



wwPDB EM Validation Summary Report ⓘ

Aug 11, 2025 – 04:20 PM JST

PDB ID : 9K3N / pdb_00009k3n
EMDB ID : EMD-62023
Title : The structure of Salmonella phage PJNS002
Authors : Hu, W.L.; Chen, Y.B.; Wei, Y.M.; Gao, Y.
Deposited on : 2024-10-19
Resolution : 2.59 Å(reported)
Based on initial model : .

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev126
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

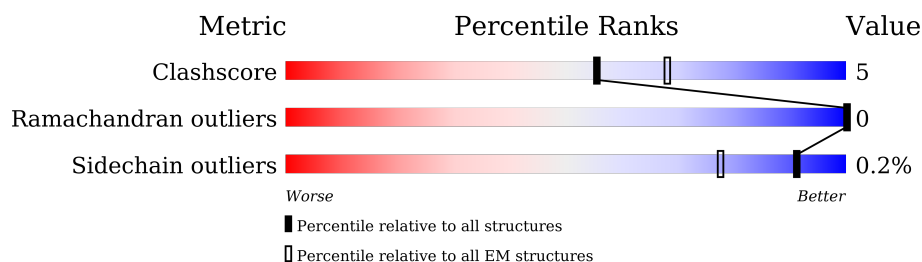
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.59 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.














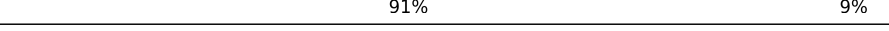







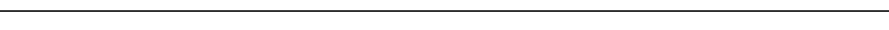

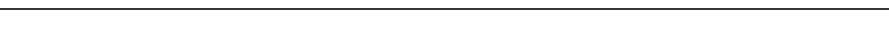
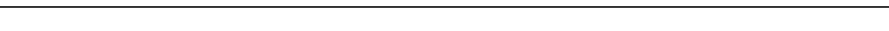


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	B	429	
1	BB	429	
1	BD	429	
1	BF	429	
1	BH	429	
1	DA	429	
1	DC	429	
1	DE	429	












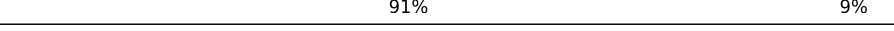







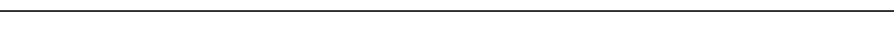

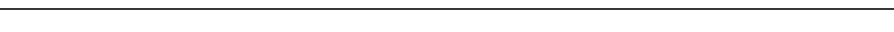
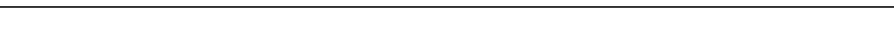


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Mol	Chain	Length	Quality of chain
1	DG	429	 91% 8%
1	DI	429	 92% 8%
1	F	429	 91% 9%
1	FB	429	 91% 9%
1	FD	429	 92% 8%
1	FF	429	 91% 9%
1	FH	429	 91% 9%
1	H	429	 91% 9%
1	HA	429	 91% 9%
1	HC	429	 91% 9%
1	HE	429	 91% 9%
1	HG	429	 91% 9%
1	JB	429	 91% 9%
1	JD	429	 91% 8%
1	JF	429	 91% 9%
1	JH	429	 91% 9%
1	LA	429	 91% 8%
1	LC	429	 91% 8%
1	LE	429	 91% 9%
1	LG	429	 91% 9%
1	M	429	 91% 9%
1	NB	429	 91% 9%
1	ND	429	 91% 9%
1	NF	429	 91% 9%
1	NH	429	 91% 9%












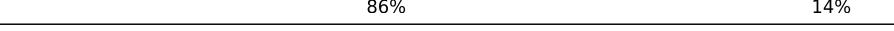







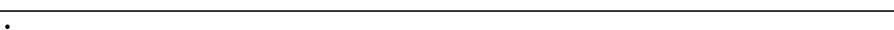

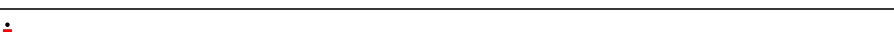
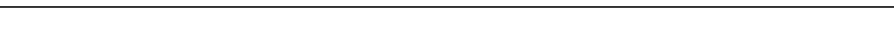


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Mol	Chain	Length	Quality of chain
1	PA	429	 91% 9%
1	PC	429	 91% 8%
1	PE	429	 91% 8%
1	PG	429	 92% 8%
1	Q	429	 91% 9%
1	RB	429	 91% 9%
1	RD	429	 91% 9%
1	RF	429	 91% 9%
1	RH	429	 91% 8%
1	TA	429	 91% 9%
1	TC	429	 91% 9%
1	TE	429	 91% 9%
1	TG	429	 91% 9%
1	V	429	 91% 9%
1	VB	429	 91% 9%
1	VD	429	 92% 8%
1	VF	429	 91% 9%
1	VH	429	 91% 9%
1	XA	429	 92% 8%
1	XC	429	 91% 9%
1	XE	429	 91% 9%
1	XG	429	 91% 9%
1	Z	429	 91% 9%
1	ZB	429	 91% 9%
1	ZD	429	 91% 9%














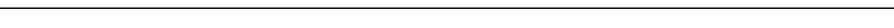











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Mol	Chain	Length	Quality of chain
1	ZF	429	 91% 9%
1	ZH	429	 91% 9%
2	AA	177	 89% 11%
2	AC	177	 88% 12%
2	AE	177	 86% 14%
2	AG	177	 86% 14%
2	AI	177	 89% 11%
2	C	177	 88% 12%
2	CB	177	 88% 12%
2	CD	177	 88% 12%
2	CF	177	 86% 14%
2	CH	177	 86% 14%
2	EA	177	 89% 11%
2	EC	177	 86% 14%
2	EE	177	 88% 12%
2	EG	177	 86% 14%
2	EI	177	 88% 12%
2	G	177	 88% 12%
2	GB	177	 86% 14%
2	GD	177	 88% 12%
2	GF	177	 86% 14%
2	GH	177	 88% 12%
2	I	177	 89% 11%
2	IA	177	 88% 12%
2	IC	177	 88% 12%


























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Mol	Chain	Length	Quality of chain
2	IE	177	 86% 14%
2	IG	177	 89% 11%
2	KB	177	 88% 12%
2	KD	177	 86% 14%
2	KF	177	 88% 12%
2	KH	177	 88% 12%
2	MA	177	 86% 14%
2	MC	177	 88% 12%
2	ME	177	 88% 12%
2	MG	177	 89% 11%
2	N	177	 89% 11%
2	OB	177	 88% 12%
2	OD	177	 89% 11%
2	OF	177	 86% 14%
2	OH	177	 86% 14%
2	QA	177	 86% 14%
2	QC	177	 86% 14%
2	QE	177	 88% 12%
2	QG	177	 88% 12%
2	R	177	 88% 12%
2	SB	177	 88% 12%
2	SD	177	 88% 12%
2	SF	177	 86% 14%
2	SH	177	 86% 14%
2	UA	177	 89% 11%





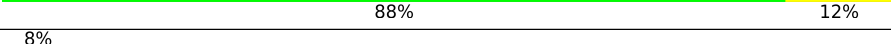
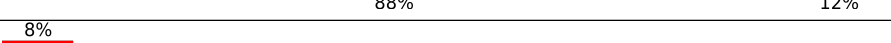








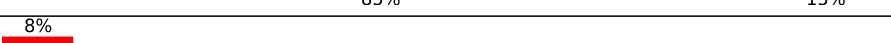






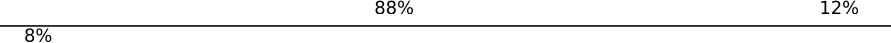



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Mol	Chain	Length	Quality of chain
2	UC	177	 89% 11%
2	UE	177	 86% 14%
2	UG	177	 86% 14%
2	W	177	 86% 14%
2	WB	177	 89% 11%
2	WD	177	 88% 12%
2	WF	177	 86% 14%
2	WH	177	 89% 11%
2	YA	177	 89% 11%
2	YC	177	 88% 12%
2	YE	177	 88% 12%
2	YG	177	 88% 12%
3	BA	26	 8% 85% 15%
3	BC	26	 8% 88% 12%
3	BE	26	 8% 85% 15%
3	BG	26	 8% 85% 15%
3	BI	26	 8% 85% 15%
3	D	26	 8% 85% 15%
3	DB	26	 8% 85% 15%
3	DD	26	 8% 88% 12%
3	DF	26	 8% 88% 12%
3	DH	26	 8% 85% 15%
3	FA	26	 8% 88% 12%
3	FC	26	 8% 88% 12%
3	FE	26	 8% 88% 12%

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Mol	Chain	Length	Quality of chain	
3	FG	26	8% 	81% 19%
3	FI	26	8% 	88% 12%
3	HB	26	8% 	88% 12%
3	HD	26	8% 	88% 12%
3	HF	26	8% 	88% 12%
3	HH	26	8% 	88% 12%
3	J	26	8% 	88% 12%
3	JA	26	8% 	85% 15%
3	JC	26	8% 	85% 15%
3	JE	26	8% 	85% 15%
3	JG	26	8% 	85% 15%
3	K	26	8% 	85% 15%
3	LB	26	8% 	85% 15%
3	LD	26	8% 	88% 12%
3	LF	26	8% 	85% 15%
3	LH	26	8% 	85% 15%
3	NA	26	8% 	88% 12%
3	NC	26	8% 	88% 12%
3	NE	26	8% 	88% 12%
3	NG	26	8% 	85% 15%
3	O	26	8% 	88% 12%
3	PB	26	8% 	85% 15%
3	PD	26	8% 	88% 12%
3	PF	26	8% 	88% 12%
3	PH	26	8% 	85% 15%



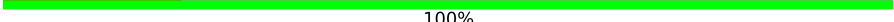

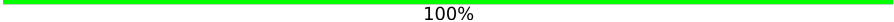

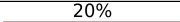


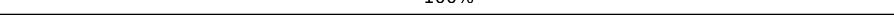

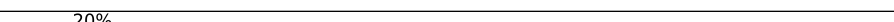
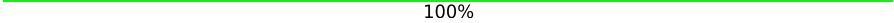

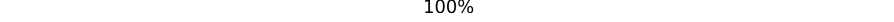
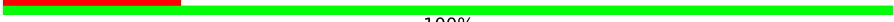

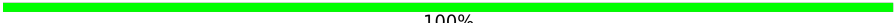






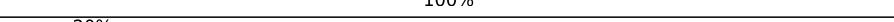


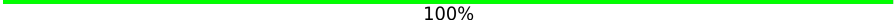


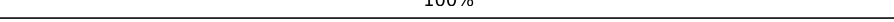

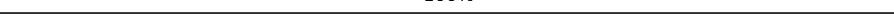
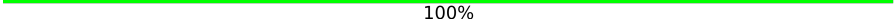

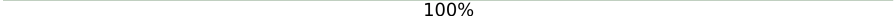
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Mol	Chain	Length	Quality of chain
3	RA	26	
3	RC	26	
3	RE	26	
3	RG	26	
3	S	26	
3	TB	26	
3	TD	26	
3	TF	26	
3	TH	26	
3	VA	26	
3	VC	26	
3	VE	26	
3	VG	26	
3	X	26	
3	XB	26	
3	XD	26	
3	XF	26	
3	XH	26	
3	ZA	26	
3	ZC	26	
3	ZE	26	
3	ZG	26	
4	A	5	
4	AB	5	
4	AD	5	

