20%)
1	GMA	eA	408	1	9,9,9	1.17	0	10,11,11	1.23	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	GMA	dB	458	1	9,9,9	1.15	1 (11%)	10,11,11	1.24	2 (20%)
1	GMA	EA	308	1	9,9,9	1.15	0	10,11,11	1.06	0
1	GMA	ZB	258	1	9,9,9	1.16	1 (11%)	10,11,11	1.24	2 (20%)
1	5CR	bB	351	1	13,14,15	1.20	2 (15%)	16,17,19	1.18	2 (12%)
1	GMA	MB	358	1	9,9,9	1.16	1 (11%)	10,11,11	1.23	1 (10%)
1	GMA	l	208	1	9,9,9	1.16	0	10,11,11	1.09	0
1	5CR	1A	51	1	13,14,15	1.21	1 (7%)	16,17,19	1.23	2 (12%)
1	GMA	qA	258	1	9,9,9	1.16	1 (11%)	10,11,11	1.25	2 (20%)
1	GMA	cB	408	1	9,9,9	1.17	0	10,11,11	1.23	1 (10%)
1	5CR	WB	101	1	13,14,15	1.22	1 (7%)	16,17,19	1.01	1 (6%)
1	GMA	LA	308	1	9,9,9	1.15	0	10,11,11	1.06	0
1	5CR	sA	351	1	13,14,15	1.20	1 (7%)	16,17,19	1.19	2 (12%)
1	GMA	c	8	1	9,9,9	1.17	1 (11%)	10,11,11	1.22	1 (10%)
1	GMA	FA	408	1	9,9,9	1.16	0	10,11,11	1.09	0
1	5CR	m	301	1	13,14,15	1.19	2 (15%)	16,17,19	1.49	3 (18%)
1	5CR	oA	151	1	13,14,15	1.20	2 (15%)	16,17,19	1.21	2 (12%)
1	GMA	2A	108	1	9,9,9	1.16	0	10,11,11	1.24	1 (10%)
1	GMA	1A	58	1	9,9,9	1.15	0	10,11,11	1.22	1 (10%)
1	5CR	U	401	1	13,14,15	1.20	2 (15%)	16,17,19	1.60	3 (18%)
1	5CR	aA	201	1	13,14,15	1.23	1 (7%)	16,17,19	1.01	1 (6%)
1	5CR	N	401	1	13,14,15	1.19	2 (15%)	16,17,19	1.59	3 (18%)
1	GMA	S	208	1	9,9,9	1.17	0	10,11,11	1.10	0
1	5CR	r	101	1	13,14,15	1.20	2 (15%)	16,17,19	1.40	3 (18%)
1	5CR	EA	301	1	13,14,15	1.18	2 (15%)	16,17,19	1.49	3 (18%)
1	GMA	b	8	1	9,9,9	1.17	1 (11%)	10,11,11	1.23	1 (10%)
1	5CR	CA	101	1	13,14,15	1.20	2 (15%)	16,17,19	1.40	3 (18%)
1	GMA	A	8	1	9,9,9	1.17	0	10,11,11	1.14	0
1	GMA	8A	408	1	9,9,9	1.17	1 (11%)	10,11,11	1.23	1 (10%)
1	5CR	pA	201	1	13,14,15	1.24	1 (7%)	16,17,19	1.01	1 (6%)
1	GMA	k	108	1	9,9,9	1.16	0	10,11,11	1.15	0
1	GMA	I	8	1	9,9,9	1.17	0	10,11,11	1.15	0
1	5CR	MA	401	1	13,14,15	1.19	2 (15%)	16,17,19	1.59	3 (18%)
1	5CR	RA	201	1	13,14,15	1.19	2 (15%)	16,17,19	1.40	3 (18%)
1	5CR	s	201	1	13,14,15	1.21	2 (15%)	16,17,19	1.40	3 (18%)
1	5CR	rA	301	1	13,14,15	1.21	1 (7%)	16,17,19	0.96	0
1	GMA	g	408	1	9,9,9	1.15	0	10,11,11	1.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	GMA	rA	308	1	9,9,9	1.17	1 (11%)	10,11,11	1.21	0
1	5CR	Y	101	1	13,14,15	1.20	2 (15%)	16,17,19	1.40	3 (18%)
1	GMA	F	8	1	9,9,9	1.17	0	10,11,11	1.14	0
1	GMA	6A	308	1	9,9,9	1.17	0	10,11,11	1.20	0
1	5CR	2A	101	1	13,14,15	1.22	1 (7%)	16,17,19	1.01	0
1	GMA	WB	108	1	9,9,9	1.17	1 (11%)	10,11,11	1.24	1 (10%)
1	5CR	SA	301	1	13,14,15	1.20	2 (15%)	16,17,19	1.49	3 (18%)
1	GMA	t	308	1	9,9,9	1.16	0	10,11,11	1.06	0
1	GMA	SA	308	1	9,9,9	1.16	1 (11%)	10,11,11	1.06	0
1	5CR	ZB	251	1	13,14,15	1.20	2 (15%)	16,17,19	1.21	2 (12%)
1	5CR	7A	351	1	13,14,15	1.20	2 (15%)	16,17,19	1.18	2 (12%)
1	GMA	OB	458	1	9,9,9	1.15	0	10,11,11	1.23	1 (10%)
1	GMA	l	408	1	9,9,9	1.15	0	10,11,11	1.09	0
1	5CR	XB	151	1	13,14,15	1.21	1 (7%)	16,17,19	1.21	2 (12%)
1	5CR	T	301	1	13,14,15	1.18	2 (15%)	16,17,19	1.49	3 (18%)
1	GMA	R	108	1	9,9,9	1.15	0	10,11,11	1.15	0
1	GMA	7A	358	1	9,9,9	1.16	1 (11%)	10,11,11	1.22	1 (10%)
1	5CR	dB	451	1	13,14,15	1.20	1 (7%)	16,17,19	1.25	2 (12%)
1	5CR	c	1	1	13,14,15	1.22	1 (7%)	16,17,19	1.02	0
1	GMA	YA	108	1	9,9,9	1.16	0	10,11,11	1.24	2 (20%)
1	5CR	k	101	1	13,14,15	1.20	2 (15%)	16,17,19	1.40	3 (18%)
1	5CR	JA	101	1	13,14,15	1.20	2 (15%)	16,17,19	1.40	3 (18%)
1	GMA	T	308	1	9,9,9	1.15	0	10,11,11	1.05	0
1	GMA	L	208	1	9,9,9	1.17	1 (11%)	10,11,11	1.09	0
1	GMA	uA	458	1	9,9,9	1.16	0	10,11,11	1.23	1 (10%)
1	GMA	sA	358	1	9,9,9	1.14	0	10,11,11	1.22	1 (10%)
1	GMA	ZA	158	1	9,9,9	1.15	1 (11%)	10,11,11	1.24	1 (10%)
1	5CR	DA	201	1	13,14,15	1.20	2 (15%)	16,17,19	1.40	3 (18%)
1	GMA	bA	258	1	9,9,9	1.15	1 (11%)	10,11,11	1.23	2 (20%)
1	GMA	GB	58	1	9,9,9	1.14	0	10,11,11	1.22	1 (10%)
1	5CR	cA	301	1	13,14,15	1.22	1 (7%)	16,17,19	0.95	0
1	GMA	J	8	1	9,9,9	1.17	0	10,11,11	1.14	0
1	GMA	D	8	1	9,9,9	1.17	0	10,11,11	1.14	0
1	GMA	cA	308	1	9,9,9	1.18	1 (11%)	10,11,11	1.21	0
1	GMA	IB	158	1	9,9,9	1.15	0	10,11,11	1.24	1 (10%)
1	GMA	mA	58	1	9,9,9	1.15	1 (11%)	10,11,11	1.23	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5CR	cB	401	1	13,14,15	1.22	1 (7%)	16,17,19	1.05	0
1	GMA	s	208	1	9,9,9	1.15	0	10,11,11	1.09	0
1	5CR	d	1	1	13,14,15	1.22	1 (7%)	16,17,19	1.03	0
1	5CR	bA	251	1	13,14,15	1.20	2 (15%)	16,17,19	1.21	2 (12%)
1	5CR	6A	301	1	13,14,15	1.22	1 (7%)	16,17,19	0.96	0
1	GMA	KA	208	1	9,9,9	1.16	0	10,11,11	1.08	0
1	GMA	LB	308	1	9,9,9	1.17	1 (11%)	10,11,11	1.21	0
1	5CR	4A	201	1	13,14,15	1.23	1 (7%)	16,17,19	1.00	1 (6%)
1	5CR	FA	401	1	13,14,15	1.20	2 (15%)	16,17,19	1.60	3 (18%)
1	5CR	tA	401	1	13,14,15	1.22	1 (7%)	16,17,19	1.04	0
1	5CR	e	1	1	13,14,15	1.22	1 (7%)	16,17,19	1.02	0
1	5CR	C	1	1	13,14,15	1.19	2 (15%)	16,17,19	1.48	3 (18%)
1	5CR	QA	101	1	13,14,15	1.19	2 (15%)	16,17,19	1.40	3 (18%)
1	5CR	XA	51	1	13,14,15	1.21	2 (15%)	16,17,19	1.23	2 (12%)
1	GMA	6	208	1	9,9,9	1.16	0	10,11,11	1.08	0
1	GMA	y	108	1	9,9,9	1.16	0	10,11,11	1.15	0
1	GMA	TA	408	1	9,9,9	1.16	0	10,11,11	1.10	0
1	5CR	8	401	1	13,14,15	1.19	2 (15%)	16,17,19	1.60	3 (18%)
1	GMA	H	8	1	9,9,9	1.17	0	10,11,11	1.15	0
1	GMA	YB	208	1	9,9,9	1.17	1 (11%)	10,11,11	1.24	2 (20%)

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	1	401	1	-	2/9/10/12	0/1/1/1
1	GMA	B	8	1	-	5/9/9/9	-
1	GMA	JB	208	1	-	7/9/9/9	-
1	5CR	g	401	1	-	2/9/10/12	0/1/1/1
1	GMA	pA	208	1	-	7/9/9/9	-
1	GMA	HB	108	1	-	8/9/9/9	-
1	5CR	F	1	1	-	2/9/10/12	0/1/1/1
1	5CR	NB	401	1	-	2/9/10/12	0/1/1/1
1	5CR	GB	51	1	-	0/9/10/12	0/1/1/1
1	5CR	8A	401	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	dA	358	1	-	4/9/9/9	-
1	5CR	S	201	1	-	2/9/10/12	0/1/1/1
1	5CR	E	1	1	-	2/9/10/12	0/1/1/1
1	5CR	a	1	1	-	2/9/10/12	0/1/1/1
1	5CR	aB	301	1	-	2/9/10/12	0/1/1/1
1	GMA	K	108	1	-	4/9/9/9	-
1	5CR	J	1	1	-	2/9/10/12	0/1/1/1
1	5CR	mA	51	1	-	0/9/10/12	0/1/1/1
1	GMA	u	408	1	-	3/9/9/9	-
1	5CR	H	1	1	-	2/9/10/12	0/1/1/1
1	GMA	n	408	1	-	3/9/9/9	-
1	GMA	e	8	1	-	7/9/9/9	-
1	5CR	qA	251	1	-	0/9/10/12	0/1/1/1
1	5CR	y	101	1	-	2/9/10/12	0/1/1/1
1	5CR	KA	201	1	-	2/9/10/12	0/1/1/1
1	GMA	QA	108	1	-	4/9/9/9	-
1	GMA	fA	458	1	-	2/9/9/9	-
1	GMA	8	408	1	-	3/9/9/9	-
1	5CR	D	1	1	-	2/9/10/12	0/1/1/1
1	5CR	MB	351	1	-	1/9/10/12	0/1/1/1
1	5CR	YB	201	1	-	2/9/10/12	0/1/1/1
1	GMA	aA	208	1	-	7/9/9/9	-
1	5CR	OB	451	1	-	0/9/10/12	0/1/1/1
1	GMA	Z	208	1	-	5/9/9/9	-
1	GMA	C	8	1	-	5/9/9/9	-
1	GMA	z	208	1	-	4/9/9/9	-
1	GMA	5A	258	1	-	2/9/9/9	-
1	GMA	XA	58	1	-	2/9/9/9	-
1	GMA	f	308	1	-	4/9/9/9	-
1	GMA	NB	408	1	-	6/9/9/9	-
1	GMA	9A	458	1	-	2/9/9/9	-
1	5CR	KB	251	1	-	0/9/10/12	0/1/1/1
1	GMA	oA	158	1	-	2/9/9/9	-
1	5CR	uA	451	1	-	0/9/10/12	0/1/1/1
1	GMA	aB	308	1	-	6/9/9/9	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5CR	z	201	1	-	2/9/10/12	0/1/1/1
1	5CR	HB	101	1	-	2/9/10/12	0/1/1/1
1	GMA	RA	208	1	-	5/9/9/9	-
1	GMA	m	308	1	-	4/9/9/9	-
1	5CR	YA	101	1	-	2/9/10/12	0/1/1/1
1	5CR	I	1	1	-	2/9/10/12	0/1/1/1
1	5CR	LA	301	1	-	2/9/10/12	0/1/1/1
1	5CR	t	301	1	-	2/9/10/12	0/1/1/1
1	5CR	TA	401	1	-	2/9/10/12	0/1/1/1
1	GMA	U	408	1	-	3/9/9/9	-
1	GMA	a	8	1	-	7/9/9/9	-
1	GMA	5	108	1	-	4/9/9/9	-
1	5CR	3A	151	1	-	0/9/10/12	0/1/1/1
1	GMA	Y	108	1	-	4/9/9/9	-
1	GMA	KB	258	1	-	2/9/9/9	-
1	GMA	M	308	1	-	4/9/9/9	-
1	GMA	bB	358	1	-	4/9/9/9	-
1	5CR	u	401	1	-	2/9/10/12	0/1/1/1
1	5CR	JB	201	1	-	2/9/10/12	0/1/1/1
1	5CR	5	101	1	-	2/9/10/12	0/1/1/1
1	5CR	b	1	1	-	2/9/10/12	0/1/1/1
1	5CR	9A	451	1	-	0/9/10/12	0/1/1/1
1	GMA	r	108	1	-	4/9/9/9	-
1	GMA	d	8	1	-	7/9/9/9	-
1	5CR	nA	101	1	-	2/9/10/12	0/1/1/1
1	5CR	LB	301	1	-	2/9/10/12	0/1/1/1
1	5CR	5A	251	1	-	0/9/10/12	0/1/1/1
1	GMA	CA	108	1	-	4/9/9/9	-
1	GMA	E	8	1	-	5/9/9/9	-
1	GMA	G	8	1	-	5/9/9/9	-
1	GMA	DA	208	1	-	4/9/9/9	-
1	GMA	JA	108	1	-	4/9/9/9	-
1	GMA	3A	158	1	-	2/9/9/9	-
1	5CR	n	401	1	-	2/9/10/12	0/1/1/1
1	5CR	dA	351	1	-	1/9/10/12	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5CR	L	201	1	-	2/9/10/12	0/1/1/1
1	5CR	IB	151	1	-	0/9/10/12	0/1/1/1
1	5CR	ZA	151	1	-	0/9/10/12	0/1/1/1
1	5CR	Z	201	1	-	2/9/10/12	0/1/1/1
1	5CR	eA	401	1	-	2/9/10/12	0/1/1/1
1	GMA	MA	408	1	-	3/9/9/9	-
1	5CR	0	301	1	-	2/9/10/12	0/1/1/1
1	GMA	N	408	1	-	3/9/9/9	-
1	GMA	4A	208	1	-	7/9/9/9	-
1	5CR	M	301	1	-	2/9/10/12	0/1/1/1
1	5CR	l	201	1	-	2/9/10/12	0/1/1/1
1	5CR	fA	451	1	-	0/9/10/12	0/1/1/1
1	5CR	f	301	1	-	2/9/10/12	0/1/1/1
1	GMA	0	308	1	-	4/9/9/9	-
1	GMA	tA	408	1	-	6/9/9/9	-
1	5CR	K	101	1	-	2/9/10/12	0/1/1/1
1	5CR	VB	51	1	-	0/9/10/12	0/1/1/1
1	GMA	nA	108	1	-	8/9/9/9	-
1	5CR	7	301	1	-	2/9/10/12	0/1/1/1
1	5CR	B	1	1	-	2/9/10/12	0/1/1/1
1	5CR	R	101	1	-	2/9/10/12	0/1/1/1
1	GMA	VB	58	1	-	2/9/9/9	-
1	5CR	6	201	1	-	2/9/10/12	0/1/1/1
1	GMA	7	308	1	-	4/9/9/9	-
1	5CR	A	1	1	-	2/9/10/12	0/1/1/1
1	5CR	G	1	1	-	2/9/10/12	0/1/1/1
1	GMA	XB	158	1	-	2/9/9/9	-
1	GMA	eA	408	1	-	6/9/9/9	-
1	GMA	dB	458	1	-	2/9/9/9	-
1	GMA	EA	308	1	-	4/9/9/9	-
1	GMA	ZB	258	1	-	2/9/9/9	-
1	5CR	bB	351	1	-	1/9/10/12	0/1/1/1
1	GMA	MB	358	1	-	4/9/9/9	-
1	GMA	l	208	1	-	5/9/9/9	-
1	5CR	1A	51	1	-	0/9/10/12	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	GMA	qA	258	1	-	2/9/9/9	-
1	GMA	cB	408	1	-	6/9/9/9	-
1	5CR	WB	101	1	-	2/9/10/12	0/1/1/1
1	GMA	LA	308	1	-	4/9/9/9	-
1	5CR	sA	351	1	-	1/9/10/12	0/1/1/1
1	GMA	c	8	1	-	7/9/9/9	-
1	GMA	FA	408	1	-	3/9/9/9	-
1	5CR	m	301	1	-	2/9/10/12	0/1/1/1
1	5CR	oA	151	1	-	0/9/10/12	0/1/1/1
1	GMA	2A	108	1	-	8/9/9/9	-
1	GMA	1A	58	1	-	2/9/9/9	-
1	5CR	U	401	1	-	2/9/10/12	0/1/1/1
1	5CR	aA	201	1	-	2/9/10/12	0/1/1/1
1	5CR	N	401	1	-	2/9/10/12	0/1/1/1
1	GMA	S	208	1	-	5/9/9/9	-
1	5CR	r	101	1	-	2/9/10/12	0/1/1/1
1	5CR	EA	301	1	-	2/9/10/12	0/1/1/1
1	GMA	b	8	1	-	7/9/9/9	-
1	5CR	CA	101	1	-	2/9/10/12	0/1/1/1
1	GMA	A	8	1	-	5/9/9/9	-
1	GMA	8A	408	1	-	6/9/9/9	-
1	5CR	pA	201	1	-	2/9/10/12	0/1/1/1
1	GMA	k	108	1	-	4/9/9/9	-
1	GMA	I	8	1	-	5/9/9/9	-
1	5CR	MA	401	1	-	2/9/10/12	0/1/1/1
1	5CR	RA	201	1	-	2/9/10/12	0/1/1/1
1	5CR	s	201	1	-	2/9/10/12	0/1/1/1
1	5CR	rA	301	1	-	2/9/10/12	0/1/1/1
1	GMA	g	408	1	-	3/9/9/9	-
1	GMA	rA	308	1	-	6/9/9/9	-
1	5CR	Y	101	1	-	2/9/10/12	0/1/1/1
1	GMA	F	8	1	-	5/9/9/9	-
1	GMA	6A	308	1	-	6/9/9/9	-
1	5CR	2A	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	WB	108	1	-	8/9/9/9	-
1	5CR	SA	301	1	-	2/9/10/12	0/1/1/1
1	GMA	t	308	1	-	4/9/9/9	-
1	GMA	SA	308	1	-	4/9/9/9	-
1	5CR	ZB	251	1	-	0/9/10/12	0/1/1/1
1	5CR	7A	351	1	-	1/9/10/12	0/1/1/1
1	GMA	OB	458	1	-	2/9/9/9	-
1	GMA	1	408	1	-	3/9/9/9	-
1	5CR	XB	151	1	-	0/9/10/12	0/1/1/1
1	5CR	T	301	1	-	2/9/10/12	0/1/1/1
1	GMA	R	108	1	-	4/9/9/9	-
1	GMA	7A	358	1	-	4/9/9/9	-
1	5CR	dB	451	1	-	0/9/10/12	0/1/1/1
1	5CR	c	1	1	-	2/9/10/12	0/1/1/1
1	GMA	YA	108	1	-	8/9/9/9	-
1	5CR	k	101	1	-	2/9/10/12	0/1/1/1
1	5CR	JA	101	1	-	2/9/10/12	0/1/1/1
1	GMA	T	308	1	-	4/9/9/9	-
1	GMA	L	208	1	-	4/9/9/9	-
1	GMA	uA	458	1	-	2/9/9/9	-
1	GMA	sA	358	1	-	4/9/9/9	-
1	GMA	ZA	158	1	-	2/9/9/9	-
1	5CR	DA	201	1	-	2/9/10/12	0/1/1/1
1	GMA	bA	258	1	-	2/9/9/9	-
1	GMA	GB	58	1	-	2/9/9/9	-
1	5CR	cA	301	1	-	2/9/10/12	0/1/1/1
1	GMA	J	8	1	-	5/9/9/9	-
1	GMA	D	8	1	-	5/9/9/9	-
1	GMA	cA	308	1	-	6/9/9/9	-
1	GMA	IB	158	1	-	2/9/9/9	-
1	GMA	mA	58	1	-	2/9/9/9	-
1	5CR	cB	401	1	-	2/9/10/12	0/1/1/1
1	GMA	s	208	1	-	4/9/9/9	-
1	5CR	d	1	1	-	2/9/10/12	0/1/1/1
1	5CR	bA	251	1	-	0/9/10/12	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5CR	6A	301	1	-	2/9/10/12	0/1/1/1
1	GMA	KA	208	1	-	4/9/9/9	-
1	GMA	LB	308	1	-	6/9/9/9	-
1	5CR	4A	201	1	-	2/9/10/12	0/1/1/1
1	5CR	FA	401	1	-	2/9/10/12	0/1/1/1
1	5CR	tA	401	1	-	2/9/10/12	0/1/1/1
1	5CR	e	1	1	-	2/9/10/12	0/1/1/1
1	5CR	C	1	1	-	2/9/10/12	0/1/1/1
1	5CR	QA	101	1	-	2/9/10/12	0/1/1/1
1	5CR	XA	51	1	-	0/9/10/12	0/1/1/1
1	GMA	6	208	1	-	4/9/9/9	-
1	GMA	y	108	1	-	4/9/9/9	-
1	GMA	TA	408	1	-	3/9/9/9	-
1	5CR	8	401	1	-	2/9/10/12	0/1/1/1
1	GMA	H	8	1	-	5/9/9/9	-
1	GMA	YB	208	1	-	7/9/9/9	-

All (194) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	pA	201	5CR	CAL-N	3.31	1.45	1.34
1	aA	201	5CR	CAL-N	3.31	1.45	1.34
1	HB	101	5CR	CAL-N	3.31	1.45	1.34
1	8A	401	5CR	CAL-N	3.31	1.45	1.34
1	nA	101	5CR	CAL-N	3.31	1.45	1.34
1	WB	101	5CR	CAL-N	3.31	1.45	1.34
1	JB	201	5CR	CAL-N	3.31	1.45	1.34