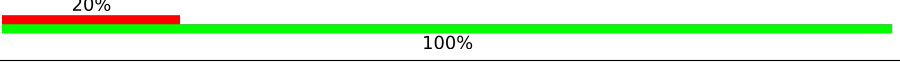
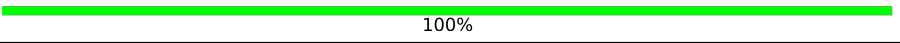
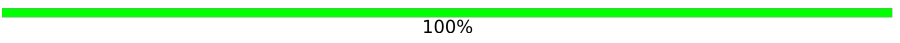
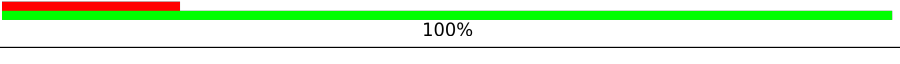
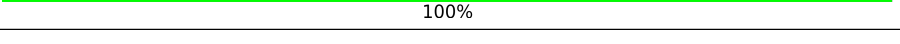
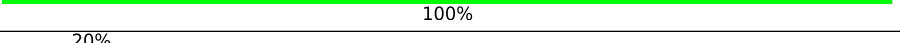
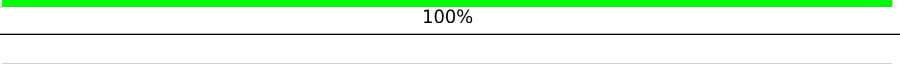
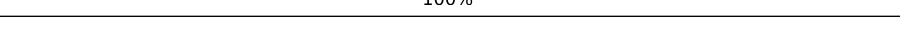
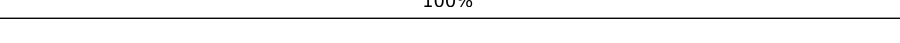
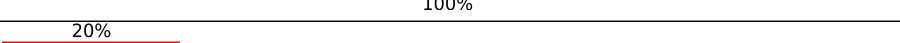
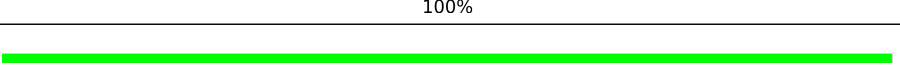

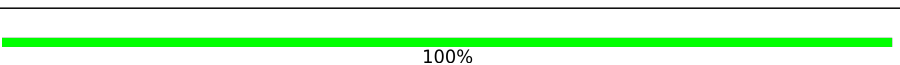
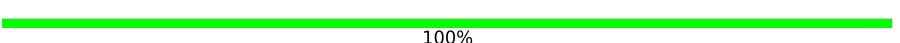
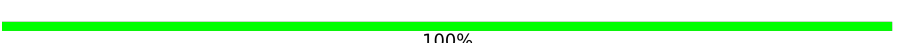
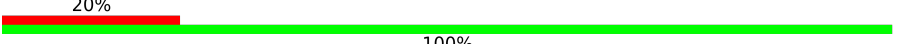
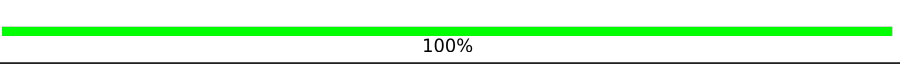
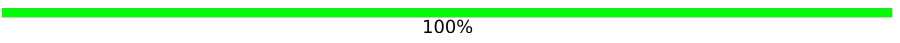
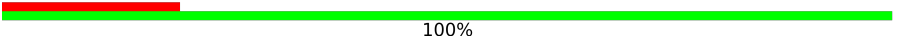
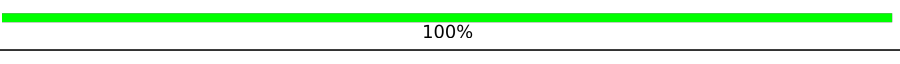
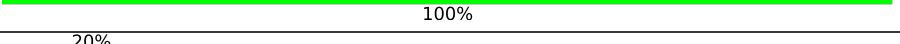
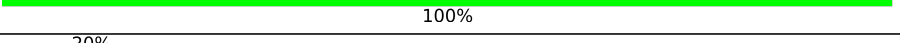
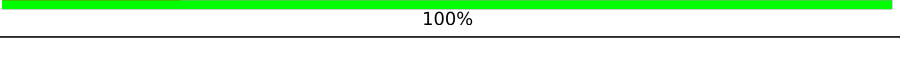
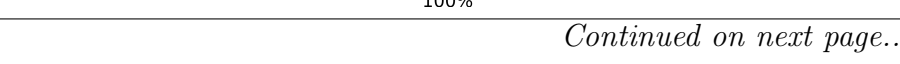

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Mol	Chain	Length	Quality of chain
4	AF	5	 100%
4	AH	5	 20%  100%
4	CA	5	 20%  100%
4	CC	5	 100%
4	CE	5	 20%  100%
4	CG	5	 100%
4	CI	5	 100%
4	E	5	 20%  100%
4	EB	5	 100%
4	ED	5	 20%  100%
4	EF	5	 100%
4	EH	5	 20%  100%
4	GA	5	 20%  100%
4	GC	5	 100%
4	GE	5	 100%
4	GG	5	 20%  100%
4	GI	5	 100%
4	IB	5	 100%
4	ID	5	 20%  100%
4	IF	5	 100%
4	IH	5	 100%
4	KA	5	 100%
4	KC	5	 20%  100%
4	KE	5	 100%
4	KG	5	 20%  100%

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Mol	Chain	Length	Quality of chain
4	L	5	
4	MB	5	
4	MD	5	
4	MF	5	
4	MH	5	
4	OA	5	
4	OC	5	
4	OE	5	
4	OG	5	
4	P	5	
4	QB	5	
4	QD	5	
4	QF	5	
4	QH	5	
4	SA	5	
4	SC	5	
4	SE	5	
4	SG	5	
4	T	5	
4	UB	5	
4	UD	5	
4	UF	5	
4	UH	5	
4	WA	5	
4	WC	5	





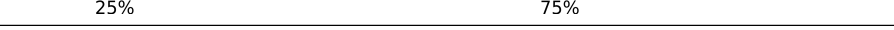
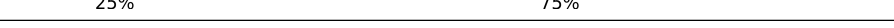

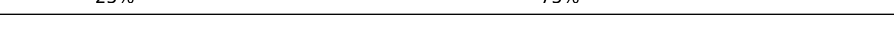
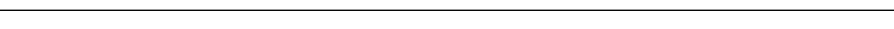
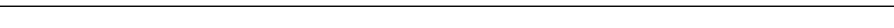




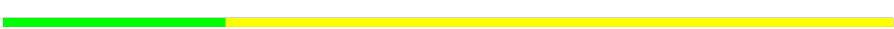
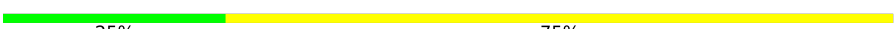


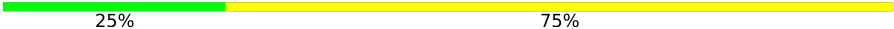






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Mol	Chain	Length	Quality of chain
4	WE	5	<div> <div>20%</div> <div>100%</div> </div>
4	WG	5	<div> <div>100%</div> </div>
4	Y	5	<div> <div>100%</div> </div>
4	YB	5	<div> <div>100%</div> </div>
4	YD	5	<div> <div>20%</div> <div>100%</div> </div>
4	YF	5	<div> <div>100%</div> </div>
4	YH	5	<div> <div>20%</div> <div>100%</div> </div>
5	0	4	<div> <div>25%</div> <div>75%</div> </div>
5	1	4	<div> <div>25%</div> <div>75%</div> </div>
5	2	4	<div> <div>25%</div> <div>75%</div> </div>
5	3	4	<div> <div>25%</div> <div>75%</div> </div>
5	4	4	<div> <div>25%</div> <div>75%</div> </div>
5	5	4	<div> <div>25%</div> <div>75%</div> </div>
5	6	4	<div> <div>25%</div> <div>75%</div> </div>
5	7	4	<div> <div>25%</div> <div>75%</div> </div>
5	8	4	<div> <div>25%</div> <div>75%</div> </div>
5	9	4	<div> <div>25%</div> <div>75%</div> </div>
5	U	4	<div> <div>25%</div> <div>75%</div> </div>
5	a	4	<div> <div>25%</div> <div>75%</div> </div>
5	aA	4	<div> <div>25%</div> <div>75%</div> </div>
5	b	4	<div> <div>25%</div> <div>75%</div> </div>
5	bA	4	<div> <div>25%</div> <div>75%</div> </div>
5	c	4	<div> <div>25%</div> <div>75%</div> </div>
5	cA	4	<div> <div>25%</div> <div>75%</div> </div>
5	d	4	<div> <div>25%</div> <div>75%</div> </div>




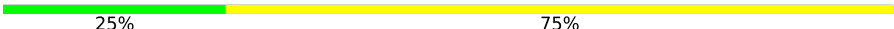
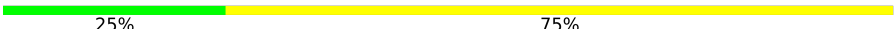
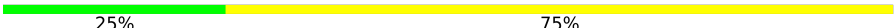
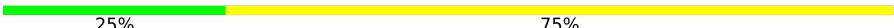


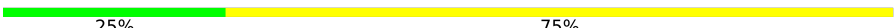
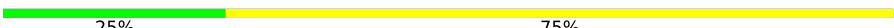
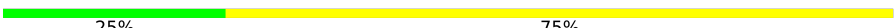




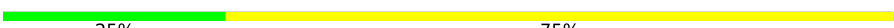
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Mol	Chain	Length	Quality of chain
5	dA	4	
5	e	4	
5	eA	4	
5	f	4	
5	fA	4	
5	g	4	
5	gA	4	
5	h	4	
5	hA	4	
5	i	4	
5	iA	4	
5	j	4	
5	jA	4	
5	k	4	
5	kA	4	
5	l	4	
5	lA	4	
5	m	4	
5	mA	4	
5	n	4	
5	nA	4	
5	o	4	
5	oA	4	
5	p	4	
5	pA	4	

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Mol	Chain	Length	Quality of chain
5	q	4	 25%75%
5	qA	4	 25%75%
5	r	4	 25%75%
5	rA	4	 25%75%
5	s	4	 25%75%
5	sA	4	 25%75%
5	t	4	 25%75%
5	tA	4	 25%75%
5	u	4	 25%75%
5	uA	4	 25%75%
5	v	4	 25%75%
5	vA	4	 25%75%
5	w	4	 25%75%
5	wA	4	 25%75%
5	x	4	 25%75%
5	y	4	 25%75%
5	z	4	 25%75%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 307380 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 capsid protein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		
1	B	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		
1	H	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		
1	M	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		
1	Q	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		
1	V	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		
1	Z	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		
1	DA	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		
1	HA	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		
1	LA	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		
1	PA	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		
1	TA	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		
1	XA	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		
1	BB	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		
1	FB	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		
1	JB	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		
1	NB	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	RB	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		
1	VB	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		
1	ZB	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		
1	DC	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		
1	HC	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		
1	LC	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		
1	PC	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		
1	TC	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		
1	XC	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		
1	BD	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		
1	FD	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		
1	JD	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		
1	ND	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		
1	RD	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		
1	VD	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		
1	ZD	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		
1	DE	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		
1	HE	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		
1	LE	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		
1	PE	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		
1	TE	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	XE	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		
1	BF	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		
1	FF	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		
1	JF	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		
1	NF	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		
1	RF	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		
1	VF	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		
1	ZF	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		
1	DG	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		
1	HG	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		
1	LG	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		
1	PG	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		
1	TG	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		
1	XG	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		
1	BH	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		
1	FH	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		
1	JH	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		
1	NH	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		
1	RH	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		
1	VH	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		
1	ZH	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	DI	428	Total	C	N	O	S	0	0
			3402	2159	586	641	16		