1	a	1	5CR	CAL-N	3.30	1.45	1.34
1	NB	401	5CR	CAL-N	3.30	1.45	1.34
1	YA	101	5CR	CAL-N	3.30	1.45	1.34
1	eA	401	5CR	CAL-N	3.30	1.45	1.34
1	YB	201	5CR	CAL-N	3.30	1.45	1.34
1	4A	201	5CR	CAL-N	3.30	1.45	1.34
1	tA	401	5CR	CAL-N	3.30	1.45	1.34
1	2A	101	5CR	CAL-N	3.30	1.45	1.34
1	b	1	5CR	CAL-N	3.30	1.45	1.34
1	c	1	5CR	CAL-N	3.29	1.45	1.34
1	aB	301	5CR	CAL-N	3.29	1.45	1.34
1	6A	301	5CR	CAL-N	3.29	1.45	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	LB	301	5CR	CAL-N	3.28	1.45	1.34
1	d	1	5CR	CAL-N	3.28	1.45	1.34
1	cB	401	5CR	CAL-N	3.27	1.45	1.34
1	e	1	5CR	CAL-N	3.27	1.45	1.34
1	cA	301	5CR	CAL-N	3.26	1.45	1.34
1	rA	301	5CR	CAL-N	3.26	1.45	1.34
1	VB	51	5CR	CAL-N	3.11	1.45	1.34
1	GB	51	5CR	CAL-N	3.10	1.45	1.34
1	ZA	151	5CR	CAL-N	3.09	1.45	1.34
1	IB	151	5CR	CAL-N	3.09	1.45	1.34
1	1A	51	5CR	CAL-N	3.09	1.45	1.34
1	XA	51	5CR	CAL-N	3.09	1.45	1.34
1	mA	51	5CR	CAL-N	3.09	1.45	1.34
1	dB	451	5CR	CAL-N	3.09	1.45	1.34
1	9A	451	5CR	CAL-N	3.09	1.45	1.34
1	dA	351	5CR	CAL-N	3.08	1.44	1.34
1	5A	251	5CR	CAL-N	3.08	1.44	1.34
1	MB	351	5CR	CAL-N	3.07	1.44	1.34
1	KB	251	5CR	CAL-N	3.07	1.44	1.34
1	sA	351	5CR	CAL-N	3.07	1.44	1.34
1	oA	151	5CR	CAL-N	3.07	1.44	1.34
1	uA	451	5CR	CAL-N	3.07	1.44	1.34
1	7A	351	5CR	CAL-N	3.07	1.44	1.34
1	ZB	251	5CR	CAL-N	3.07	1.44	1.34
1	bB	351	5CR	CAL-N	3.07	1.44	1.34
1	XB	151	5CR	CAL-N	3.06	1.44	1.34
1	OB	451	5CR	CAL-N	3.06	1.44	1.34
1	fA	451	5CR	CAL-N	3.06	1.44	1.34
1	3A	151	5CR	CAL-N	3.06	1.44	1.34
1	bA	251	5CR	CAL-N	3.05	1.44	1.34
1	qA	251	5CR	CAL-N	3.04	1.44	1.34
1	JA	101	5CR	CAL-N	3.01	1.44	1.34
1	KA	201	5CR	CAL-N	3.01	1.44	1.34
1	s	201	5CR	CAL-N	3.00	1.44	1.34
1	QA	101	5CR	CAL-N	3.00	1.44	1.34
1	K	101	5CR	CAL-N	2.99	1.44	1.34
1	z	201	5CR	CAL-N	2.99	1.44	1.34
1	S	201	5CR	CAL-N	2.99	1.44	1.34
1	5	101	5CR	CAL-N	2.99	1.44	1.34
1	k	101	5CR	CAL-N	2.99	1.44	1.34
1	J	1	5CR	CAL-N	2.99	1.44	1.34
1	u	401	5CR	CAL-N	2.98	1.44	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	6	201	5CR	CAL-N	2.98	1.44	1.34
1	r	101	5CR	CAL-N	2.98	1.44	1.34
1	0	301	5CR	CAL-N	2.98	1.44	1.34
1	U	401	5CR	CAL-N	2.98	1.44	1.34
1	7	301	5CR	CAL-N	2.98	1.44	1.34
1	CA	101	5CR	CAL-N	2.98	1.44	1.34
1	L	201	5CR	CAL-N	2.98	1.44	1.34
1	l	201	5CR	CAL-N	2.98	1.44	1.34
1	Z	201	5CR	CAL-N	2.98	1.44	1.34
1	G	1	5CR	CAL-N	2.98	1.44	1.34
1	DA	201	5CR	CAL-N	2.98	1.44	1.34
1	t	301	5CR	CAL-N	2.98	1.44	1.34
1	R	101	5CR	CAL-N	2.97	1.44	1.34
1	y	101	5CR	CAL-N	2.97	1.44	1.34
1	I	1	5CR	CAL-N	2.97	1.44	1.34
1	SA	301	5CR	CAL-N	2.97	1.44	1.34
1	8	401	5CR	CAL-N	2.97	1.44	1.34
1	RA	201	5CR	CAL-N	2.97	1.44	1.34
1	f	301	5CR	CAL-N	2.97	1.44	1.34
1	n	401	5CR	CAL-N	2.97	1.44	1.34
1	Y	101	5CR	CAL-N	2.97	1.44	1.34
1	FA	401	5CR	CAL-N	2.97	1.44	1.34
1	M	301	5CR	CAL-N	2.96	1.44	1.34
1	MA	401	5CR	CAL-N	2.96	1.44	1.34
1	N	401	5CR	CAL-N	2.96	1.44	1.34
1	TA	401	5CR	CAL-N	2.96	1.44	1.34
1	g	401	5CR	CAL-N	2.96	1.44	1.34
1	m	301	5CR	CAL-N	2.95	1.44	1.34
1	T	301	5CR	CAL-N	2.95	1.44	1.34
1	LA	301	5CR	CAL-N	2.95	1.44	1.34
1	B	1	5CR	CAL-N	2.95	1.44	1.34
1	H	1	5CR	CAL-N	2.95	1.44	1.34
1	C	1	5CR	CAL-N	2.95	1.44	1.34
1	F	1	5CR	CAL-N	2.95	1.44	1.34
1	A	1	5CR	CAL-N	2.95	1.44	1.34
1	E	1	5CR	CAL-N	2.95	1.44	1.34
1	1	401	5CR	CAL-N	2.94	1.44	1.34
1	D	1	5CR	CAL-N	2.94	1.44	1.34
1	EA	301	5CR	CAL-N	2.94	1.44	1.34
1	s	201	5CR	OAB-CAL	-2.14	1.18	1.23
1	z	201	5CR	OAB-CAL	-2.14	1.18	1.23
1	u	401	5CR	OAB-CAL	-2.13	1.18	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CA	101	5CR	OAB-CAL	-2.13	1.18	1.23
1	5	101	5CR	OAB-CAL	-2.13	1.18	1.23
1	K	101	5CR	OAB-CAL	-2.13	1.18	1.23
1	FA	401	5CR	OAB-CAL	-2.13	1.18	1.23
1	KA	201	5CR	OAB-CAL	-2.13	1.18	1.23
1	n	401	5CR	OAB-CAL	-2.13	1.18	1.23
1	SA	301	5CR	OAB-CAL	-2.13	1.18	1.23
1	1	401	5CR	OAB-CAL	-2.12	1.18	1.23
1	JA	101	5CR	OAB-CAL	-2.12	1.18	1.23
1	6	201	5CR	OAB-CAL	-2.12	1.18	1.23
1	U	401	5CR	OAB-CAL	-2.12	1.18	1.23
1	G	1	5CR	OAB-CAL	-2.12	1.18	1.23
1	J	1	5CR	OAB-CAL	-2.12	1.18	1.23
1	I	1	5CR	OAB-CAL	-2.12	1.18	1.23
1	l	201	5CR	OAB-CAL	-2.11	1.18	1.23
1	r	101	5CR	OAB-CAL	-2.11	1.18	1.23
1	DA	201	5CR	OAB-CAL	-2.11	1.18	1.23
1	g	401	5CR	OAB-CAL	-2.11	1.18	1.23
1	N	401	5CR	OAB-CAL	-2.11	1.18	1.23
1	S	201	5CR	OAB-CAL	-2.11	1.18	1.23
1	m	301	5CR	OAB-CAL	-2.11	1.18	1.23
1	y	101	5CR	OAB-CAL	-2.11	1.18	1.23
1	0	301	5CR	OAB-CAL	-2.11	1.18	1.23
1	M	301	5CR	OAB-CAL	-2.11	1.18	1.23
1	k	101	5CR	OAB-CAL	-2.11	1.18	1.23
1	MA	401	5CR	OAB-CAL	-2.11	1.18	1.23
1	Y	101	5CR	OAB-CAL	-2.10	1.18	1.23
1	Z	201	5CR	OAB-CAL	-2.10	1.18	1.23
1	E	1	5CR	OAB-CAL	-2.10	1.18	1.23
1	7	301	5CR	OAB-CAL	-2.09	1.18	1.23
1	D	1	5CR	OAB-CAL	-2.09	1.18	1.23
1	B	1	5CR	OAB-CAL	-2.09	1.18	1.23
1	F	1	5CR	OAB-CAL	-2.09	1.18	1.23
1	L	201	5CR	OAB-CAL	-2.09	1.18	1.23
1	t	301	5CR	OAB-CAL	-2.09	1.18	1.23
1	H	1	5CR	OAB-CAL	-2.09	1.18	1.23
1	C	1	5CR	OAB-CAL	-2.09	1.18	1.23
1	EA	301	5CR	OAB-CAL	-2.09	1.18	1.23
1	RA	201	5CR	OAB-CAL	-2.09	1.18	1.23
1	8	401	5CR	OAB-CAL	-2.09	1.18	1.23
1	QA	101	5CR	OAB-CAL	-2.08	1.18	1.23
1	A	1	5CR	OAB-CAL	-2.08	1.18	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	TA	401	5CR	OAB-CAL	-2.08	1.18	1.23
1	T	301	5CR	OAB-CAL	-2.08	1.18	1.23
1	LA	301	5CR	OAB-CAL	-2.07	1.18	1.23
1	R	101	5CR	OAB-CAL	-2.07	1.18	1.23
1	f	301	5CR	OAB-CAL	-2.06	1.18	1.23
1	ZA	151	5CR	OAB-CAL	-2.04	1.18	1.23
1	YB	208	GMA	C-N2	2.04	1.38	1.32
1	dA	351	5CR	OAB-CAL	-2.04	1.18	1.23
1	ZB	258	GMA	C-N2	2.03	1.38	1.32
1	3A	151	5CR	OAB-CAL	-2.03	1.18	1.23
1	WB	108	GMA	C-N2	2.03	1.38	1.32
1	IB	151	5CR	OAB-CAL	-2.03	1.18	1.23
1	KB	258	GMA	C-N2	2.03	1.38	1.32
1	HB	108	GMA	C-N2	2.02	1.38	1.32
1	LB	308	GMA	C-N2	2.02	1.38	1.32
1	bB	351	5CR	OAB-CAL	-2.02	1.18	1.23
1	cA	308	GMA	C-N2	2.02	1.38	1.32
1	MB	358	GMA	C-N2	2.02	1.38	1.32
1	fA	458	GMA	C-N2	2.02	1.38	1.32
1	4A	208	GMA	C-N2	2.02	1.38	1.32
1	qA	258	GMA	C-N2	2.02	1.38	1.32
1	aA	208	GMA	C-N2	2.02	1.38	1.32
1	7A	351	5CR	OAB-CAL	-2.02	1.18	1.23
1	rA	308	GMA	C-N2	2.02	1.38	1.32
1	d	8	GMA	C-N2	2.02	1.38	1.32
1	c	8	GMA	C-N2	2.02	1.38	1.32
1	JB	208	GMA	C-N2	2.02	1.38	1.32
1	VB	51	5CR	OAB-CAL	-2.01	1.18	1.23
1	7A	358	GMA	C-N2	2.01	1.38	1.32
1	XA	51	5CR	OAB-CAL	-2.01	1.18	1.23
1	8A	408	GMA	C-N2	2.01	1.38	1.32
1	aB	308	GMA	C-N2	2.01	1.38	1.32
1	bA	251	5CR	OAB-CAL	-2.01	1.18	1.23
1	bB	358	GMA	C-N2	2.01	1.38	1.32
1	SA	308	GMA	C-N2	2.01	1.38	1.32
1	3A	158	GMA	C-N2	2.01	1.38	1.32
1	MB	351	5CR	OAB-CAL	-2.01	1.18	1.23
1	ZA	158	GMA	C-N2	2.01	1.38	1.32
1	mA	58	GMA	C-N2	2.00	1.38	1.32
1	e	8	GMA	C-N2	2.00	1.38	1.32
1	oA	151	5CR	OAB-CAL	-2.00	1.18	1.23
1	b	8	GMA	C-N2	2.00	1.38	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	ZB	251	5CR	OAB-CAL	-2.00	1.18	1.23
1	a	8	GMA	C-N2	2.00	1.38	1.32
1	XA	58	GMA	C-N2	2.00	1.38	1.32
1	dB	458	GMA	C-N2	2.00	1.38	1.32
1	GB	51	5CR	OAB-CAL	-2.00	1.18	1.23
1	L	208	GMA	C-N2	2.00	1.38	1.32
1	bA	258	GMA	C-N2	2.00	1.38	1.32