- Molecule 2 is a protein called spike protein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		
2	C	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		
2	I	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		
2	N	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		
2	R	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		
2	W	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		
2	AA	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		
2	EA	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		
2	IA	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		
2	MA	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		
2	QA	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		
2	UA	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		
2	YA	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		
2	CB	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		
2	GB	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		
2	KB	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		
2	OB	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		
2	SB	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	WB	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		
2	AC	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		
2	EC	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		
2	IC	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		
2	MC	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		
2	QC	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		
2	UC	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		
2	YC	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		
2	CD	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		
2	GD	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		
2	KD	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		
2	OD	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		
2	SD	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		
2	WD	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		
2	AE	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		
2	EE	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		
2	IE	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		
2	ME	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		
2	QE	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		
2	UE	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		
2	YE	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	CF	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		
2	GF	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		
2	KF	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		
2	OF	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		
2	SF	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		
2	WF	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		
2	AG	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		
2	EG	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		
2	IG	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		
2	MG	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		
2	QG	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		
2	UG	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		
2	YG	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		
2	CH	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		
2	GH	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		
2	KH	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		
2	OH	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		
2	SH	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		
2	WH	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		
2	AI	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		
2	EI	177	Total	C	N	O	S	0	0
			1327	854	214	254	5		

- Molecule 3 is a protein called DNA-binding protein J.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	26	Total 205	C 129	N 41	O 34	S 1	0	0
3	D	26	Total 205	C 129	N 41	O 34	S 1	0	0
3	K	26	Total 205	C 129	N 41	O 34	S 1	0	0
3	O	26	Total 205	C 129	N 41	O 34	S 1	0	0
3	S	26	Total 205	C 129	N 41	O 34	S 1	0	0
3	X	26	Total 205	C 129	N 41	O 34	S 1	0	0
3	BA	26	Total 205	C 129	N 41	O 34	S 1	0	0
3	FA	26	Total 205	C 129	N 41	O 34	S 1	0	0
3	JA	26	Total 205	C 129	N 41	O 34	S 1	0	0
3	NA	26	Total 205	C 129	N 41	O 34	S 1	0	0
3	RA	26	Total 205	C 129	N 41	O 34	S 1	0	0
3	VA	26	Total 205	C 129	N 41	O 34	S 1	0	0
3	ZA	26	Total 205	C 129	N 41	O 34	S 1	0	0
3	DB	26	Total 205	C 129	N 41	O 34	S 1	0	0
3	HB	26	Total 205	C 129	N 41	O 34	S 1	0	0
3	LB	26	Total 205	C 129	N 41	O 34	S 1	0	0
3	PB	26	Total 205	C 129	N 41	O 34	S 1	0	0
3	TB	26	Total 205	C 129	N 41	O 34	S 1	0	0
3	XB	26	Total 205	C 129	N 41	O 34	S 1	0	0
3	BC	26	Total 205	C 129	N 41	O 34	S 1	0	0
3	FC	26	Total 205	C 129	N 41	O 34	S 1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	JC	26	Total 205	C 129	N 41	O 34	S 1	0	0
3	NC	26	Total 205	C 129	N 41	O 34	S 1	0	0
3	RC	26	Total 205	C 129	N 41	O 34	S 1	0	0
3	VC	26	Total 205	C 129	N 41	O 34	S 1	0	0
3	ZC	26	Total 205	C 129	N 41	O 34	S 1	0	0
3	DD	26	Total 205	C 129	N 41	O 34	S 1	0	0
3	HD	26	Total 205	C 129	N 41	O 34	S 1	0	0
3	LD	26	Total 205	C 129	N 41	O 34	S 1	0	0
3	PD	26	Total 205	C 129	N 41	O 34	S 1	0	0
3	TD	26	Total 205	C 129	N 41	O 34	S 1	0	0
3	XD	26	Total 205	C 129	N 41	O 34	S 1	0	0
3	BE	26	Total 205	C 129	N 41	O 34	S 1	0	0
3	FE	26	Total 205	C 129	N 41	O 34	S 1	0	0
3	JE	26	Total 205	C 129	N 41	O 34	S 1	0	0
3	NE	26	Total 205	C 129	N 41	O 34	S 1	0	0
3	RE	26	Total 205	C 129	N 41	O 34	S 1	0	0
3	VE	26	Total 205	C 129	N 41	O 34	S 1	0	0
3	ZE	26	Total 205	C 129	N 41	O 34	S 1	0	0
3	DF	26	Total 205	C 129	N 41	O 34	S 1	0	0
3	HF	26	Total 205	C 129	N 41	O 34	S 1	0	0
3	LF	26	Total 205	C 129	N 41	O 34	S 1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	PF	26	Total 205	C 129	N 41	O 34	S 1	0	0
3	TF	26	Total 205	C 129	N 41	O 34	S 1	0	0
3	XF	26	Total 205	C 129	N 41	O 34	S 1	0	0
3	BG	26	Total 205	C 129	N 41	O 34	S 1	0	0
3	FG	26	Total 205	C 129	N 41	O 34	S 1	0	0
3	JG	26	Total 205	C 129	N 41	O 34	S 1	0	0
3	NG	26	Total 205	C 129	N 41	O 34	S 1	0	0
3	RG	26	Total 205	C 129	N 41	O 34	S 1	0	0
3	VG	26	Total 205	C 129	N 41	O 34	S 1	0	0
3	ZG	26	Total 205	C 129	N 41	O 34	S 1	0	0
3	DH	26	Total 205	C 129	N 41	O 34	S 1	0	0
3	HH	26	Total 205	C 129	N 41	O 34	S 1	0	0
3	LH	26	Total 205	C 129	N 41	O 34	S 1	0	0
3	PH	26	Total 205	C 129	N 41	O 34	S 1	0	0
3	TH	26	Total 205	C 129	N 41	O 34	S 1	0	0
3	XH	26	Total 205	C 129	N 41	O 34	S 1	0	0
3	BI	26	Total 205	C 129	N 41	O 34	S 1	0	0
3	FI	26	Total 205	C 129	N 41	O 34	S 1	0	0

- Molecule 4 is a DNA chain called DNA (5'-D(P*AP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	5	Total 105	C 50	N 25	O 25	P 5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	5	Total 105	C 50	N 25	O 25	P 5	0	0
4	L	5	Total 105	C 50	N 25	O 25	P 5	0	0
4	P	5	Total 105	C 50	N 25	O 25	P 5	0	0
4	T	5	Total 105	C 50	N 25	O 25	P 5	0	0
4	Y	5	Total 105	C 50	N 25	O 25	P 5	0	0
4	CA	5	Total 105	C 50	N 25	O 25	P 5	0	0
4	GA	5	Total 105	C 50	N 25	O 25	P 5	0	0
4	KA	5	Total 105	C 50	N 25	O 25	P 5	0	0
4	OA	5	Total 105	C 50	N 25	O 25	P 5	0	0
4	SA	5	Total 105	C 50	N 25	O 25	P 5	0	0
4	WA	5	Total 105	C 50	N 25	O 25	P 5	0	0
4	AB	5	Total 105	C 50	N 25	O 25	P 5	0	0
4	EB	5	Total 105	C 50	N 25	O 25	P 5	0	0
4	IB	5	Total 105	C 50	N 25	O 25	P 5	0	0
4	MB	5	Total 105	C 50	N 25	O 25	P 5	0	0
4	QB	5	Total 105	C 50	N 25	O 25	P 5	0	0
4	UB	5	Total 105	C 50	N 25	O 25	P 5	0	0
4	YB	5	Total 105	C 50	N 25	O 25	P 5	0	0
4	CC	5	Total 105	C 50	N 25	O 25	P 5	0	0
4	GC	5	Total 105	C 50	N 25	O 25	P 5	0	0
4	KC	5	Total 105	C 50	N 25	O 25	P 5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	OC	5	Total 105	C 50	N 25	O 25	P 5	0	0
4	SC	5	Total 105	C 50	N 25	O 25	P 5	0	0
4	WC	5	Total 105	C 50	N 25	O 25	P 5	0	0
4	AD	5	Total 105	C 50	N 25	O 25	P 5	0	0
4	ED	5	Total 105	C 50	N 25	O 25	P 5	0	0
4	ID	5	Total 105	C 50	N 25	O 25	P 5	0	0
4	MD	5	Total 105	C 50	N 25	O 25	P 5	0	0
4	QD	5	Total 105	C 50	N 25	O 25	P 5	0	0
4	UD	5	Total 105	C 50	N 25	O 25	P 5	0	0
4	YD	5	Total 105	C 50	N 25	O 25	P 5	0	0
4	CE	5	Total 105	C 50	N 25	O 25	P 5	0	0
4	GE	5	Total 105	C 50	N 25	O 25	P 5	0	0
4	KE	5	Total 105	C 50	N 25	O 25	P 5	0	0
4	OE	5	Total 105	C 50	N 25	O 25	P 5	0	0
4	SE	5	Total 105	C 50	N 25	O 25	P 5	0	0
4	WE	5	Total 105	C 50	N 25	O 25	P 5	0	0
4	AF	5	Total 105	C 50	N 25	O 25	P 5	0	0
4	EF	5	Total 105	C 50	N 25	O 25	P 5	0	0
4	IF	5	Total 105	C 50	N 25	O 25	P 5	0	0
4	MF	5	Total 105	C 50	N 25	O 25	P 5	0	0
4	QF	5	Total 105	C 50	N 25	O 25	P 5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	UF	5	Total 105	C 50	N 25	O 25	P 5	0	0
4	YF	5	Total 105	C 50	N 25	O 25	P 5	0	0
4	CG	5	Total 105	C 50	N 25	O 25	P 5	0	0
4	GG	5	Total 105	C 50	N 25	O 25	P 5	0	0
4	KG	5	Total 105	C 50	N 25	O 25	P 5	0	0
4	OG	5	Total 105	C 50	N 25	O 25	P 5	0	0
4	SG	5	Total 105	C 50	N 25	O 25	P 5	0	0
4	WG	5	Total 105	C 50	N 25	O 25	P 5	0	0
4	AH	5	Total 105	C 50	N 25	O 25	P 5	0	0
4	EH	5	Total 105	C 50	N 25	O 25	P 5	0	0
4	IH	5	Total 105	C 50	N 25	O 25	P 5	0	0
4	MH	5	Total 105	C 50	N 25	O 25	P 5	0	0
4	QH	5	Total 105	C 50	N 25	O 25	P 5	0	0
4	UH	5	Total 105	C 50	N 25	O 25	P 5	0	0
4	YH	5	Total 105	C 50	N 25	O 25	P 5	0	0
4	CI	5	Total 105	C 50	N 25	O 25	P 5	0	0
4	GI	5	Total 105	C 50	N 25	O 25	P 5	0	0