All (265) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	U	401	5CR	CA-N-CAL	-3.94	115.89	123.15
1	u	401	5CR	CA-N-CAL	-3.93	115.89	123.15
1	n	401	5CR	CA-N-CAL	-3.93	115.89	123.15
1	FA	401	5CR	CA-N-CAL	-3.93	115.90	123.15
1	MA	401	5CR	CA-N-CAL	-3.93	115.90	123.15
1	g	401	5CR	CA-N-CAL	-3.93	115.91	123.15
1	8	401	5CR	CA-N-CAL	-3.92	115.91	123.15
1	N	401	5CR	CA-N-CAL	-3.92	115.92	123.15
1	TA	401	5CR	CA-N-CAL	-3.92	115.92	123.15
1	l	401	5CR	CA-N-CAL	-3.91	115.94	123.15
1	m	301	5CR	CA-N-CAL	-3.69	116.34	123.15
1	t	301	5CR	CA-N-CAL	-3.69	116.35	123.15
1	SA	301	5CR	CA-N-CAL	-3.69	116.35	123.15
1	0	301	5CR	CA-N-CAL	-3.68	116.36	123.15
1	J	1	5CR	CA-N-CAL	-3.68	116.37	123.15
1	M	301	5CR	CA-N-CAL	-3.67	116.38	123.15
1	7	301	5CR	CA-N-CAL	-3.67	116.38	123.15
1	T	301	5CR	CA-N-CAL	-3.67	116.39	123.15
1	I	1	5CR	CA-N-CAL	-3.66	116.39	123.15
1	f	301	5CR	CA-N-CAL	-3.66	116.39	123.15
1	F	1	5CR	CA-N-CAL	-3.66	116.39	123.15
1	E	1	5CR	CA-N-CAL	-3.66	116.39	123.15
1	EA	301	5CR	CA-N-CAL	-3.65	116.41	123.15
1	A	1	5CR	CA-N-CAL	-3.65	116.41	123.15
1	D	1	5CR	CA-N-CAL	-3.65	116.41	123.15
1	H	1	5CR	CA-N-CAL	-3.65	116.41	123.15
1	LA	301	5CR	CA-N-CAL	-3.65	116.41	123.15
1	C	1	5CR	CA-N-CAL	-3.65	116.42	123.15
1	G	1	5CR	CA-N-CAL	-3.65	116.42	123.15
1	B	1	5CR	CA-N-CAL	-3.64	116.43	123.15
1	K	101	5CR	CA-N-CAL	-3.50	116.69	123.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	101	5CR	CA-N-CAL	-3.50	116.70	123.15
1	5	101	5CR	CA-N-CAL	-3.49	116.72	123.15
1	QA	101	5CR	CA-N-CAL	-3.48	116.72	123.15
1	CA	101	5CR	CA-N-CAL	-3.48	116.73	123.15
1	JA	101	5CR	CA-N-CAL	-3.47	116.74	123.15
1	k	101	5CR	CA-N-CAL	-3.47	116.75	123.15
1	y	101	5CR	CA-N-CAL	-3.46	116.76	123.15
1	r	101	5CR	CA-N-CAL	-3.46	116.76	123.15
1	R	101	5CR	CA-N-CAL	-3.46	116.77	123.15
1	L	201	5CR	CA-N-CAL	-3.38	116.91	123.15
1	6	201	5CR	CA-N-CAL	-3.38	116.92	123.15
1	KA	201	5CR	CA-N-CAL	-3.37	116.92	123.15
1	Z	201	5CR	CA-N-CAL	-3.37	116.94	123.15
1	DA	201	5CR	CA-N-CAL	-3.37	116.94	123.15
1	l	201	5CR	CA-N-CAL	-3.36	116.95	123.15
1	s	201	5CR	CA-N-CAL	-3.36	116.95	123.15
1	z	201	5CR	CA-N-CAL	-3.36	116.95	123.15
1	RA	201	5CR	CA-N-CAL	-3.35	116.97	123.15
1	S	201	5CR	CA-N-CAL	-3.34	116.98	123.15
1	uA	451	5CR	CA-N-CAL	-3.19	117.26	123.15
1	9A	451	5CR	CA-N-CAL	-3.19	117.26	123.15
1	dB	451	5CR	CA-N-CAL	-3.18	117.27	123.15
1	fA	451	5CR	CA-N-CAL	-3.18	117.28	123.15
1	OB	451	5CR	CA-N-CAL	-3.17	117.29	123.15
1	mA	51	5CR	CA-N-CAL	-3.00	117.62	123.15
1	1A	51	5CR	CA-N-CAL	-3.00	117.62	123.15
1	8	401	5CR	CG-CB-CA	-2.98	109.36	113.63
1	VB	51	5CR	CA-N-CAL	-2.98	117.66	123.15
1	XA	51	5CR	CA-N-CAL	-2.97	117.66	123.15
1	N	401	5CR	CG-CB-CA	-2.97	109.38	113.63
1	1	401	5CR	CG-CB-CA	-2.97	109.38	113.63
1	sA	351	5CR	CA-N-CAL	-2.97	117.67	123.15
1	u	401	5CR	CG-CB-CA	-2.97	109.38	113.63
1	U	401	5CR	CG-CB-CA	-2.97	109.39	113.63
1	GB	51	5CR	CA-N-CAL	-2.96	117.68	123.15
1	FA	401	5CR	CG-CB-CA	-2.96	109.39	113.63
1	TA	401	5CR	CG-CB-CA	-2.96	109.40	113.63
1	7A	351	5CR	CA-N-CAL	-2.96	117.69	123.15
1	dA	351	5CR	CA-N-CAL	-2.96	117.69	123.15
1	MA	401	5CR	CG-CB-CA	-2.96	109.40	113.63
1	g	401	5CR	CG-CB-CA	-2.95	109.41	113.63
1	bB	351	5CR	CA-N-CAL	-2.95	117.71	123.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	n	401	5CR	CG-CB-CA	-2.95	109.41	113.63
1	ZA	151	5CR	CA-N-CAL	-2.94	117.72	123.15
1	3A	151	5CR	CA-N-CAL	-2.94	117.72	123.15
1	oA	151	5CR	CA-N-CAL	-2.93	117.74	123.15
1	MB	351	5CR	CA-N-CAL	-2.93	117.75	123.15
1	IB	151	5CR	CA-N-CAL	-2.93	117.75	123.15
1	XB	151	5CR	CA-N-CAL	-2.91	117.78	123.15
1	KB	251	5CR	CA-N-CAL	-2.89	117.83	123.15
1	bA	251	5CR	CA-N-CAL	-2.88	117.83	123.15
1	5A	251	5CR	CA-N-CAL	-2.88	117.84	123.15
1	ZB	251	5CR	CA-N-CAL	-2.87	117.86	123.15
1	qA	251	5CR	CA-N-CAL	-2.86	117.87	123.15
1	TA	401	5CR	CAA-CAL-N	2.71	120.69	116.10
1	l	401	5CR	CAA-CAL-N	2.70	120.68	116.10
1	g	401	5CR	CAA-CAL-N	2.70	120.67	116.10
1	8	401	5CR	CAA-CAL-N	2.70	120.67	116.10
1	n	401	5CR	CAA-CAL-N	2.70	120.67	116.10
1	U	401	5CR	CAA-CAL-N	2.69	120.65	116.10
1	FA	401	5CR	CAA-CAL-N	2.68	120.64	116.10
1	N	401	5CR	CAA-CAL-N	2.68	120.63	116.10
1	MA	401	5CR	CAA-CAL-N	2.67	120.62	116.10
1	u	401	5CR	CAA-CAL-N	2.66	120.61	116.10
1	7	301	5CR	CG-CB-CA	-2.66	109.83	113.63
1	SA	301	5CR	CG-CB-CA	-2.65	109.84	113.63
1	t	301	5CR	CG-CB-CA	-2.64	109.85	113.63
1	M	301	5CR	CG-CB-CA	-2.64	109.85	113.63
1	0	301	5CR	CG-CB-CA	-2.64	109.86	113.63
1	m	301	5CR	CG-CB-CA	-2.63	109.86	113.63
1	LA	301	5CR	CG-CB-CA	-2.63	109.86	113.63
1	C	1	5CR	CAA-CAL-N	2.63	120.55	116.10
1	EA	301	5CR	CG-CB-CA	-2.63	109.87	113.63
1	T	301	5CR	CG-CB-CA	-2.62	109.88	113.63
1	f	301	5CR	CG-CB-CA	-2.62	109.88	113.63
1	H	1	5CR	CAA-CAL-N	2.62	120.53	116.10
1	B	1	5CR	CAA-CAL-N	2.61	120.52	116.10
1	LA	301	5CR	CAA-CAL-N	2.61	120.52	116.10
1	E	1	5CR	CAA-CAL-N	2.61	120.52	116.10
1	G	1	5CR	CAA-CAL-N	2.61	120.52	116.10
1	F	1	5CR	CAA-CAL-N	2.61	120.52	116.10
1	f	301	5CR	CAA-CAL-N	2.61	120.51	116.10
1	D	1	5CR	CAA-CAL-N	2.61	120.51	116.10
1	EA	301	5CR	CAA-CAL-N	2.60	120.51	116.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	5CR	CAA-CAL-N	2.60	120.50	116.10
1	J	1	5CR	CAA-CAL-N	2.60	120.50	116.10
1	t	301	5CR	CAA-CAL-N	2.60	120.50	116.10
1	T	301	5CR	CAA-CAL-N	2.60	120.50	116.10
1	7	301	5CR	CAA-CAL-N	2.59	120.48	116.10
1	I	1	5CR	CAA-CAL-N	2.59	120.48	116.10
1	m	301	5CR	CAA-CAL-N	2.58	120.46	116.10
1	S	201	5CR	CAA-CAL-N	2.58	120.46	116.10
1	M	301	5CR	CAA-CAL-N	2.57	120.46	116.10
1	0	301	5CR	CAA-CAL-N	2.57	120.46	116.10
1	l	201	5CR	CAA-CAL-N	2.57	120.44	116.10
1	SA	301	5CR	CAA-CAL-N	2.56	120.44	116.10
1	Z	201	5CR	CAA-CAL-N	2.55	120.42	116.10
1	RA	201	5CR	CAA-CAL-N	2.55	120.42	116.10
1	s	201	5CR	CAA-CAL-N	2.55	120.42	116.10
1	9A	451	5CR	CAA-CAL-N	2.55	120.41	116.10
1	L	201	5CR	CAA-CAL-N	2.55	120.41	116.10
1	fA	451	5CR	CAA-CAL-N	2.55	120.41	116.10
1	6	201	5CR	CAA-CAL-N	2.54	120.41	116.10
1	DA	201	5CR	CAA-CAL-N	2.54	120.40	116.10
1	z	201	5CR	CAA-CAL-N	2.54	120.40	116.10
1	OB	451	5CR	CAA-CAL-N	2.54	120.39	116.10
1	R	101	5CR	CAA-CAL-N	2.53	120.39	116.10
1	uA	451	5CR	CAA-CAL-N	2.53	120.39	116.10
1	dB	451	5CR	CAA-CAL-N	2.53	120.39	116.10
1	k	101	5CR	CAA-CAL-N	2.53	120.38	116.10
1	y	101	5CR	CAA-CAL-N	2.53	120.38	116.10
1	r	101	5CR	CAA-CAL-N	2.52	120.37	116.10
1	KA	201	5CR	CAA-CAL-N	2.51	120.35	116.10
1	Y	101	5CR	CAA-CAL-N	2.50	120.34	116.10
1	CA	101	5CR	CAA-CAL-N	2.50	120.34	116.10
1	JA	101	5CR	CAA-CAL-N	2.50	120.34	116.10
1	QA	101	5CR	CAA-CAL-N	2.50	120.34	116.10
1	B	1	5CR	CG-CB-CA	-2.50	110.05	113.63
1	K	101	5CR	CAA-CAL-N	2.50	120.33	116.10
1	J	1	5CR	CG-CB-CA	-2.49	110.06	113.63
1	A	1	5CR	CG-CB-CA	-2.49	110.07	113.63
1	1A	51	5CR	CAA-CAL-N	2.49	120.31	116.10
1	E	1	5CR	CG-CB-CA	-2.49	110.07	113.63
1	5	101	5CR	CAA-CAL-N	2.48	120.30	116.10
1	GB	51	5CR	CAA-CAL-N	2.48	120.30	116.10
1	C	1	5CR	CG-CB-CA	-2.48	110.09	113.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	1	5CR	CG-CB-CA	-2.47	110.09	113.63
1	XA	51	5CR	CAA-CAL-N	2.47	120.28	116.10
1	D	1	5CR	CG-CB-CA	-2.47	110.10	113.63
1	VB	51	5CR	CAA-CAL-N	2.46	120.27	116.10
1	MB	351	5CR	CAA-CAL-N	2.46	120.26	116.10
1	XB	151	5CR	CAA-CAL-N	2.46	120.26	116.10
1	mA	51	5CR	CAA-CAL-N	2.46	120.26	116.10
1	5A	251	5CR	CAA-CAL-N	2.46	120.26	116.10
1	F	1	5CR	CG-CB-CA	-2.45	110.12	113.63
1	bA	251	5CR	CAA-CAL-N	2.45	120.25	116.10
1	I	1	5CR	CG-CB-CA	-2.45	110.12	113.63
1	oA	151	5CR	CAA-CAL-N	2.45	120.25	116.10
1	qA	251	5CR	CAA-CAL-N	2.45	120.25	116.10
1	G	1	5CR	CG-CB-CA	-2.45	110.12	113.63
1	IB	151	5CR	CAA-CAL-N	2.44	120.24	116.10
1	KB	251	5CR	CAA-CAL-N	2.44	120.24	116.10
1	bB	351	5CR	CAA-CAL-N	2.44	120.24	116.10
1	ZB	251	5CR	CAA-CAL-N	2.44	120.23	116.10
1	7A	351	5CR	CAA-CAL-N	2.44	120.23	116.10
1	sA	351	5CR	CAA-CAL-N	2.43	120.22	116.10
1	dA	351	5CR	CAA-CAL-N	2.43	120.22	116.10
1	ZA	151	5CR	CAA-CAL-N	2.42	120.20	116.10
1	3A	151	5CR	CAA-CAL-N	2.42	120.19	116.10
1	l	201	5CR	CG-CB-CA	-2.22	110.46	113.63
1	Z	201	5CR	CG-CB-CA	-2.21	110.47	113.63
1	z	201	5CR	CG-CB-CA	-2.20	110.48	113.63
1	6	201	5CR	CG-CB-CA	-2.20	110.48	113.63
1	s	201	5CR	CG-CB-CA	-2.20	110.48	113.63
1	L	201	5CR	CG-CB-CA	-2.20	110.48	113.63
1	DA	201	5CR	CG-CB-CA	-2.20	110.48	113.63
1	S	201	5CR	CG-CB-CA	-2.20	110.49	113.63
1	RA	201	5CR	CG-CB-CA	-2.20	110.49	113.63
1	dB	458	GMA	O-C-N2	-2.19	119.19	123.00
1	oA	158	GMA	O-C-N2	-2.19	119.19	123.00
1	KA	201	5CR	CG-CB-CA	-2.19	110.50	113.63
1	XB	158	GMA	O-C-N2	-2.18	119.20	123.00
1	3A	158	GMA	O-C-N2	-2.18	119.21	123.00
1	fA	458	GMA	O-C-N2	-2.18	119.21	123.00
1	ZA	158	GMA	O-C-N2	-2.18	119.21	123.00
1	R	101	5CR	CG-CB-CA	-2.18	110.52	113.63
1	CA	101	5CR	CG-CB-CA	-2.18	110.52	113.63
1	IB	158	GMA	O-C-N2	-2.17	119.22	123.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	qA	258	GMA	O-C-N2	-2.17	119.22	123.00
1	OB	458	GMA	O-C-N2	-2.17	119.22	123.00
1	9A	458	GMA	O-C-N2	-2.17	119.23	123.00
1	r	101	5CR	CG-CB-CA	-2.16	110.54	113.63
1	mA	58	GMA	O-C-N2	-2.16	119.25	123.00
1	Y	101	5CR	CG-CB-CA	-2.16	110.55	113.63
1	ZB	258	GMA	O-C-N2	-2.16	119.25	123.00
1	uA	458	GMA	O-C-N2	-2.15	119.25	123.00
1	5	101	5CR	CG-CB-CA	-2.15	110.55	113.63
1	y	101	5CR	CG-CB-CA	-2.15	110.56	113.63
1	XA	58	GMA	O-C-N2	-2.14	119.28	123.00
1	VB	58	GMA	O-C-N2	-2.14	119.28	123.00
1	MB	358	GMA	O-C-N2	-2.14	119.28	123.00
1	K	101	5CR	CG-CB-CA	-2.14	110.57	113.63
1	QA	101	5CR	CG-CB-CA	-2.14	110.58	113.63
1	JA	101	5CR	CG-CB-CA	-2.13	110.58	113.63
1	KB	258	GMA	O-C-N2	-2.13	119.29	123.00
1	k	101	5CR	CG-CB-CA	-2.13	110.58	113.63
1	bA	258	GMA	O-C-N2	-2.12	119.31	123.00
1	sA	358	GMA	O-C-N2	-2.12	119.31	123.00
1	5A	258	GMA	O-C-N2	-2.12	119.31	123.00
1	7A	358	GMA	O-C-N2	-2.12	119.32	123.00
1	GB	58	GMA	O-C-N2	-2.12	119.32	123.00
1	1A	58	GMA	O-C-N2	-2.11	119.32	123.00
1	e	8	GMA	O-C-CA	2.11	123.39	120.30
1	bB	358	GMA	O-C-N2	-2.10	119.34	123.00
1	dA	358	GMA	O-C-N2	-2.08	119.38	123.00
1	JB	208	GMA	O-C-N2	-2.07	119.40	123.00
1	b	8	GMA	O-C-CA	2.07	123.33	120.30
1	HB	108	GMA	O-C-CA	2.07	123.33	120.30
1	a	8	GMA	O-C-CA	2.06	123.33	120.30
1	c	8	GMA	O-C-CA	2.05	123.31	120.30
1	d	8	GMA	O-C-CA	2.05	123.31	120.30
1	4A	201	5CR	CAA-CAL-N	2.05	119.56	116.10
1	4A	208	GMA	O-C-N2	-2.05	119.44	123.00
1	aA	208	GMA	O-C-N2	-2.04	119.45	123.00
1	aA	201	5CR	CAA-CAL-N	2.04	119.56	116.10
1	8A	408	GMA	O-C-N2	-2.04	119.45	123.00
1	WB	108	GMA	O-C-CA	2.04	123.29	120.30
1	pA	208	GMA	O-C-N2	-2.04	119.45	123.00
1	ZB	258	GMA	O-C-CA	2.04	123.29	120.30
1	JB	208	GMA	O-C-CA	2.04	123.28	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	qA	258	GMA	O-C-CA	2.04	123.28	120.30
1	YB	208	GMA	O-C-N2	-2.03	119.46	123.00
1	YB	201	5CR	CAA-CAL-N	2.03	119.54	116.10
1	nA	108	GMA	O-C-CA	2.03	123.27	120.30
1	fA	458	GMA	O-C-CA	2.03	123.27	120.30
1	NB	408	GMA	O-C-N2	-2.03	119.47	123.00
1	JB	201	5CR	CAA-CAL-N	2.03	119.53	116.10
1	tA	408	GMA	O-C-N2	-2.03	119.48	123.00
1	KB	258	GMA	O-C-CA	2.02	123.26	120.30
1	dB	458	GMA	O-C-CA	2.02	123.26	120.30
1	4A	208	GMA	O-C-CA	2.02	123.26	120.30
1	HB	108	GMA	O-C-N2	-2.02	119.49	123.00
1	YA	108	GMA	O-C-CA	2.02	123.26	120.30
1	cB	408	GMA	O-C-N2	-2.02	119.49	123.00
1	pA	201	5CR	CAA-CAL-N	2.01	119.51	116.10
1	aA	208	GMA	O-C-CA	2.01	123.25	120.30
1	bA	258	GMA	O-C-CA	2.01	123.25	120.30
1	9A	458	GMA	O-C-CA	2.01	123.25	120.30
1	YB	208	GMA	O-C-CA	2.01	123.25	120.30
1	2A	108	GMA	O-C-CA	2.01	123.25	120.30
1	XB	158	GMA	O-C-CA	2.01	123.25	120.30
1	eA	408	GMA	O-C-N2	-2.00	119.52	123.00
1	WB	101	5CR	CAA-CAL-N	2.00	119.49	116.10
1	YA	108	GMA	O-C-N2	-2.00	119.52	123.00

There are no chirality outliers.

All (589) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	a	1	5CR	C-CA-N-CAL
1	a	1	5CR	CB-CA-N-CAL
1	YA	101	5CR	C-CA-N-CAL
1	YA	101	5CR	CB-CA-N-CAL
1	aA	201	5CR	C-CA-N-CAL
1	aA	201	5CR	CB-CA-N-CAL
1	cA	301	5CR	C-CA-N-CAL
1	cA	301	5CR	CB-CA-N-CAL
1	dA	351	5CR	O-C-CA-CB
1	eA	401	5CR	C-CA-N-CAL
1	eA	401	5CR	CB-CA-N-CAL
1	b	1	5CR	C-CA-N-CAL
1	b	1	5CR	CB-CA-N-CAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	nA	101	5CR	C-CA-N-CAL
1	nA	101	5CR	CB-CA-N-CAL
1	pA	201	5CR	C-CA-N-CAL
1	pA	201	5CR	CB-CA-N-CAL
1	rA	301	5CR	C-CA-N-CAL
1	rA	301	5CR	CB-CA-N-CAL
1	sA	351	5CR	O-C-CA-CB
1	tA	401	5CR	C-CA-N-CAL
1	tA	401	5CR	CB-CA-N-CAL
1	c	1	5CR	C-CA-N-CAL
1	c	1	5CR	CB-CA-N-CAL
1	2A	101	5CR	C-CA-N-CAL
1	2A	101	5CR	CB-CA-N-CAL
1	4A	201	5CR	C-CA-N-CAL
1	4A	201	5CR	CB-CA-N-CAL
1	6A	301	5CR	C-CA-N-CAL
1	6A	301	5CR	CB-CA-N-CAL
1	7A	351	5CR	O-C-CA-CB
1	8A	401	5CR	C-CA-N-CAL
1	8A	401	5CR	CB-CA-N-CAL
1	d	1	5CR	C-CA-N-CAL
1	d	1	5CR	CB-CA-N-CAL
1	HB	101	5CR	C-CA-N-CAL
1	HB	101	5CR	CB-CA-N-CAL
1	JB	201	5CR	C-CA-N-CAL
1	JB	201	5CR	CB-CA-N-CAL
1	LB	301	5CR	C-CA-N-CAL
1	LB	301	5CR	CB-CA-N-CAL
1	MB	351	5CR	O-C-CA-CB
1	NB	401	5CR	C-CA-N-CAL
1	NB	401	5CR	CB-CA-N-CAL
1	e	1	5CR	C-CA-N-CAL
1	e	1	5CR	CB-CA-N-CAL
1	WB	101	5CR	C-CA-N-CAL
1	WB	101	5CR	CB-CA-N-CAL
1	YB	201	5CR	C-CA-N-CAL
1	YB	201	5CR	CB-CA-N-CAL
1	aB	301	5CR	C-CA-N-CAL
1	aB	301	5CR	CB-CA-N-CAL
1	bB	351	5CR	O-C-CA-CB
1	cB	401	5CR	C-CA-N-CAL
1	cB	401	5CR	CB-CA-N-CAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	A	8	GMA	N-CA-CB-CG
1	A	8	GMA	C-CA-CB-CG
1	K	108	GMA	N-CA-CB-CG
1	K	108	GMA	C-CA-CB-CG
1	L	208	GMA	N2-C-CA-N
1	L	208	GMA	N-CA-CB-CG
1	L	208	GMA	C-CA-CB-CG
1	B	8	GMA	N-CA-CB-CG
1	B	8	GMA	C-CA-CB-CG
1	R	108	GMA	N-CA-CB-CG
1	R	108	GMA	C-CA-CB-CG
1	S	208	GMA	N2-C-CA-N
1	S	208	GMA	N-CA-CB-CG
1	S	208	GMA	C-CA-CB-CG
1	C	8	GMA	N-CA-CB-CG
1	C	8	GMA	C-CA-CB-CG
1	Y	108	GMA	N-CA-CB-CG
1	Y	108	GMA	C-CA-CB-CG
1	Z	208	GMA	N2-C-CA-N
1	Z	208	GMA	N-CA-CB-CG
1	Z	208	GMA	C-CA-CB-CG
1	D	8	GMA	N-CA-CB-CG
1	D	8	GMA	C-CA-CB-CG
1	k	108	GMA	N-CA-CB-CG
1	k	108	GMA	C-CA-CB-CG
1	l	208	GMA	N2-C-CA-N
1	l	208	GMA	N-CA-CB-CG
1	l	208	GMA	C-CA-CB-CG
1	E	8	GMA	N-CA-CB-CG
1	E	8	GMA	C-CA-CB-CG
1	r	108	GMA	N-CA-CB-CG
1	r	108	GMA	C-CA-CB-CG
1	s	208	GMA	N2-C-CA-N
1	s	208	GMA	N-CA-CB-CG
1	s	208	GMA	C-CA-CB-CG
1	F	8	GMA	N-CA-CB-CG
1	F	8	GMA	C-CA-CB-CG
1	y	108	GMA	N-CA-CB-CG
1	y	108	GMA	C-CA-CB-CG
1	z	208	GMA	N2-C-CA-N
1	z	208	GMA	N-CA-CB-CG
1	z	208	GMA	C-CA-CB-CG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	G	8	GMA	N-CA-CB-CG
1	G	8	GMA	C-CA-CB-CG
1	5	108	GMA	N-CA-CB-CG
1	5	108	GMA	C-CA-CB-CG
1	6	208	GMA	N2-C-CA-N
1	6	208	GMA	N-CA-CB-CG
1	6	208	GMA	C-CA-CB-CG
1	H	8	GMA	N-CA-CB-CG
1	H	8	GMA	C-CA-CB-CG
1	CA	108	GMA	N-CA-CB-CG
1	CA	108	GMA	C-CA-CB-CG
1	DA	208	GMA	N2-C-CA-N
1	DA	208	GMA	N-CA-CB-CG
1	DA	208	GMA	C-CA-CB-CG
1	I	8	GMA	N-CA-CB-CG
1	I	8	GMA	C-CA-CB-CG
1	JA	108	GMA	N-CA-CB-CG
1	JA	108	GMA	C-CA-CB-CG
1	KA	208	GMA	N2-C-CA-N
1	KA	208	GMA	N-CA-CB-CG
1	KA	208	GMA	C-CA-CB-CG
1	J	8	GMA	N-CA-CB-CG
1	J	8	GMA	C-CA-CB-CG
1	QA	108	GMA	N-CA-CB-CG
1	QA	108	GMA	C-CA-CB-CG
1	RA	208	GMA	N2-C-CA-N
1	RA	208	GMA	N-CA-CB-CG
1	RA	208	GMA	C-CA-CB-CG
1	a	8	GMA	N-CA-CB-CG
1	a	8	GMA	C-CA-CB-CG
1	YA	108	GMA	N-CA-CB-CG
1	YA	108	GMA	C-CA-CB-CG
1	aA	208	GMA	N-CA-CB-CG
1	aA	208	GMA	C-CA-CB-CG
1	cA	308	GMA	N-CA-CB-CG
1	cA	308	GMA	C-CA-CB-CG
1	eA	408	GMA	N-CA-CB-CG
1	eA	408	GMA	C-CA-CB-CG
1	b	8	GMA	N-CA-CB-CG
1	b	8	GMA	C-CA-CB-CG
1	nA	108	GMA	N-CA-CB-CG
1	nA	108	GMA	C-CA-CB-CG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	pA	208	GMA	N-CA-CB-CG
1	pA	208	GMA	C-CA-CB-CG
1	rA	308	GMA	N-CA-CB-CG
1	rA	308	GMA	C-CA-CB-CG
1	tA	408	GMA	N-CA-CB-CG
1	tA	408	GMA	C-CA-CB-CG
1	c	8	GMA	N-CA-CB-CG
1	c	8	GMA	C-CA-CB-CG
1	2A	108	GMA	N-CA-CB-CG
1	2A	108	GMA	C-CA-CB-CG
1	4A	208	GMA	N-CA-CB-CG
1	4A	208	GMA	C-CA-CB-CG
1	6A	308	GMA	N-CA-CB-CG
1	6A	308	GMA	C-CA-CB-CG
1	8A	408	GMA	N-CA-CB-CG
1	8A	408	GMA	C-CA-CB-CG
1	d	8	GMA	N-CA-CB-CG
1	d	8	GMA	C-CA-CB-CG
1	HB	108	GMA	N-CA-CB-CG
1	HB	108	GMA	C-CA-CB-CG
1	JB	208	GMA	N-CA-CB-CG
1	JB	208	GMA	C-CA-CB-CG
1	LB	308	GMA	N-CA-CB-CG
1	LB	308	GMA	C-CA-CB-CG
1	NB	408	GMA	N-CA-CB-CG
1	NB	408	GMA	C-CA-CB-CG
1	e	8	GMA	N-CA-CB-CG
1	e	8	GMA	C-CA-CB-CG
1	WB	108	GMA	N-CA-CB-CG
1	WB	108	GMA	C-CA-CB-CG
1	YB	208	GMA	N-CA-CB-CG
1	YB	208	GMA	C-CA-CB-CG
1	aB	308	GMA	N-CA-CB-CG
1	aB	308	GMA	C-CA-CB-CG
1	cB	408	GMA	N-CA-CB-CG
1	cB	408	GMA	C-CA-CB-CG
1	L	208	GMA	CA-CB-CG-CD
1	S	208	GMA	CA-CB-CG-CD
1	Z	208	GMA	CA-CB-CG-CD
1	l	208	GMA	CA-CB-CG-CD
1	s	208	GMA	CA-CB-CG-CD
1	z	208	GMA	CA-CB-CG-CD

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	6	208	GMA	CA-CB-CG-CD
1	DA	208	GMA	CA-CB-CG-CD
1	KA	208	GMA	CA-CB-CG-CD
1	RA	208	GMA	CA-CB-CG-CD
1	XA	58	GMA	CA-CB-CG-CD
1	mA	58	GMA	CA-CB-CG-CD
1	1A	58	GMA	CA-CB-CG-CD
1	GB	58	GMA	CA-CB-CG-CD
1	VB	58	GMA	CA-CB-CG-CD
1	K	108	GMA	CA-CB-CG-CD
1	M	308	GMA	CA-CB-CG-CD
1	N	408	GMA	CA-CB-CG-CD
1	R	108	GMA	CA-CB-CG-CD
1	T	308	GMA	CA-CB-CG-CD
1	U	408	GMA	CA-CB-CG-CD
1	Y	108	GMA	CA-CB-CG-CD
1	f	308	GMA	CA-CB-CG-CD
1	g	408	GMA	CA-CB-CG-CD
1	k	108	GMA	CA-CB-CG-CD
1	m	308	GMA	CA-CB-CG-CD
1	n	408	GMA	CA-CB-CG-CD
1	r	108	GMA	CA-CB-CG-CD
1	t	308	GMA	CA-CB-CG-CD
1	y	108	GMA	CA-CB-CG-CD
1	0	308	GMA	CA-CB-CG-CD
1	1	408	GMA	CA-CB-CG-CD
1	5	108	GMA	CA-CB-CG-CD
1	7	308	GMA	CA-CB-CG-CD
1	8	408	GMA	CA-CB-CG-CD
1	CA	108	GMA	CA-CB-CG-CD
1	EA	308	GMA	CA-CB-CG-CD
1	FA	408	GMA	CA-CB-CG-CD
1	JA	108	GMA	CA-CB-CG-CD
1	LA	308	GMA	CA-CB-CG-CD
1	MA	408	GMA	CA-CB-CG-CD
1	QA	108	GMA	CA-CB-CG-CD
1	SA	308	GMA	CA-CB-CG-CD
1	TA	408	GMA	CA-CB-CG-CD
1	fA	458	GMA	CA-CB-CG-CD
1	sA	358	GMA	CA-CB-CG-CD
1	uA	458	GMA	CA-CB-CG-CD
1	7A	358	GMA	CA-CB-CG-CD