- Molecule 5 is a DNA chain called DNA (5'-D(P*AP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
5	U	4	Total 84	C 40	N 20	O 20	P 4	0	0
5	a	4	Total 84	C 40	N 20	O 20	P 4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	b	4	Total 84	C 40	N 20	O 20	P 4	0	0
5	c	4	Total 84	C 40	N 20	O 20	P 4	0	0
5	d	4	Total 84	C 40	N 20	O 20	P 4	0	0
5	e	4	Total 84	C 40	N 20	O 20	P 4	0	0
5	f	4	Total 84	C 40	N 20	O 20	P 4	0	0
5	g	4	Total 84	C 40	N 20	O 20	P 4	0	0
5	h	4	Total 84	C 40	N 20	O 20	P 4	0	0
5	i	4	Total 84	C 40	N 20	O 20	P 4	0	0
5	j	4	Total 84	C 40	N 20	O 20	P 4	0	0
5	k	4	Total 84	C 40	N 20	O 20	P 4	0	0
5	l	4	Total 84	C 40	N 20	O 20	P 4	0	0
5	m	4	Total 84	C 40	N 20	O 20	P 4	0	0
5	n	4	Total 84	C 40	N 20	O 20	P 4	0	0
5	o	4	Total 84	C 40	N 20	O 20	P 4	0	0
5	p	4	Total 84	C 40	N 20	O 20	P 4	0	0
5	q	4	Total 84	C 40	N 20	O 20	P 4	0	0
5	r	4	Total 84	C 40	N 20	O 20	P 4	0	0
5	s	4	Total 84	C 40	N 20	O 20	P 4	0	0
5	t	4	Total 84	C 40	N 20	O 20	P 4	0	0
5	u	4	Total 84	C 40	N 20	O 20	P 4	0	0
5	v	4	Total 84	C 40	N 20	O 20	P 4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	w	4	Total 84	C 40	N 20	O 20	P 4	0	0
5	x	4	Total 84	C 40	N 20	O 20	P 4	0	0
5	y	4	Total 84	C 40	N 20	O 20	P 4	0	0
5	z	4	Total 84	C 40	N 20	O 20	P 4	0	0
5	0	4	Total 84	C 40	N 20	O 20	P 4	0	0
5	1	4	Total 84	C 40	N 20	O 20	P 4	0	0
5	2	4	Total 84	C 40	N 20	O 20	P 4	0	0
5	3	4	Total 84	C 40	N 20	O 20	P 4	0	0
5	4	4	Total 84	C 40	N 20	O 20	P 4	0	0
5	5	4	Total 84	C 40	N 20	O 20	P 4	0	0
5	6	4	Total 84	C 40	N 20	O 20	P 4	0	0
5	7	4	Total 84	C 40	N 20	O 20	P 4	0	0
5	8	4	Total 84	C 40	N 20	O 20	P 4	0	0
5	9	4	Total 84	C 40	N 20	O 20	P 4	0	0
5	aA	4	Total 84	C 40	N 20	O 20	P 4	0	0
5	bA	4	Total 84	C 40	N 20	O 20	P 4	0	0
5	cA	4	Total 84	C 40	N 20	O 20	P 4	0	0
5	dA	4	Total 84	C 40	N 20	O 20	P 4	0	0
5	eA	4	Total 84	C 40	N 20	O 20	P 4	0	0
5	fA	4	Total 84	C 40	N 20	O 20	P 4	0	0
5	gA	4	Total 84	C 40	N 20	O 20	P 4	0	0

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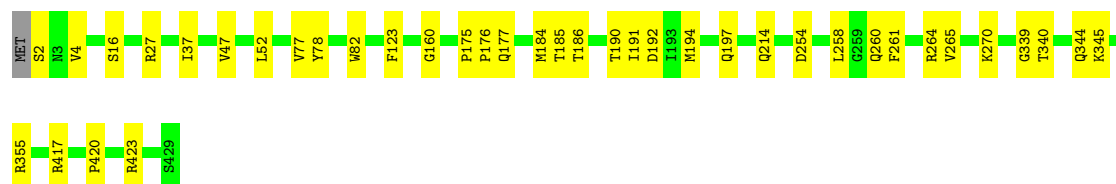
Mol	Chain	Residues	Atoms					AltConf	Trace
5	hA	4	Total 84	C 40	N 20	O 20	P 4	0	0
5	iA	4	Total 84	C 40	N 20	O 20	P 4	0	0
5	jA	4	Total 84	C 40	N 20	O 20	P 4	0	0
5	kA	4	Total 84	C 40	N 20	O 20	P 4	0	0
5	lA	4	Total 84	C 40	N 20	O 20	P 4	0	0
5	mA	4	Total 84	C 40	N 20	O 20	P 4	0	0
5	nA	4	Total 84	C 40	N 20	O 20	P 4	0	0
5	oA	4	Total 84	C 40	N 20	O 20	P 4	0	0
5	pA	4	Total 84	C 40	N 20	O 20	P 4	0	0
5	qA	4	Total 84	C 40	N 20	O 20	P 4	0	0
5	rA	4	Total 84	C 40	N 20	O 20	P 4	0	0
5	sA	4	Total 84	C 40	N 20	O 20	P 4	0	0
5	tA	4	Total 84	C 40	N 20	O 20	P 4	0	0
5	uA	4	Total 84	C 40	N 20	O 20	P 4	0	0
5	vA	4	Total 84	C 40	N 20	O 20	P 4	0	0
5	wA	4	Total 84	C 40	N 20	O 20	P 4	0	0

3 Residue-property plots

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.

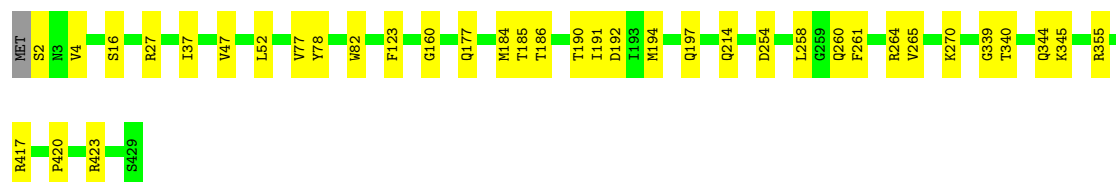
- Molecule 1: capsid protein F

Chain F: 



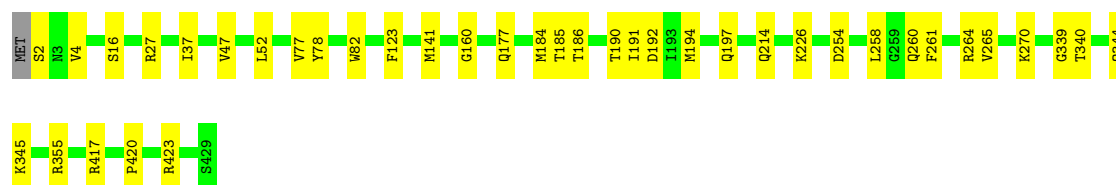
- Molecule 1: capsid protein F

Chain B: 



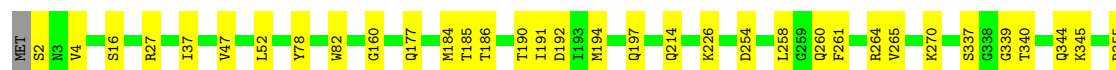
- Molecule 1: capsid protein F

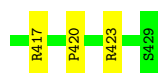
Chain H: 



- Molecule 1: capsid protein F

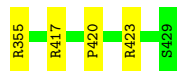
Chain M: 





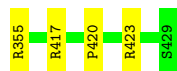
- Molecule 1: capsid protein F

Chain Q: 91% 9%



- Molecule 1: capsid protein F

Chain V: 91% 9%



- Molecule 1: capsid protein F

Chain Z: 91% 9%



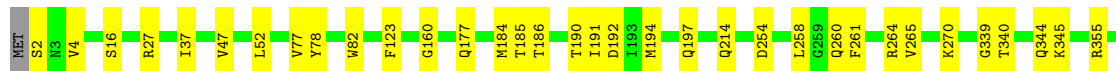
- Molecule 1: capsid protein F

Chain DA: 91% 9%



- Molecule 1: capsid protein F

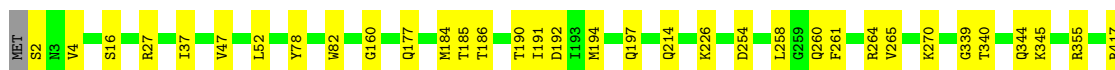
Chain HA: 91% 9%





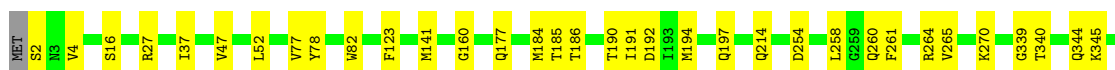
- Molecule 1: capsid protein F

Chain LA: 91% 8%



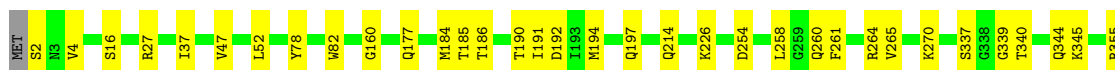
- Molecule 1: capsid protein F

Chain PA: 91% 9%



- Molecule 1: capsid protein F

Chain TA: 91% 9%



- Molecule 1: capsid protein F

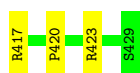
Chain XA: 92% 8%



- Molecule 1: capsid protein F

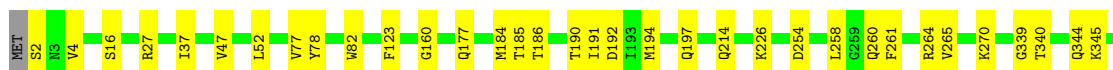
Chain BB: 91% 9%





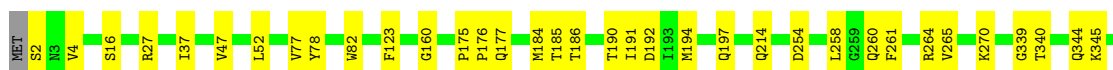
- Molecule 1: capsid protein F

Chain FB: 91% 9%



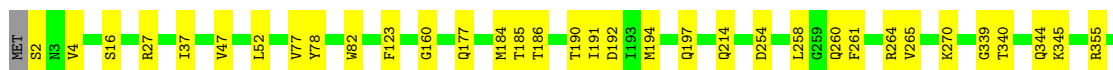
- Molecule 1: capsid protein F

Chain JB: 91% 9%



- Molecule 1: capsid protein F

Chain NB: 91% 9%



- Molecule 1: capsid protein F

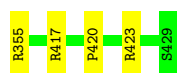
Chain RB: 91% 9%



- Molecule 1: capsid protein F

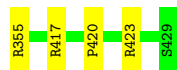
Chain VB: 91% 9%





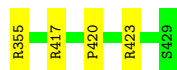
- Molecule 1: capsid protein F

Chain ZB: 91% 9%



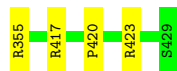
- Molecule 1: capsid protein F

Chain DC: 91% 9%



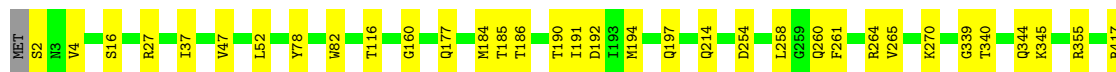
- Molecule 1: capsid protein F

Chain HC: 91% 9%



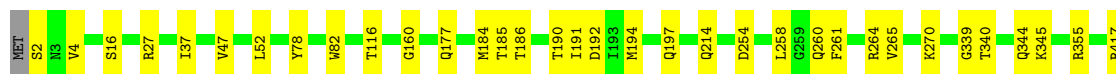
- Molecule 1: capsid protein F

Chain LC: 91% 8%



- Molecule 1: capsid protein F

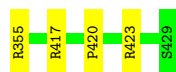
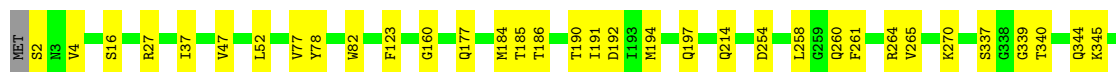
Chain PC: 91% 8%