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	9A	458	GMA	CA-CB-CG-CD
1	OB	458	GMA	CA-CB-CG-CD
1	dB	458	GMA	CA-CB-CG-CD
1	M	308	GMA	C-CA-CB-CG
1	T	308	GMA	C-CA-CB-CG
1	f	308	GMA	C-CA-CB-CG
1	m	308	GMA	C-CA-CB-CG
1	t	308	GMA	C-CA-CB-CG
1	0	308	GMA	C-CA-CB-CG
1	7	308	GMA	C-CA-CB-CG
1	EA	308	GMA	C-CA-CB-CG
1	LA	308	GMA	C-CA-CB-CG
1	SA	308	GMA	C-CA-CB-CG
1	u	408	GMA	CA-CB-CG-CD
1	ZA	158	GMA	CA-CB-CG-CD
1	bA	258	GMA	CA-CB-CG-CD
1	dA	358	GMA	CA-CB-CG-CD
1	oA	158	GMA	CA-CB-CG-CD
1	qA	258	GMA	CA-CB-CG-CD
1	3A	158	GMA	CA-CB-CG-CD
1	5A	258	GMA	CA-CB-CG-CD
1	IB	158	GMA	CA-CB-CG-CD
1	KB	258	GMA	CA-CB-CG-CD
1	MB	358	GMA	CA-CB-CG-CD
1	XB	158	GMA	CA-CB-CG-CD
1	ZB	258	GMA	CA-CB-CG-CD
1	bB	358	GMA	CA-CB-CG-CD
1	a	8	GMA	O-C-CA-N
1	YA	108	GMA	O-C-CA-N
1	aA	208	GMA	O-C-CA-N
1	b	8	GMA	O-C-CA-N
1	nA	108	GMA	O-C-CA-N
1	pA	208	GMA	O-C-CA-N
1	c	8	GMA	O-C-CA-N
1	2A	108	GMA	O-C-CA-N
1	4A	208	GMA	O-C-CA-N
1	d	8	GMA	O-C-CA-N
1	HB	108	GMA	O-C-CA-N
1	JB	208	GMA	O-C-CA-N
1	e	8	GMA	O-C-CA-N
1	WB	108	GMA	O-C-CA-N
1	YB	208	GMA	O-C-CA-N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	g	401	5CR	CA-CB-CG-CD2
1	n	401	5CR	CA-CB-CG-CD2
1	u	401	5CR	CA-CB-CG-CD2
1	1	401	5CR	CA-CB-CG-CD2
1	8	401	5CR	CA-CB-CG-CD2
1	MA	401	5CR	CA-CB-CG-CD2
1	TA	401	5CR	CA-CB-CG-CD2
1	N	401	5CR	CA-CB-CG-CD2
1	U	401	5CR	CA-CB-CG-CD2
1	FA	401	5CR	CA-CB-CG-CD2
1	A	1	5CR	CA-CB-CG-CD2
1	B	1	5CR	CA-CB-CG-CD2
1	C	1	5CR	CA-CB-CG-CD2
1	D	1	5CR	CA-CB-CG-CD2
1	E	1	5CR	CA-CB-CG-CD2
1	F	1	5CR	CA-CB-CG-CD2
1	G	1	5CR	CA-CB-CG-CD2
1	H	1	5CR	CA-CB-CG-CD2
1	I	1	5CR	CA-CB-CG-CD2
1	J	1	5CR	CA-CB-CG-CD2
1	K	101	5CR	CA-CB-CG-CD2
1	R	101	5CR	CA-CB-CG-CD2
1	Y	101	5CR	CA-CB-CG-CD2
1	k	101	5CR	CA-CB-CG-CD2
1	r	101	5CR	CA-CB-CG-CD2
1	y	101	5CR	CA-CB-CG-CD2
1	5	101	5CR	CA-CB-CG-CD2
1	CA	101	5CR	CA-CB-CG-CD2
1	JA	101	5CR	CA-CB-CG-CD2
1	QA	101	5CR	CA-CB-CG-CD2
1	R	101	5CR	CA-CB-CG-CD1
1	Y	101	5CR	CA-CB-CG-CD1
1	5	101	5CR	CA-CB-CG-CD1
1	K	101	5CR	CA-CB-CG-CD1
1	N	401	5CR	CA-CB-CG-CD1
1	g	401	5CR	CA-CB-CG-CD1
1	k	101	5CR	CA-CB-CG-CD1
1	r	101	5CR	CA-CB-CG-CD1
1	u	401	5CR	CA-CB-CG-CD1
1	y	101	5CR	CA-CB-CG-CD1
1	1	401	5CR	CA-CB-CG-CD1
1	8	401	5CR	CA-CB-CG-CD1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	CA	101	5CR	CA-CB-CG-CD1
1	FA	401	5CR	CA-CB-CG-CD1
1	JA	101	5CR	CA-CB-CG-CD1
1	QA	101	5CR	CA-CB-CG-CD1
1	TA	401	5CR	CA-CB-CG-CD1
1	A	1	5CR	CA-CB-CG-CD1
1	B	1	5CR	CA-CB-CG-CD1
1	T	301	5CR	CA-CB-CG-CD2
1	U	401	5CR	CA-CB-CG-CD1
1	C	1	5CR	CA-CB-CG-CD1
1	f	301	5CR	CA-CB-CG-CD2
1	D	1	5CR	CA-CB-CG-CD1
1	m	301	5CR	CA-CB-CG-CD2
1	n	401	5CR	CA-CB-CG-CD1
1	E	1	5CR	CA-CB-CG-CD1
1	F	1	5CR	CA-CB-CG-CD1
1	0	301	5CR	CA-CB-CG-CD2
1	G	1	5CR	CA-CB-CG-CD1
1	H	1	5CR	CA-CB-CG-CD1
1	EA	301	5CR	CA-CB-CG-CD2
1	I	1	5CR	CA-CB-CG-CD1
1	LA	301	5CR	CA-CB-CG-CD2
1	MA	401	5CR	CA-CB-CG-CD1
1	J	1	5CR	CA-CB-CG-CD1
1	SA	301	5CR	CA-CB-CG-CD2
1	L	201	5CR	CA-CB-CG-CD1
1	M	301	5CR	CA-CB-CG-CD1
1	M	301	5CR	CA-CB-CG-CD2
1	S	201	5CR	CA-CB-CG-CD1
1	T	301	5CR	CA-CB-CG-CD1
1	Z	201	5CR	CA-CB-CG-CD1
1	f	301	5CR	CA-CB-CG-CD1
1	l	201	5CR	CA-CB-CG-CD1
1	m	301	5CR	CA-CB-CG-CD1
1	s	201	5CR	CA-CB-CG-CD1
1	t	301	5CR	CA-CB-CG-CD1
1	t	301	5CR	CA-CB-CG-CD2
1	z	201	5CR	CA-CB-CG-CD1
1	0	301	5CR	CA-CB-CG-CD1
1	6	201	5CR	CA-CB-CG-CD1
1	7	301	5CR	CA-CB-CG-CD1
1	7	301	5CR	CA-CB-CG-CD2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	DA	201	5CR	CA-CB-CG-CD1
1	EA	301	5CR	CA-CB-CG-CD1
1	KA	201	5CR	CA-CB-CG-CD1
1	LA	301	5CR	CA-CB-CG-CD1
1	RA	201	5CR	CA-CB-CG-CD1
1	SA	301	5CR	CA-CB-CG-CD1
1	A	8	GMA	CA-CB-CG-CD
1	B	8	GMA	CA-CB-CG-CD
1	C	8	GMA	CA-CB-CG-CD
1	D	8	GMA	CA-CB-CG-CD
1	E	8	GMA	CA-CB-CG-CD
1	F	8	GMA	CA-CB-CG-CD
1	G	8	GMA	CA-CB-CG-CD
1	H	8	GMA	CA-CB-CG-CD
1	I	8	GMA	CA-CB-CG-CD
1	J	8	GMA	CA-CB-CG-CD
1	l	201	5CR	CA-CB-CG-CD2
1	s	201	5CR	CA-CB-CG-CD2
1	L	201	5CR	CA-CB-CG-CD2
1	S	201	5CR	CA-CB-CG-CD2
1	Z	201	5CR	CA-CB-CG-CD2
1	z	201	5CR	CA-CB-CG-CD2
1	6	201	5CR	CA-CB-CG-CD2
1	DA	201	5CR	CA-CB-CG-CD2
1	KA	201	5CR	CA-CB-CG-CD2
1	RA	201	5CR	CA-CB-CG-CD2
1	aA	208	GMA	O-C-CA-CB
1	aA	208	GMA	N2-C-CA-CB
1	pA	208	GMA	O-C-CA-CB
1	pA	208	GMA	N2-C-CA-CB
1	4A	208	GMA	O-C-CA-CB
1	4A	208	GMA	N2-C-CA-CB
1	JB	208	GMA	O-C-CA-CB
1	JB	208	GMA	N2-C-CA-CB
1	YB	208	GMA	O-C-CA-CB
1	YB	208	GMA	N2-C-CA-CB
1	fA	458	GMA	C-CA-CB-CG
1	uA	458	GMA	C-CA-CB-CG
1	9A	458	GMA	C-CA-CB-CG
1	OB	458	GMA	C-CA-CB-CG
1	dB	458	GMA	C-CA-CB-CG
1	XA	58	GMA	C-CA-CB-CG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	bA	258	GMA	C-CA-CB-CG
1	mA	58	GMA	C-CA-CB-CG
1	qA	258	GMA	C-CA-CB-CG
1	1A	58	GMA	C-CA-CB-CG
1	5A	258	GMA	C-CA-CB-CG
1	GB	58	GMA	C-CA-CB-CG
1	KB	258	GMA	C-CA-CB-CG
1	VB	58	GMA	C-CA-CB-CG
1	ZB	258	GMA	C-CA-CB-CG
1	N	408	GMA	C-CA-CB-CG
1	U	408	GMA	C-CA-CB-CG
1	g	408	GMA	C-CA-CB-CG
1	n	408	GMA	C-CA-CB-CG
1	u	408	GMA	C-CA-CB-CG
1	l	408	GMA	C-CA-CB-CG
1	8	408	GMA	C-CA-CB-CG
1	FA	408	GMA	C-CA-CB-CG
1	MA	408	GMA	C-CA-CB-CG
1	TA	408	GMA	C-CA-CB-CG
1	M	308	GMA	N-CA-CB-CG
1	N	408	GMA	N-CA-CB-CG
1	T	308	GMA	N-CA-CB-CG
1	U	408	GMA	N-CA-CB-CG
1	f	308	GMA	N-CA-CB-CG
1	g	408	GMA	N-CA-CB-CG
1	m	308	GMA	N-CA-CB-CG
1	n	408	GMA	N-CA-CB-CG
1	t	308	GMA	N-CA-CB-CG
1	u	408	GMA	N-CA-CB-CG
1	0	308	GMA	N-CA-CB-CG
1	1	408	GMA	N-CA-CB-CG
1	7	308	GMA	N-CA-CB-CG
1	8	408	GMA	N-CA-CB-CG
1	EA	308	GMA	N-CA-CB-CG
1	FA	408	GMA	N-CA-CB-CG
1	LA	308	GMA	N-CA-CB-CG
1	MA	408	GMA	N-CA-CB-CG
1	SA	308	GMA	N-CA-CB-CG
1	TA	408	GMA	N-CA-CB-CG
1	cA	308	GMA	O-C-CA-N
1	rA	308	GMA	O-C-CA-N
1	6A	308	GMA	O-C-CA-N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	LB	308	GMA	O-C-CA-N
1	aB	308	GMA	O-C-CA-N
1	a	8	GMA	N2-C-CA-CB
1	YA	108	GMA	N2-C-CA-CB
1	cA	308	GMA	O-C-CA-CB
1	b	8	GMA	N2-C-CA-CB
1	nA	108	GMA	N2-C-CA-CB
1	rA	308	GMA	O-C-CA-CB
1	c	8	GMA	N2-C-CA-CB
1	2A	108	GMA	N2-C-CA-CB
1	6A	308	GMA	O-C-CA-CB
1	d	8	GMA	N2-C-CA-CB
1	HB	108	GMA	N2-C-CA-CB
1	LB	308	GMA	O-C-CA-CB
1	e	8	GMA	N2-C-CA-CB
1	WB	108	GMA	N2-C-CA-CB
1	aB	308	GMA	O-C-CA-CB
1	ZA	158	GMA	C-CA-CB-CG
1	oA	158	GMA	C-CA-CB-CG
1	3A	158	GMA	C-CA-CB-CG
1	IB	158	GMA	C-CA-CB-CG
1	XB	158	GMA	C-CA-CB-CG
1	a	8	GMA	O-C-CA-CB
1	YA	108	GMA	O-C-CA-CB
1	b	8	GMA	O-C-CA-CB
1	nA	108	GMA	O-C-CA-CB
1	c	8	GMA	O-C-CA-CB
1	2A	108	GMA	O-C-CA-CB
1	d	8	GMA	O-C-CA-CB
1	HB	108	GMA	O-C-CA-CB
1	e	8	GMA	O-C-CA-CB
1	WB	108	GMA	O-C-CA-CB
1	eA	408	GMA	OE2-CD-CG-CB
1	tA	408	GMA	OE2-CD-CG-CB
1	8A	408	GMA	OE2-CD-CG-CB
1	NB	408	GMA	OE2-CD-CG-CB
1	cB	408	GMA	OE2-CD-CG-CB
1	b	8	GMA	OE2-CD-CG-CB
1	c	8	GMA	OE2-CD-CG-CB
1	e	8	GMA	OE2-CD-CG-CB
1	WB	108	GMA	OE2-CD-CG-CB
1	a	8	GMA	OE2-CD-CG-CB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	YA	108	GMA	OE2-CD-CG-CB
1	d	8	GMA	OE2-CD-CG-CB
1	sA	358	GMA	C-CA-CB-CG
1	MB	358	GMA	C-CA-CB-CG
1	bB	358	GMA	C-CA-CB-CG
1	cA	308	GMA	OE2-CD-CG-CB
1	nA	108	GMA	OE2-CD-CG-CB
1	2A	108	GMA	OE2-CD-CG-CB
1	HB	108	GMA	OE2-CD-CG-CB
1	LB	308	GMA	OE2-CD-CG-CB
1	rA	308	GMA	OE2-CD-CG-CB
1	6A	308	GMA	OE2-CD-CG-CB
1	aB	308	GMA	OE2-CD-CG-CB
1	YA	108	GMA	CA-CB-CG-CD
1	nA	108	GMA	CA-CB-CG-CD
1	2A	108	GMA	CA-CB-CG-CD
1	WB	108	GMA	CA-CB-CG-CD
1	eA	408	GMA	OE1-CD-CG-CB
1	tA	408	GMA	OE1-CD-CG-CB
1	c	8	GMA	OE1-CD-CG-CB
1	8A	408	GMA	OE1-CD-CG-CB
1	dA	358	GMA	C-CA-CB-CG
1	7A	358	GMA	C-CA-CB-CG
1	a	8	GMA	OE1-CD-CG-CB
1	b	8	GMA	OE1-CD-CG-CB
1	d	8	GMA	OE1-CD-CG-CB
1	NB	408	GMA	OE1-CD-CG-CB
1	e	8	GMA	OE1-CD-CG-CB
1	cB	408	GMA	OE1-CD-CG-CB
1	YA	108	GMA	OE1-CD-CG-CB
1	nA	108	GMA	OE1-CD-CG-CB
1	2A	108	GMA	OE1-CD-CG-CB
1	HB	108	GMA	OE1-CD-CG-CB
1	WB	108	GMA	OE1-CD-CG-CB
1	aA	208	GMA	OE2-CD-CG-CB
1	pA	208	GMA	OE2-CD-CG-CB
1	4A	208	GMA	OE2-CD-CG-CB
1	JB	208	GMA	OE2-CD-CG-CB
1	YB	208	GMA	OE2-CD-CG-CB
1	HB	108	GMA	CA-CB-CG-CD
1	D	8	GMA	OE1-CD-CG-CB
1	J	8	GMA	OE1-CD-CG-CB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	A	8	GMA	OE1-CD-CG-CB
1	B	8	GMA	OE1-CD-CG-CB
1	C	8	GMA	OE1-CD-CG-CB
1	E	8	GMA	OE1-CD-CG-CB
1	F	8	GMA	OE1-CD-CG-CB
1	G	8	GMA	OE1-CD-CG-CB
1	H	8	GMA	OE1-CD-CG-CB
1	I	8	GMA	OE1-CD-CG-CB
1	eA	408	GMA	O-C-CA-CB
1	tA	408	GMA	O-C-CA-CB
1	8A	408	GMA	O-C-CA-CB
1	NB	408	GMA	O-C-CA-CB
1	cB	408	GMA	O-C-CA-CB
1	cA	308	GMA	OE1-CD-CG-CB
1	rA	308	GMA	OE1-CD-CG-CB
1	6A	308	GMA	OE1-CD-CG-CB
1	LB	308	GMA	OE1-CD-CG-CB
1	aB	308	GMA	OE1-CD-CG-CB
1	pA	208	GMA	OE1-CD-CG-CB
1	aA	208	GMA	OE1-CD-CG-CB
1	4A	208	GMA	OE1-CD-CG-CB
1	JB	208	GMA	OE1-CD-CG-CB
1	YB	208	GMA	OE1-CD-CG-CB
1	dA	358	GMA	OE1-CD-CG-CB
1	sA	358	GMA	OE1-CD-CG-CB
1	7A	358	GMA	OE1-CD-CG-CB
1	A	8	GMA	OE2-CD-CG-CB
1	B	8	GMA	OE2-CD-CG-CB
1	C	8	GMA	OE2-CD-CG-CB
1	D	8	GMA	OE2-CD-CG-CB
1	E	8	GMA	OE2-CD-CG-CB
1	F	8	GMA	OE2-CD-CG-CB
1	G	8	GMA	OE2-CD-CG-CB
1	H	8	GMA	OE2-CD-CG-CB
1	I	8	GMA	OE2-CD-CG-CB
1	J	8	GMA	OE2-CD-CG-CB
1	eA	408	GMA	CA-CB-CG-CD
1	tA	408	GMA	CA-CB-CG-CD
1	8A	408	GMA	CA-CB-CG-CD
1	NB	408	GMA	CA-CB-CG-CD
1	cB	408	GMA	CA-CB-CG-CD
1	MB	358	GMA	OE1-CD-CG-CB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	bB	358	GMA	OE1-CD-CG-CB
1	M	308	GMA	OE1-CD-CG-CB
1	LA	308	GMA	OE1-CD-CG-CB
1	sA	358	GMA	OE2-CD-CG-CB
1	R	108	GMA	OE1-CD-CG-CB
1	T	308	GMA	OE1-CD-CG-CB
1	m	308	GMA	OE1-CD-CG-CB
1	t	308	GMA	OE1-CD-CG-CB
1	y	108	GMA	OE1-CD-CG-CB
1	0	308	GMA	OE1-CD-CG-CB
1	CA	108	GMA	OE1-CD-CG-CB
1	EA	308	GMA	OE1-CD-CG-CB
1	QA	108	GMA	OE1-CD-CG-CB
1	SA	308	GMA	OE1-CD-CG-CB
1	dA	358	GMA	OE2-CD-CG-CB
1	7A	358	GMA	OE2-CD-CG-CB
1	MB	358	GMA	OE2-CD-CG-CB
1	bB	358	GMA	OE2-CD-CG-CB
1	K	108	GMA	OE1-CD-CG-CB
1	S	208	GMA	OE1-CD-CG-CB
1	Y	108	GMA	OE1-CD-CG-CB
1	Z	208	GMA	OE1-CD-CG-CB
1	f	308	GMA	OE1-CD-CG-CB
1	k	108	GMA	OE1-CD-CG-CB
1	l	208	GMA	OE1-CD-CG-CB
1	r	108	GMA	OE1-CD-CG-CB
1	5	108	GMA	OE1-CD-CG-CB
1	7	308	GMA	OE1-CD-CG-CB
1	JA	108	GMA	OE1-CD-CG-CB
1	RA	208	GMA	OE1-CD-CG-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