- Molecule 1: capsid protein F

Chain TC: 91% 9%



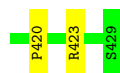
- Molecule 1: capsid protein F

Chain XC: 91% 9%



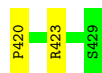
- Molecule 1: capsid protein F

Chain BD: 91% 8%



- Molecule 1: capsid protein F

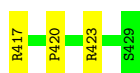
Chain FD: 92% 8%



- Molecule 1: capsid protein F

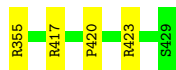
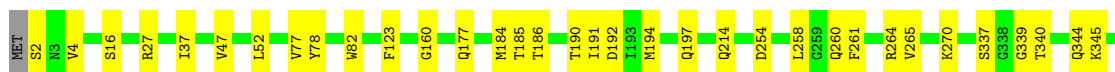
Chain JD: 91% 8%





- Molecule 1: capsid protein F

Chain ND: 91% 9%



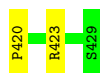
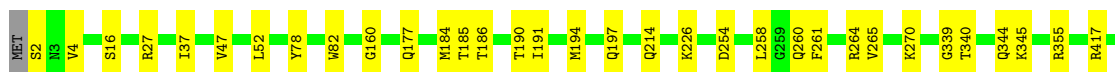
- Molecule 1: capsid protein F

Chain RD: 91% 9%



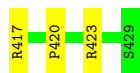
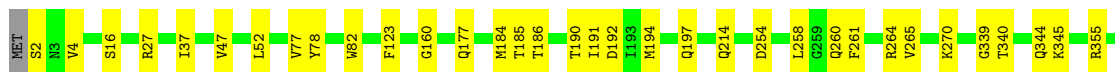
- Molecule 1: capsid protein F

Chain VD: 92% 8%



- Molecule 1: capsid protein F

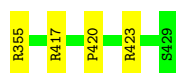
Chain ZD: 91% 9%



- Molecule 1: capsid protein F

Chain DE: 91% 9%





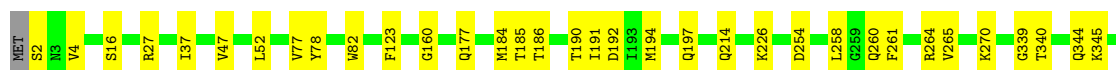
- Molecule 1: capsid protein F

Chain HE: 91% 9%



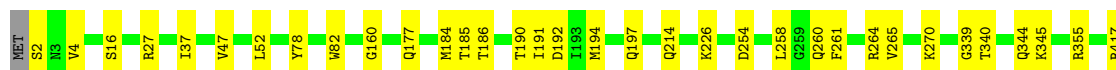
- Molecule 1: capsid protein F

Chain LE: 91% 9%



- Molecule 1: capsid protein F

Chain PE: 91% 8%



- Molecule 1: capsid protein F

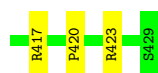
Chain TE: 91% 9%



- Molecule 1: capsid protein F

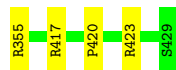
Chain XE: 91% 9%





- Molecule 1: capsid protein F

Chain BF:  91% 9%



- Molecule 1: capsid protein F

Chain FF:  91% 9%



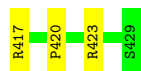
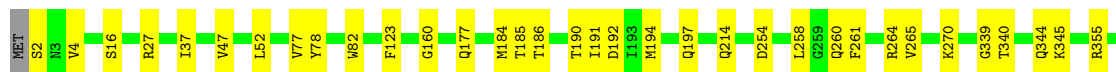
- Molecule 1: capsid protein F

Chain JF:  91% 9%



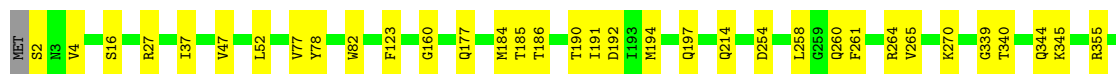
- Molecule 1: capsid protein F

Chain NF:  91% 9%



- Molecule 1: capsid protein F

Chain RF:  91% 9%





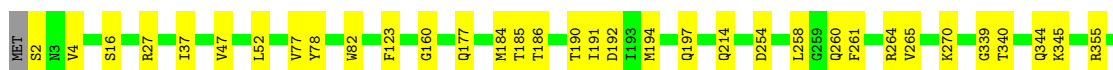
- Molecule 1: capsid protein F

Chain VF:  91% 9%



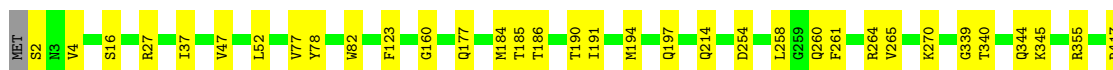
- Molecule 1: capsid protein F

Chain ZF:  91% 9%



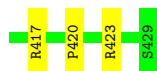
- Molecule 1: capsid protein F

Chain DG:  91% 8%



- Molecule 1: capsid protein F

Chain HG:  91% 9%



- Molecule 1: capsid protein F

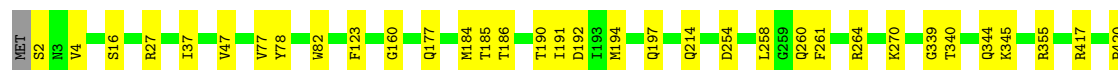
Chain LG:  91% 9%





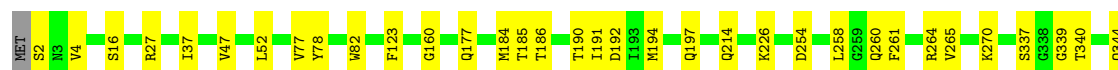
- Molecule 1: capsid protein F

Chain PG:  92% 8%



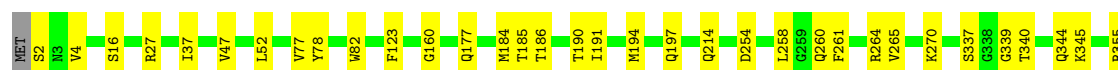
- Molecule 1: capsid protein F

Chain TG:  91% 9%



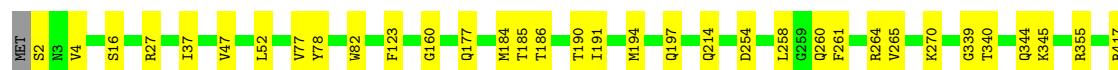
- Molecule 1: capsid protein F

Chain XG:  91% 9%



- Molecule 1: capsid protein F

Chain BH:  91% 8%



- Molecule 1: capsid protein F

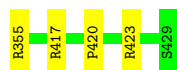
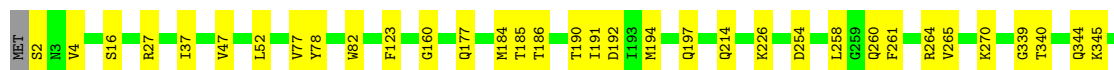
Chain FH:  91% 9%





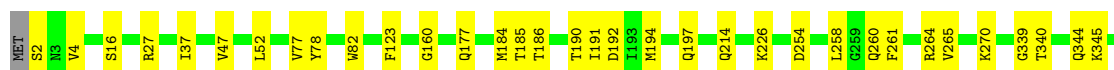
- Molecule 1: capsid protein F

Chain JH:  91% 9%



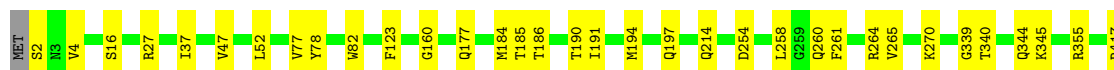
- Molecule 1: capsid protein F

Chain NH:  91% 9%



- Molecule 1: capsid protein F

Chain RH:  91% 8%



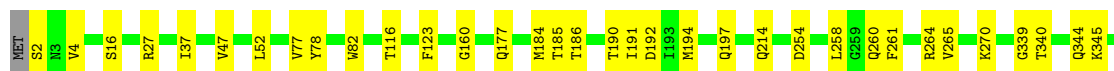
- Molecule 1: capsid protein F

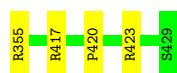
Chain VH:  91% 9%



- Molecule 1: capsid protein F

Chain ZH:  91% 9%





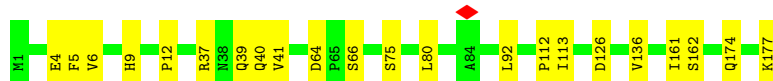
- Molecule 1: capsid protein F

Chain DI: 92% 8%



- Molecule 2: spike protein G

Chain G: 88% 12%



- Molecule 2: spike protein G

Chain C: 88% 12%



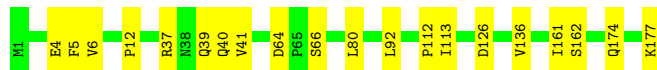
- Molecule 2: spike protein G

Chain I: 89% 11%



- Molecule 2: spike protein G

Chain N: 89% 11%

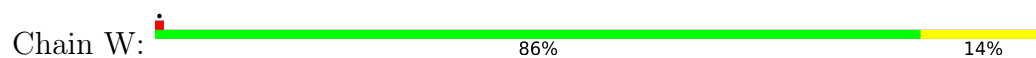


- Molecule 2: spike protein G

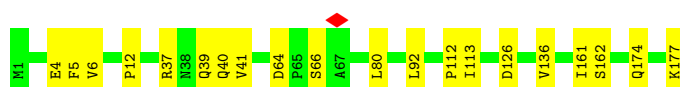
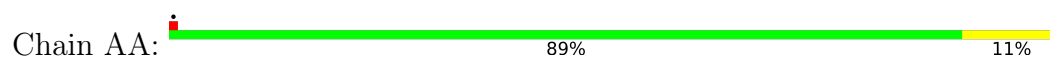
Chain R: 88% 12%



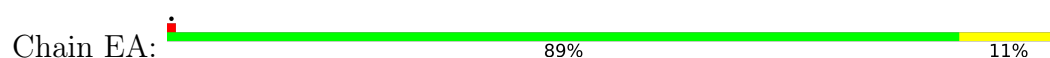
• Molecule 2: spike protein G



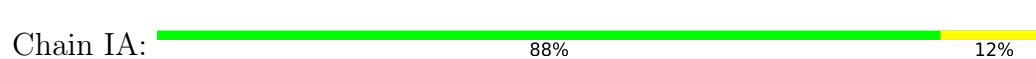
• Molecule 2: spike protein G



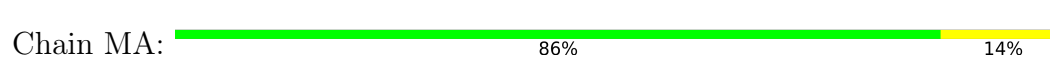
• Molecule 2: spike protein G



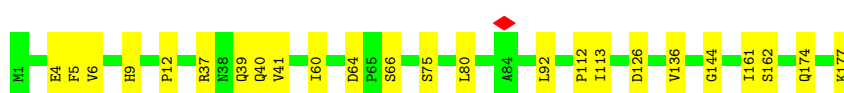
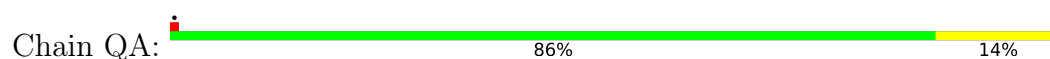
• Molecule 2: spike protein G



• Molecule 2: spike protein G



• Molecule 2: spike protein G

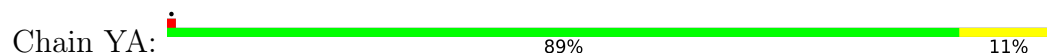


• Molecule 2: spike protein G





- Molecule 2: spike protein G



- Molecule 2: spike protein G



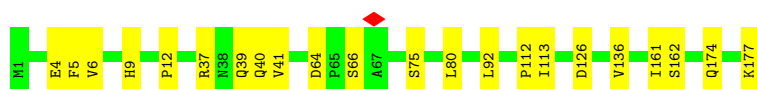
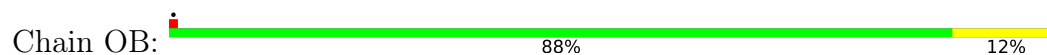
- Molecule 2: spike protein G



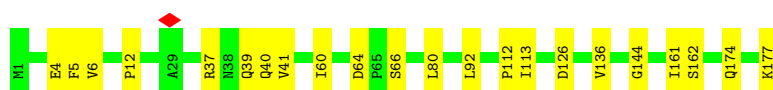
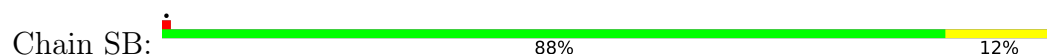
- Molecule 2: spike protein G



- Molecule 2: spike protein G

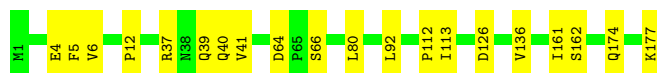


- Molecule 2: spike protein G




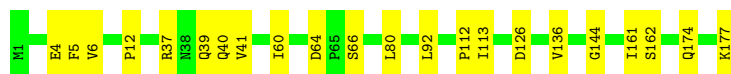
- Molecule 2: spike protein G

Chain WB:  89% 11%



- Molecule 2: spike protein G

Chain AC:  88% 12%




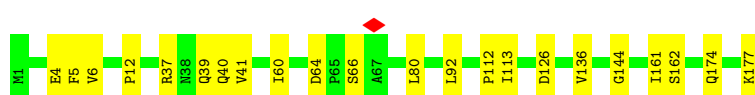
- Molecule 2: spike protein G

Chain EC:  86% 14%



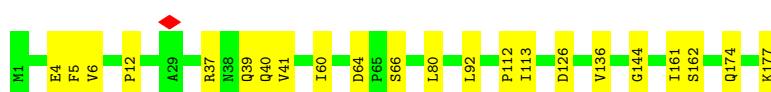
- Molecule 2: spike protein G

Chain IC:  88% 12%




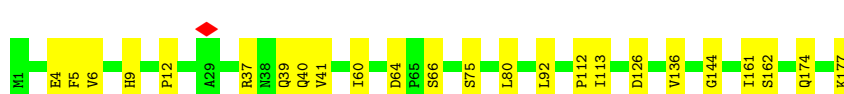
- Molecule 2: spike protein G

Chain MC:  88% 12%



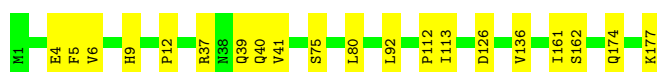
- Molecule 2: spike protein G

Chain QC:  86% 14%

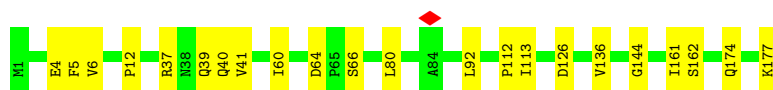


- Molecule 2: spike protein G

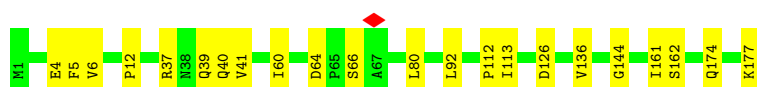
Chain UC:  89% 11%




● Molecule 2: spike protein G

Chain YC:  88% 12%


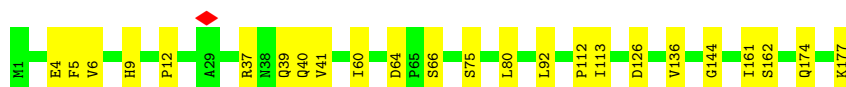
● Molecule 2: spike protein G

Chain CD:  88% 12%

● Molecule 2: spike protein G

Chain GD:  88% 12%


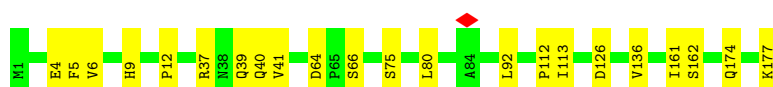
● Molecule 2: spike protein G

Chain KD:  86% 14%

● Molecule 2: spike protein G

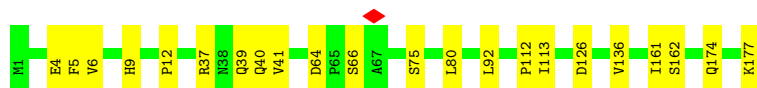
Chain OD:  89% 11%

● Molecule 2: spike protein G

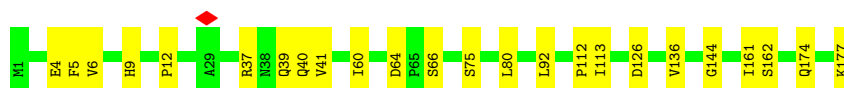
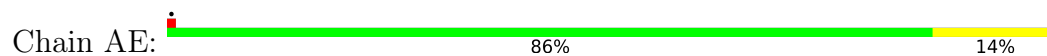
Chain SD:  88% 12%

● Molecule 2: spike protein G

Chain WD:  88% 12%



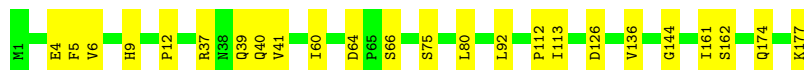
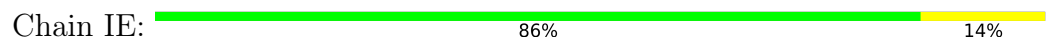
- Molecule 2: spike protein G



- Molecule 2: spike protein G



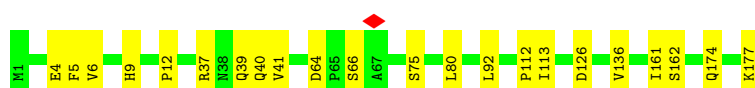
- Molecule 2: spike protein G



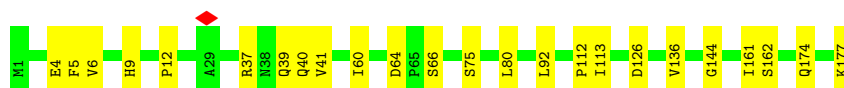
- Molecule 2: spike protein G



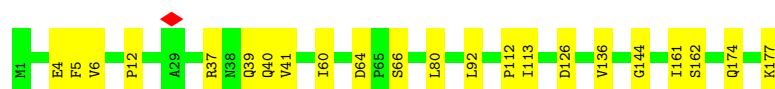
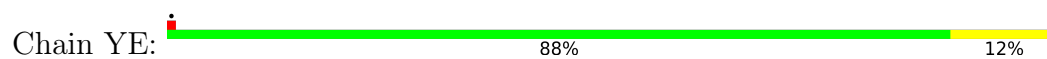
- Molecule 2: spike protein G



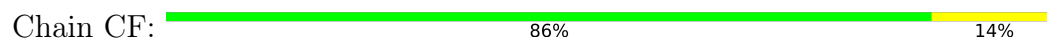
- Molecule 2: spike protein G



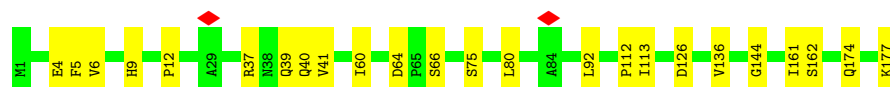
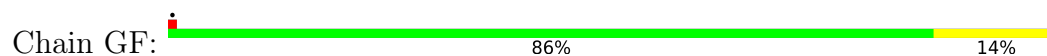
- Molecule 2: spike protein G



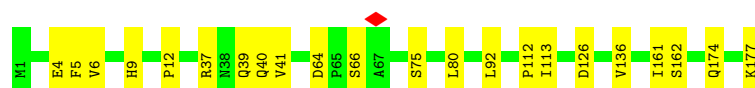
- Molecule 2: spike protein G



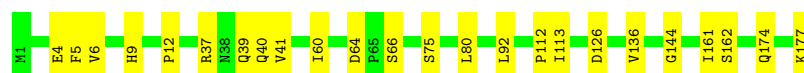
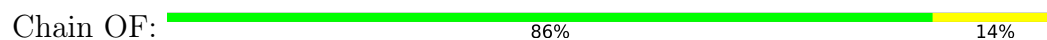
- Molecule 2: spike protein G



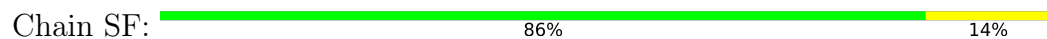
- Molecule 2: spike protein G



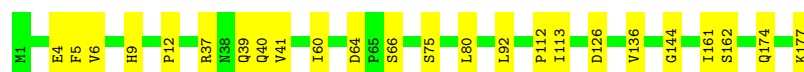
- Molecule 2: spike protein G




- Molecule 2: spike protein G



- Molecule 2: spike protein G



- Molecule 2: spike protein G

Chain AG:  86% 14%




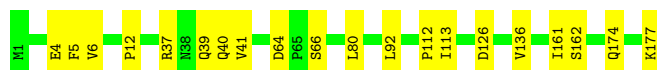
- Molecule 2: spike protein G

Chain EG:  86% 14%



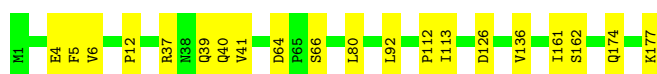
- Molecule 2: spike protein G

Chain IG:  89% 11%




- Molecule 2: spike protein G

Chain MG:  89% 11%




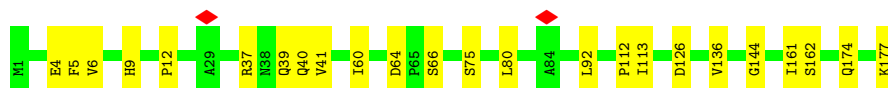
- Molecule 2: spike protein G

Chain QG:  88% 12%



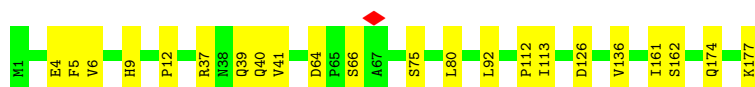
- Molecule 2: spike protein G

Chain UG:  86% 14%

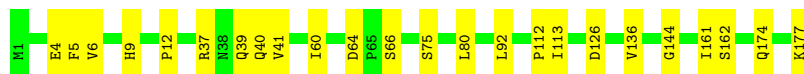


- Molecule 2: spike protein G

Chain YG:  88% 12%



• Molecule 2: spike protein G

Chain CH:  86% 14%

• Molecule 2: spike protein G

Chain GH:  88% 12%


• Molecule 2: spike protein G

Chain KH:  88% 12%

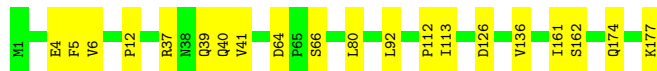
• Molecule 2: spike protein G

Chain OH:  86% 14%


• Molecule 2: spike protein G

Chain SH:  86% 14%


• Molecule 2: spike protein G

Chain WH:  89% 11%

• Molecule 2: spike protein G


Chain AI:  89% 11%

- Molecule 2: spike protein G

Chain EI:  88% 12%




- Molecule 3: DNA-binding protein J

Chain J:  8% 88% 12%




- Molecule 3: DNA-binding protein J

Chain D:  8% 85% 15%




- Molecule 3: DNA-binding protein J

Chain K:  8% 85% 15%




- Molecule 3: DNA-binding protein J

Chain O:  8% 88% 12%




- Molecule 3: DNA-binding protein J

Chain S:  8% 88% 12%

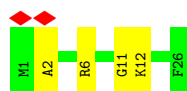
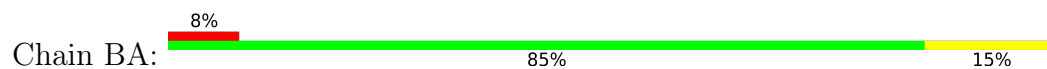