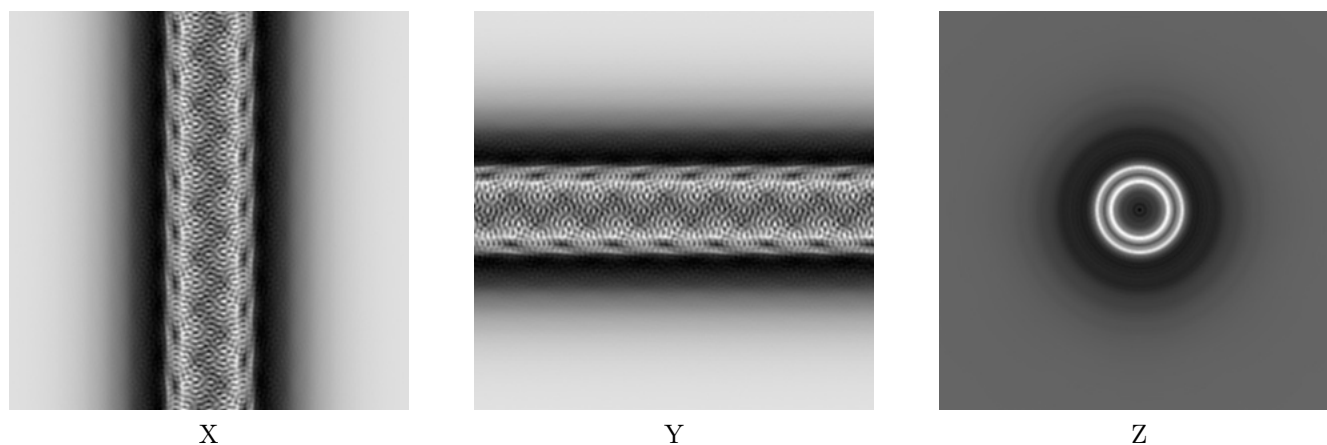
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23487. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

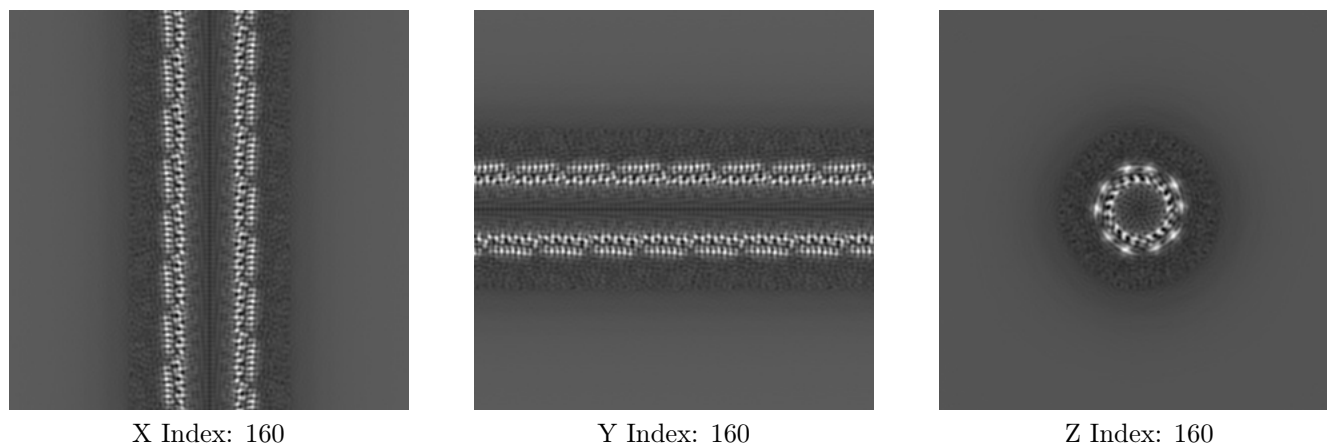
6.1.1 Primary map



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

6.2 Central slices [i](#)

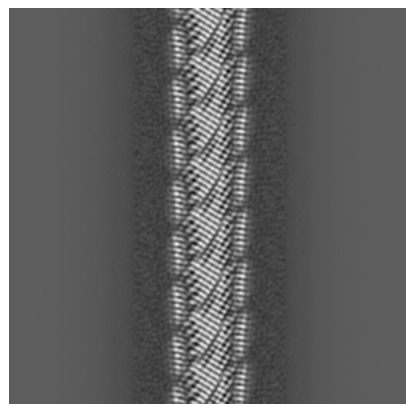
6.2.1 Primary map



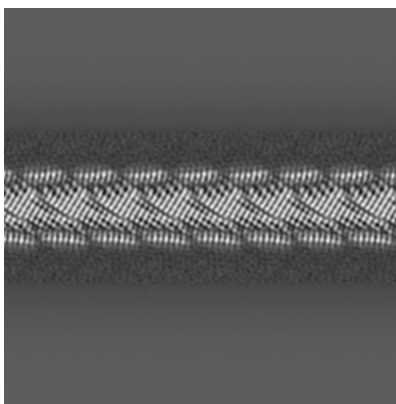
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

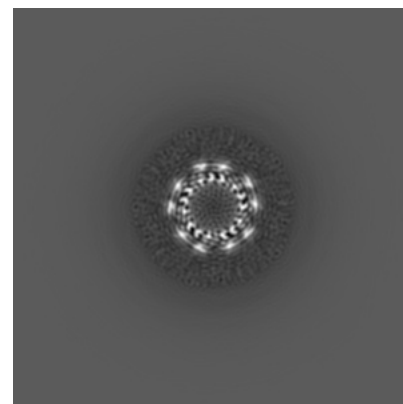
6.3.1 Primary map



X Index: 138



Y Index: 138



Z Index: 285

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

6.4 Orthogonal surface views [i](#)

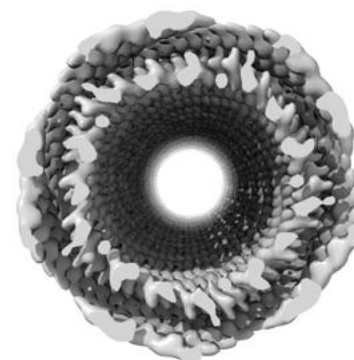
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.000542. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

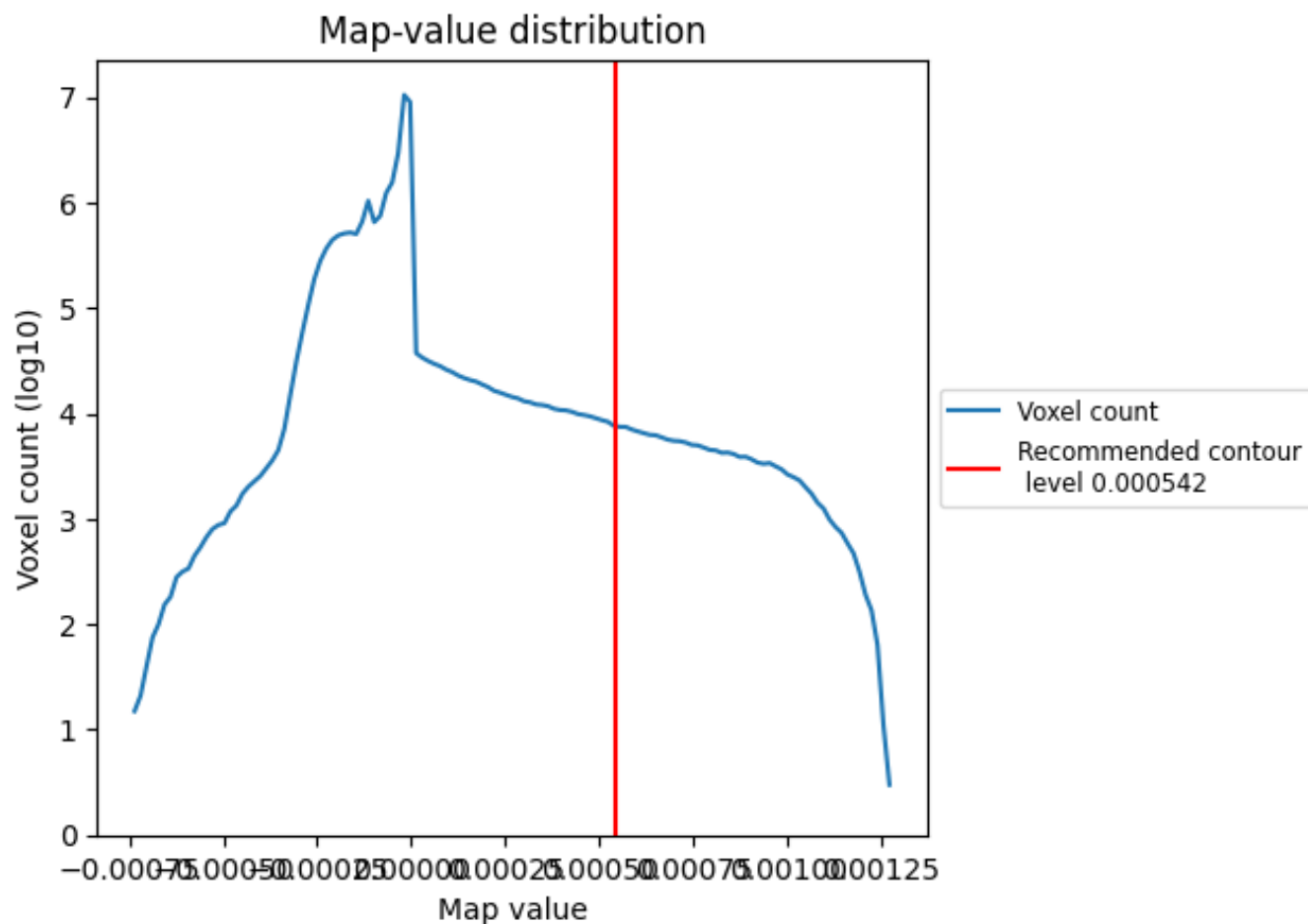
6.5 Mask visualisation

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

7 Map analysis [i](#)

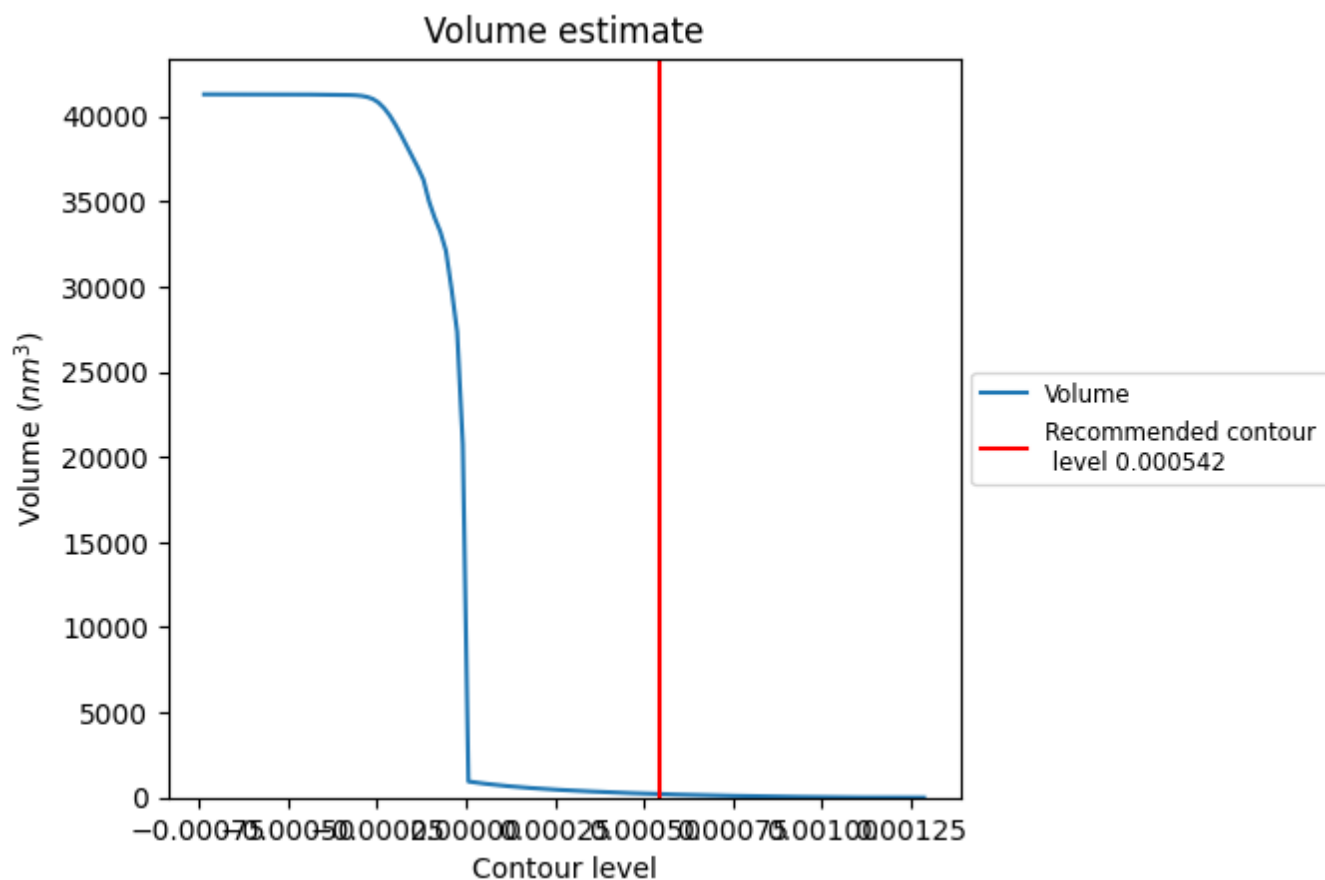
This section contains the results of statistical analysis of the map.

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.

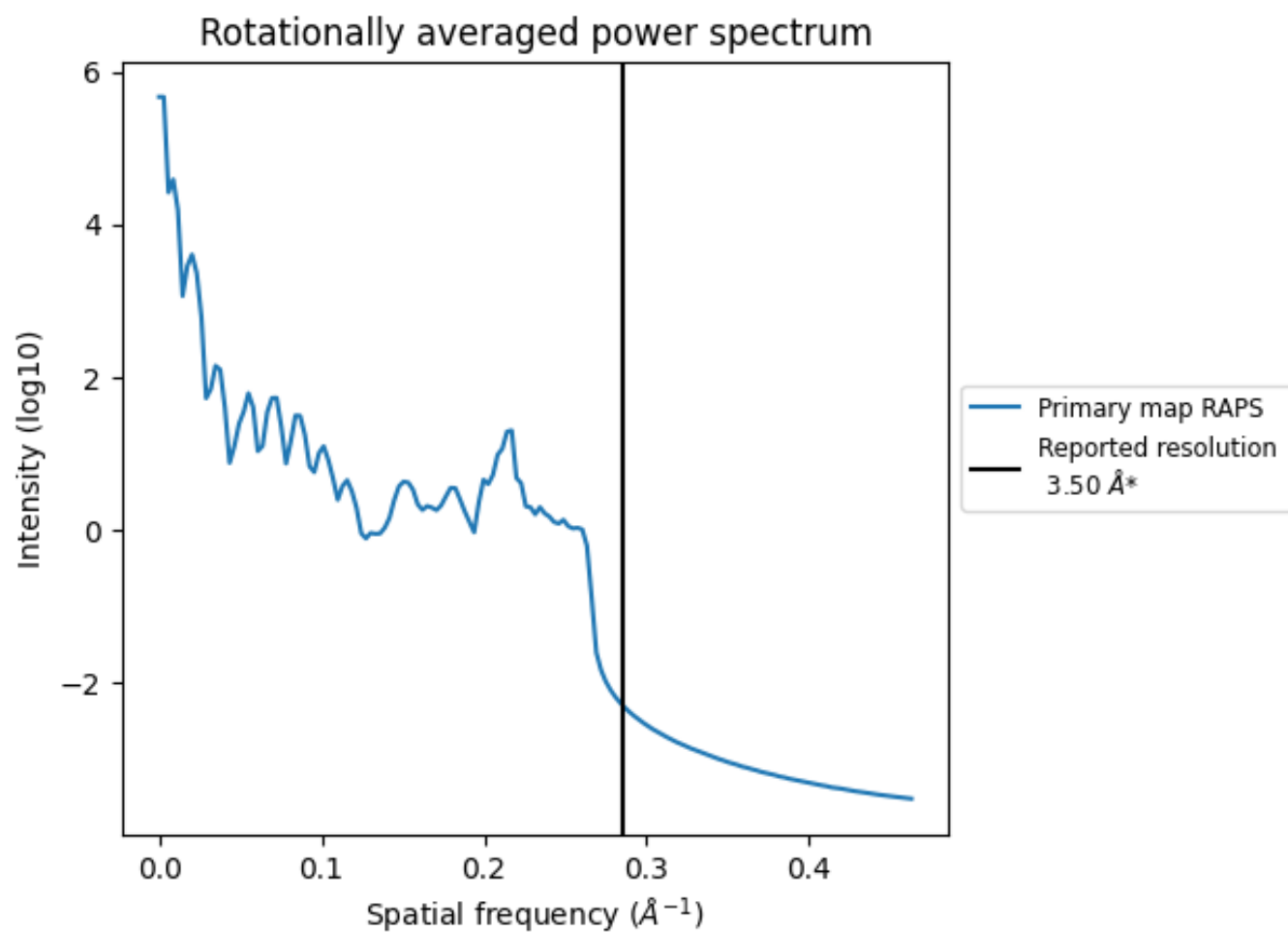
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 206 nm³; this corresponds to an approximate mass of 187 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 0.286 Å⁻¹

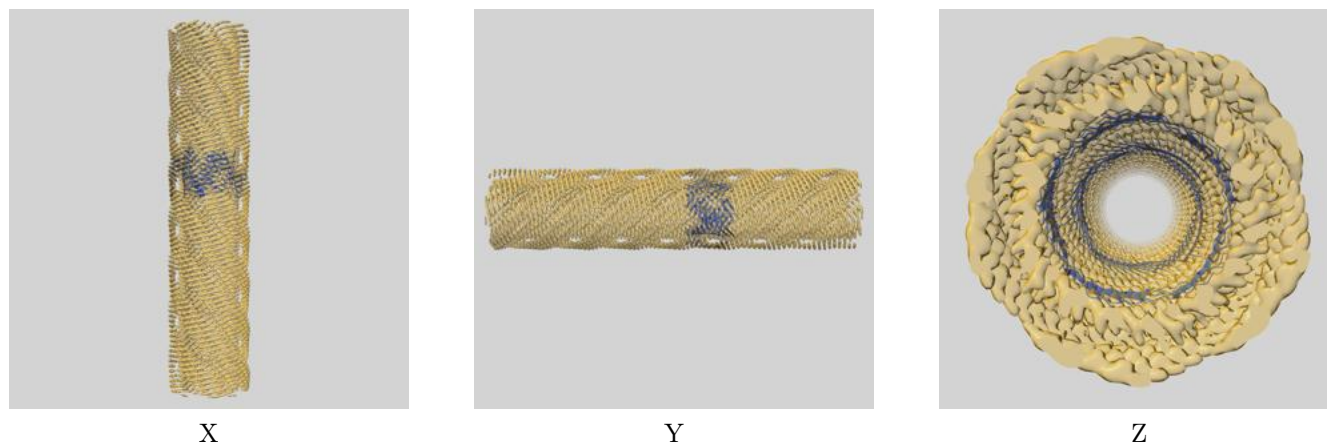
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

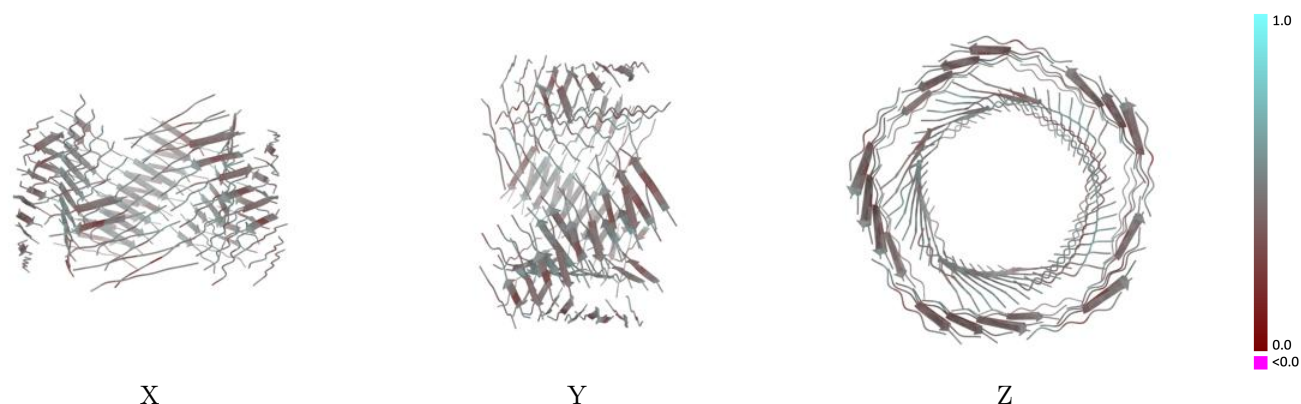
This section contains information regarding the fit between EMDB map EMD-23487 and PDB model 7LQI. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

9.1 Map-model overlay [i](#)



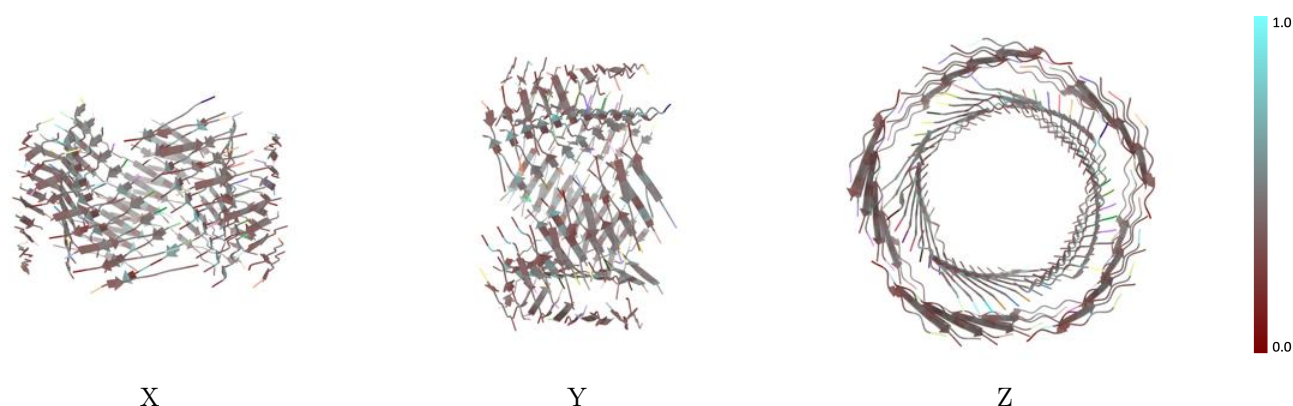
The images above show the 3D surface view of the map at the recommended contour level 0.000542 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



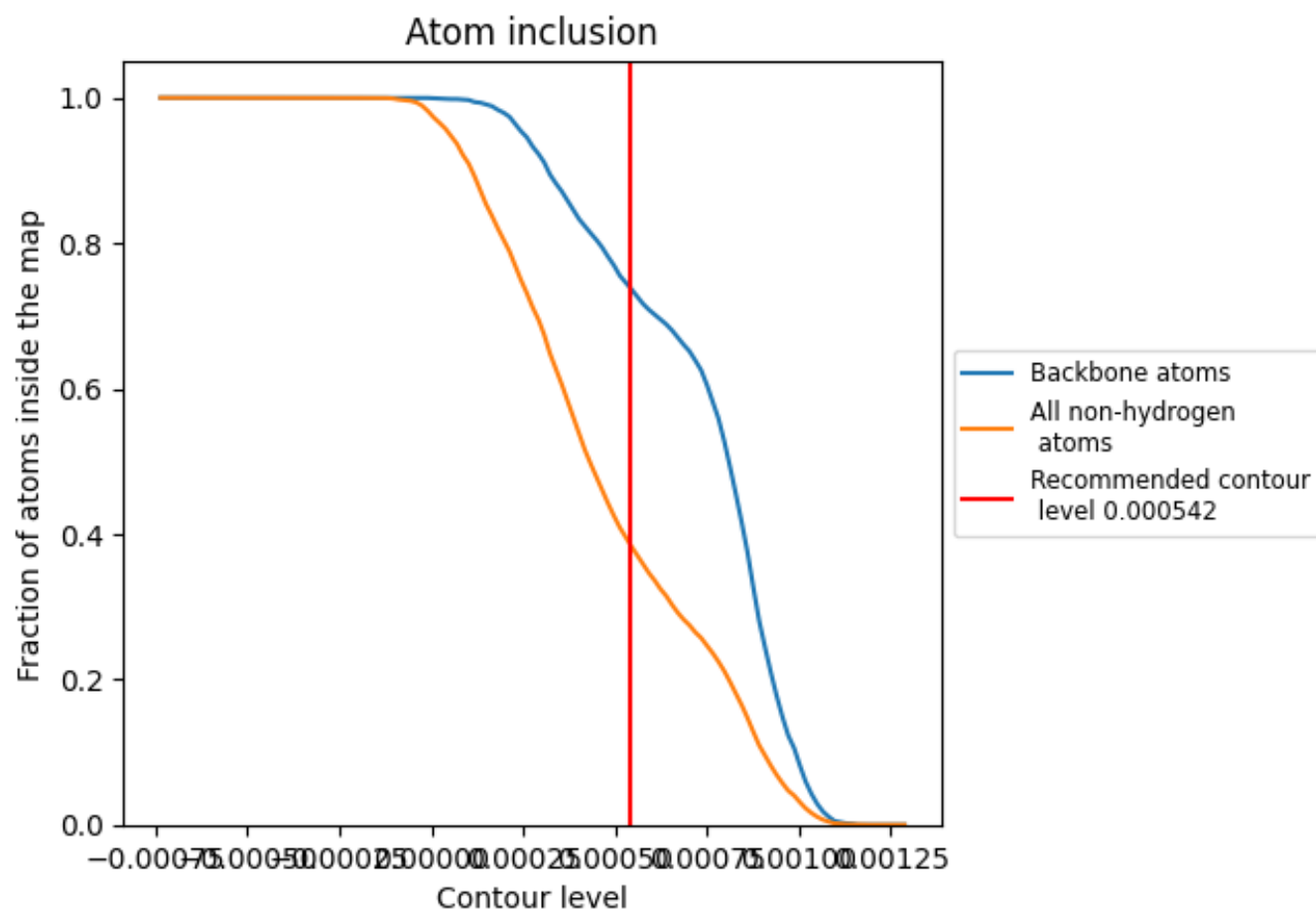
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.000542).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 38% 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 (0.000542) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3848	 0.4640
0	 0.4048	 0.5110
1	 0.4167	 0.5010
1A	 0.3095	 0.4330
2A	 0.3690	 0.4590
3A	 0.3214	 0.4380
4A	 0.3690	 0.4500
5	 0.4286	 0.5090
5A	 0.3214	 0.4250
6	 0.4405	 0.5180
6A	 0.3452	 0.4410
7	 0.4524	 0.5170
7A	 0.3214	 0.4390
8	 0.4167	 0.5020
8A	 0.3333	 0.4430
9A	 0.3333	 0.4500
A	 0.4405	 0.4750
B	 0.4167	 0.5180
C	 0.4405	 0.5110
CA	 0.4048	 0.4330
D	 0.4048	 0.5050
DA	 0.4286	 0.4610
E	 0.3810	 0.4930
EA	 0.4524	 0.4760
F	 0.4286	 0.5020
FA	 0.4286	 0.4610
G	 0.4286	 0.5010
GB	 0.3214	 0.4440
H	 0.4167	 0.4380
HB	 0.3690	 0.4640
I	 0.4286	 0.4520
IB	 0.3333	 0.4350
J	 0.4405	 0.4190
JA	 0.4524	 0.4720
JB	 0.3690	 0.4600



















































Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
K	 0.4286	 0.4600
KA	 0.4643	 0.4110
KB	 0.3214	 0.4430
L	 0.4405	 0.4530
LA	 0.4405	 0.3670
LB	 0.3571	 0.4440
M	 0.4286	 0.4650
MA	 0.4286	 0.3750
MB	 0.3214	 0.4380
N	 0.4286	 0.4810
NB	 0.3571	 0.4490
OB	 0.3333	 0.4430
QA	 0.4524	 0.4140
R	 0.4286	 0.5170
RA	 0.4405	 0.4040
S	 0.4286	 0.5150
SA	 0.4405	 0.4020
T	 0.4167	 0.5100
TA	 0.4524	 0.4100
U	 0.4167	 0.5140
VB	 0.3333	 0.4450
WB	 0.3690	 0.4630
XA	 0.3214	 0.4400
XB	 0.3333	 0.4400
Y	 0.4286	 0.5190
YA	 0.3333	 0.4630
YB	 0.3571	 0.4530
Z	 0.4524	 0.5180
ZA	 0.3333	 0.4410
ZB	 0.3214	 0.4500
a	 0.3333	 0.4660
aA	 0.3810	 0.4550
aB	 0.3690	 0.4520
b	 0.3571	 0.4580
bA	 0.3214	 0.4320
bB	 0.3333	 0.4550
c	 0.3571	 0.4620
cA	 0.3452	 0.4410
cB	 0.3571	 0.4450
d	 0.3452	 0.4590
dA	 0.3333	 0.4350
dB	 0.3214	 0.4500

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
e	 0.3571	 0.4660
eA	 0.3452	 0.4480
f	 0.4286	 0.5190
fA	 0.3214	 0.4460
g	 0.4167	 0.5140
k	 0.4286	 0.5180
l	 0.4167	 0.5130
m	 0.4286	 0.5080
mA	 0.3214	 0.4420
n	 0.4405	 0.5010
nA	 0.3571	 0.4550
oA	 0.3452	 0.4490
pA	 0.3452	 0.4550
qA	 0.3214	 0.4460
r	 0.4405	 0.5030
rA	 0.3333	 0.4370
s	 0.4405	 0.5060
sA	 0.3333	 0.4400
t	 0.4286	 0.5040
tA	 0.3333	 0.4290
u	 0.4167	 0.5120
uA	 0.3214	 0.4490
y	 0.4167	 0.5230
z	 0.4048	 0.5200