- Molecule 3: DNA-binding protein J

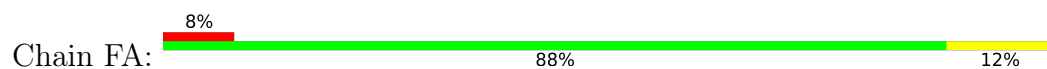
Chain X:  8% 88% 12%



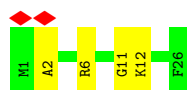
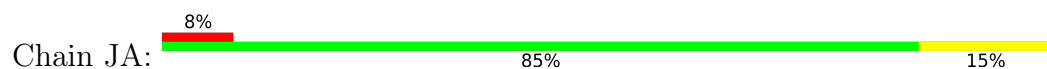
- Molecule 3: DNA-binding protein J



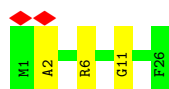
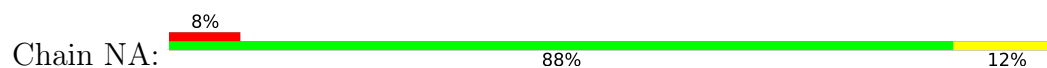
- Molecule 3: DNA-binding protein J



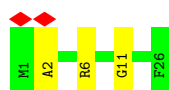
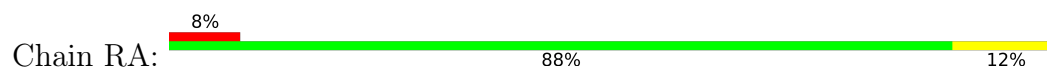
- Molecule 3: DNA-binding protein J



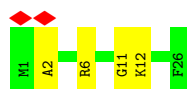
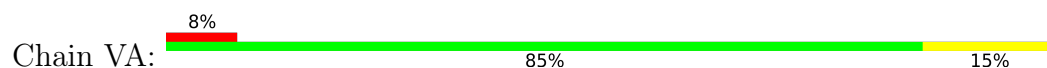
- Molecule 3: DNA-binding protein J



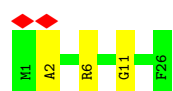
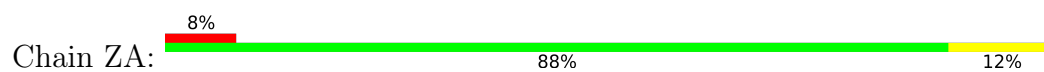
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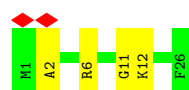
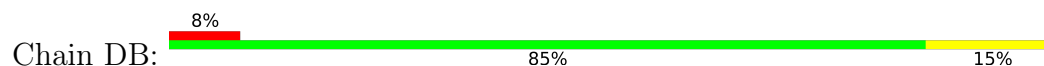
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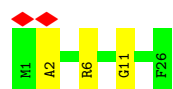
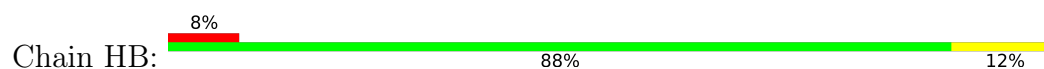
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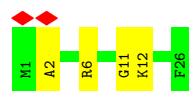
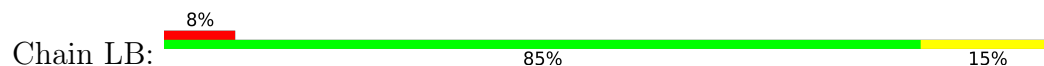
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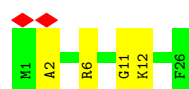
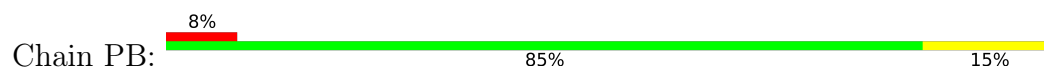
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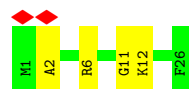
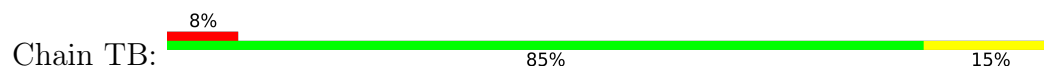
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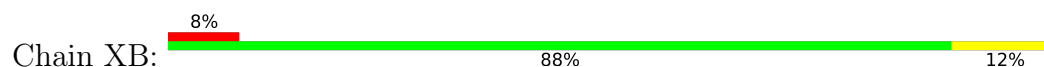
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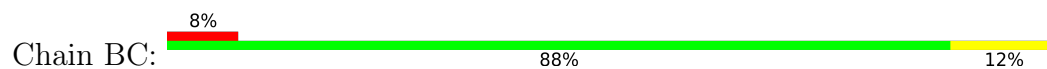
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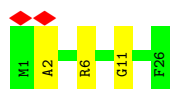
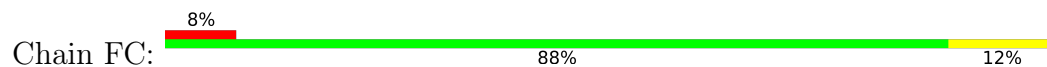
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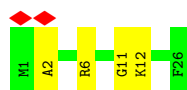
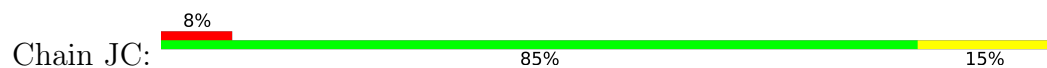
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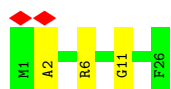
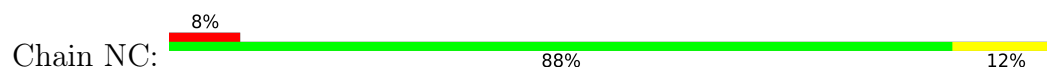
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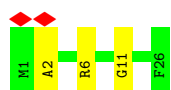
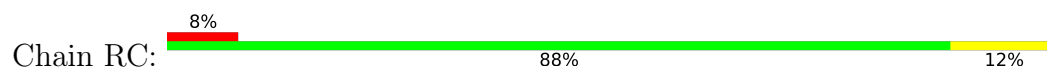
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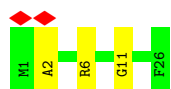
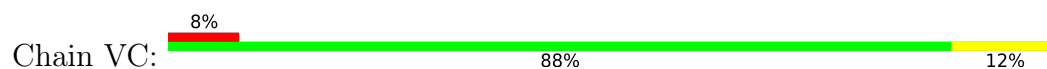
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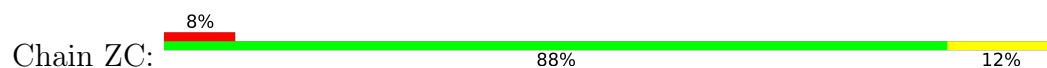
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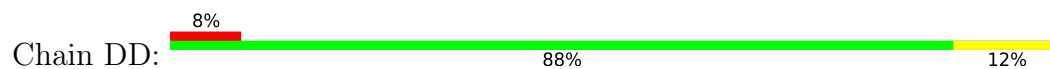


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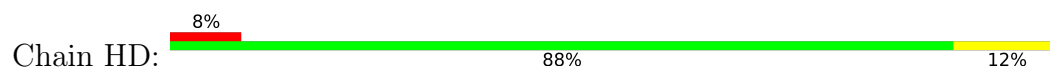




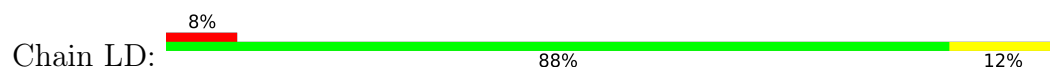
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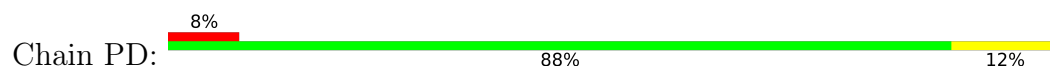
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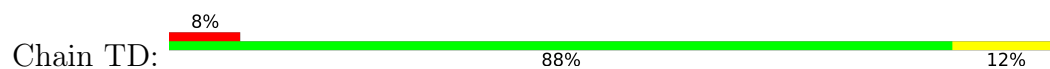
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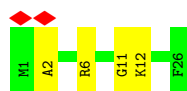
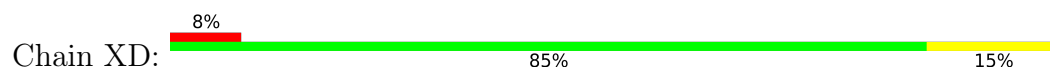
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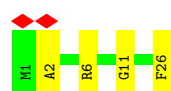
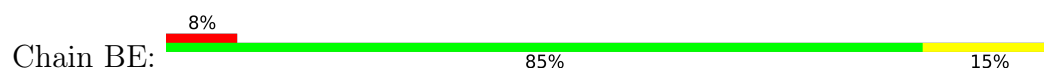
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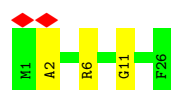
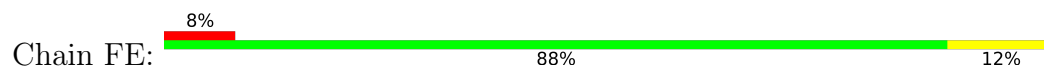
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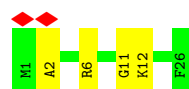
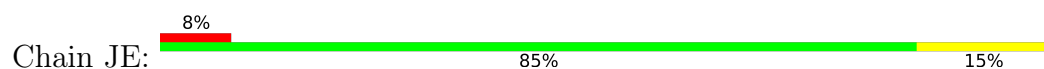
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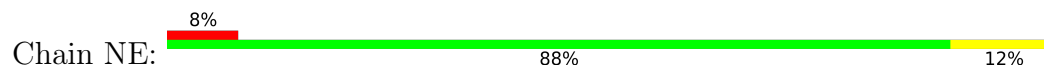
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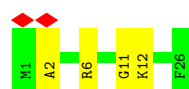
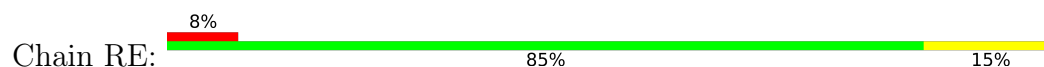
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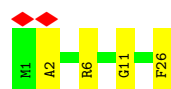
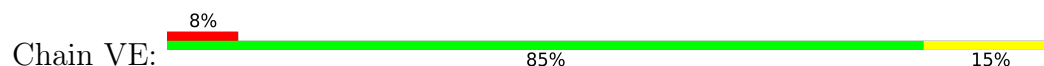
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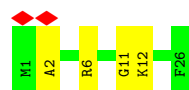
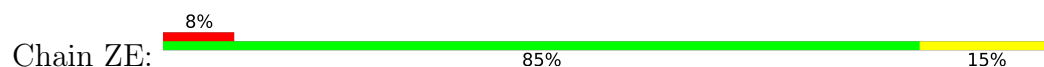
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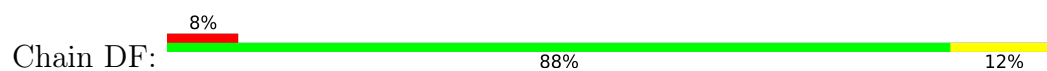
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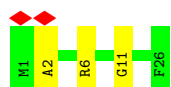
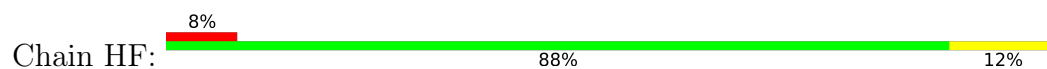
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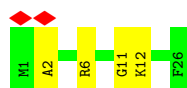
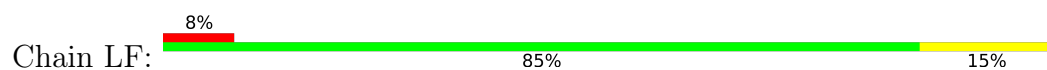
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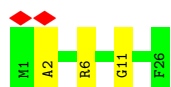
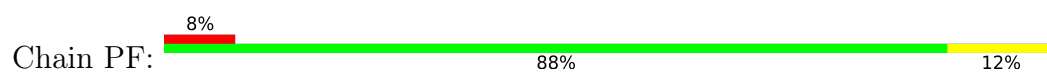
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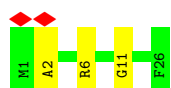
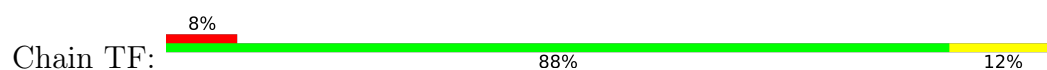
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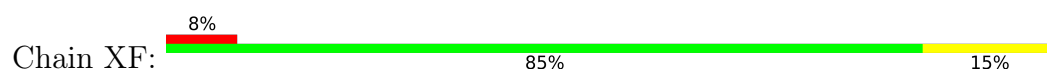
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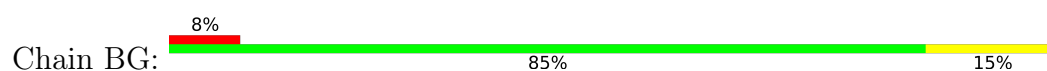
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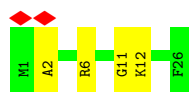


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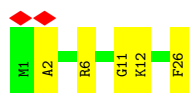
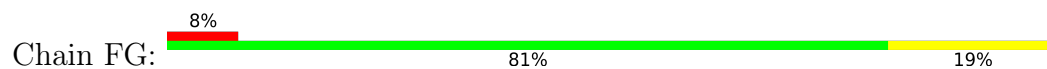


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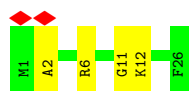
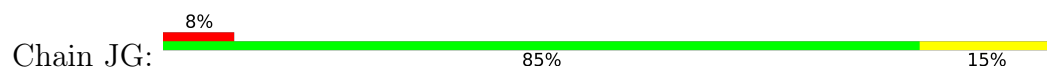




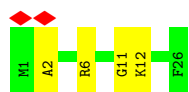
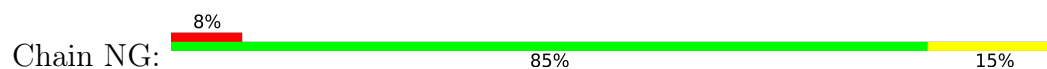
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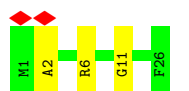
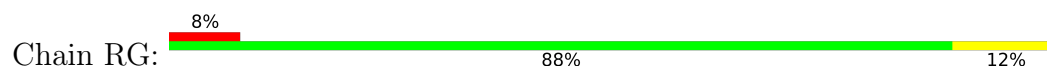
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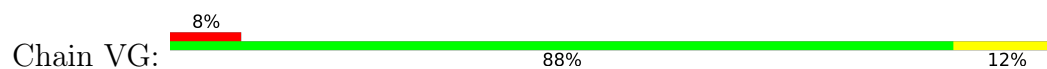
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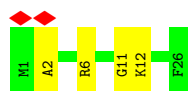
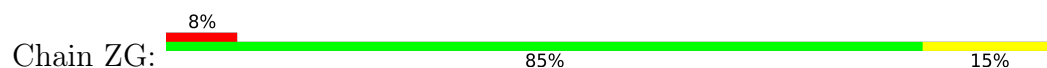
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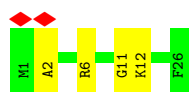
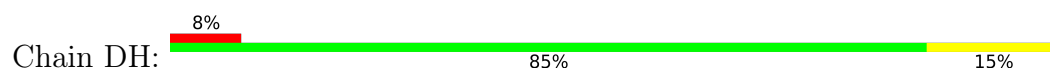
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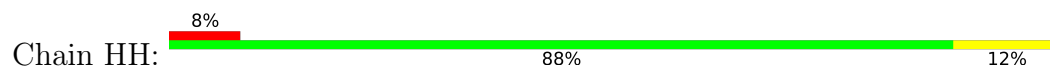
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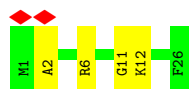
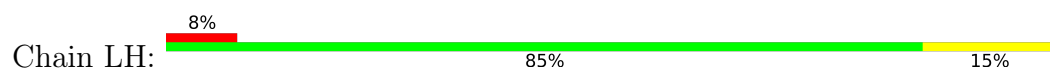
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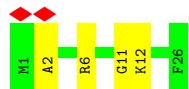
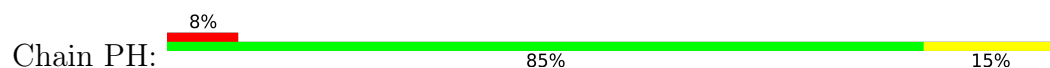
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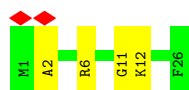
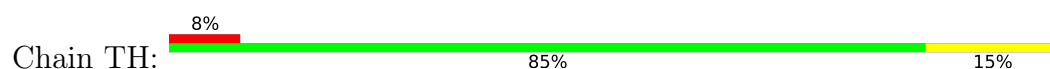
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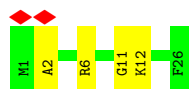
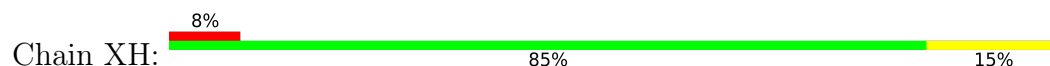
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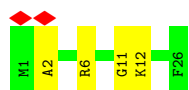
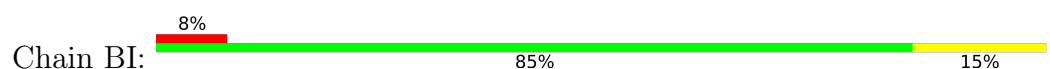
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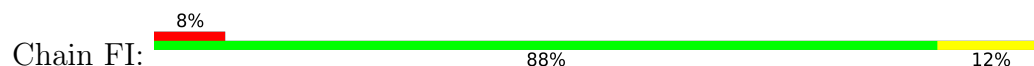
- Molecule 3: DNA-binding protein J



- Molecule 3: DNA-binding protein J



- Molecule 3: DNA-binding protein J



- Molecule 4: DNA (5'-D(P*AP*AP*AP*AP*A)-3')



There are no outlier residues recorded for this chain.

- Molecule 4: DNA (5'-D(P*AP*AP*AP*AP*A)-3')



- Molecule 4: DNA (5'-D(P*AP*AP*AP*AP*A)-3')



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- Molecule 4: DNA (5'-D(P*AP*AP*AP*AP*A)-3')

Chain GA:  20% 100%



- Molecule 4: DNA (5'-D(P*AP*AP*AP*AP*A)-3')

Chain KA:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: DNA (5'-D(P*AP*AP*AP*AP*A)-3')

Chain OA:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: DNA (5'-D(P*AP*AP*AP*AP*A)-3')

Chain SA:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: DNA (5'-D(P*AP*AP*AP*AP*A)-3')

Chain WA:  20% 100%



- Molecule 4: DNA (5'-D(P*AP*AP*AP*AP*A)-3')

Chain AB:  20% 100%



- Molecule 4: DNA (5'-D(P*AP*AP*AP*AP*A)-3')

Chain EB:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: DNA (5'-D(P*AP*AP*AP*AP*A)-3')

Chain IB:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: DNA (5'-D(P*AP*AP*AP*AP*A)-3')

Chain MB:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: DNA (5'-D(P*AP*AP*AP*AP*A)-3')

Chain QB:  20% 100%



- Molecule 4: DNA (5'-D(P*AP*AP*AP*AP*A)-3')

Chain UB:  20% 100%



- Molecule 4: DNA (5'-D(P*AP*AP*AP*AP*A)-3')

Chain YB:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: DNA (5'-D(P*AP*AP*AP*AP*A)-3')

Chain CC:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: DNA (5'-D(P*AP*AP*AP*AP*A)-3')

Chain GC:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: DNA (5'-D(P*AP*AP*AP*AP*A)-3')

Chain KC:  20% 100%



- Molecule 4: DNA (5'-D(P*AP*AP*AP*AP*A)-3')



- Molecule 4: DNA (5'-D(P*AP*AP*AP*AP*A)-3')



There are no outlier residues recorded for this chain.

- Molecule 4: DNA (5'-D(P*AP*AP*AP*AP*A)-3')



There are no outlier residues recorded for this chain.

- Molecule 4: DNA (5'-D(P*AP*AP*AP*AP*A)-3')



There are no outlier residues recorded for this chain.

- Molecule 4: DNA (5'-D(P*AP*AP*AP*AP*A)-3')



- Molecule 4: DNA (5'-D(P*AP*AP*AP*AP*A)-3')



- Molecule 4: DNA (5'-D(P*AP*AP*AP*AP*A)-3')




There are no outlier residues recorded for this chain.

- Molecule 4: DNA (5'-D(P*AP*AP*AP*AP*A)-3')



There are no outlier residues recorded for this chain.

- Molecule 4: DNA (5'-D(P*AP*AP*AP*AP*A)-3')

Chain UD:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: DNA (5'-D(P*AP*AP*AP*AP*A)-3')

Chain YD:  20%  100%



- Molecule 4: DNA (5'-D(P*AP*AP*AP*AP*A)-3')

Chain CE:  20%  100%



- Molecule 4: DNA (5'-D(P*AP*AP*AP*AP*A)-3')

Chain GE:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: DNA (5'-D(P*AP*AP*AP*AP*A)-3')

Chain KE:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: DNA (5'-D(P*AP*AP*AP*AP*A)-3')

Chain OE:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: DNA (5'-D(P*AP*AP*AP*AP*A)-3')

Chain SE:  20%  100%



- Molecule 4: DNA (5'-D(P*AP*AP*AP*AP*A)-3')

Chain WE:  20%  100%



- Molecule 4: DNA (5'-D(P*AP*AP*AP*AP*A)-3')

Chain AF:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: DNA (5'-D(P*AP*AP*AP*AP*A)-3')

Chain EF:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: DNA (5'-D(P*AP*AP*AP*AP*A)-3')

Chain IF:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: DNA (5'-D(P*AP*AP*AP*AP*A)-3')

Chain MF:  20% 100%



- Molecule 4: DNA (5'-D(P*AP*AP*AP*AP*A)-3')

Chain QF:  20% 100%



- Molecule 4: DNA (5'-D(P*AP*AP*AP*AP*A)-3')

Chain UF:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: DNA (5'-D(P*AP*AP*AP*AP*A)-3')

Chain YF:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: DNA (5'-D(P*AP*AP*AP*AP*A)-3')

Chain CG:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: DNA (5'-D(P*AP*AP*AP*AP*A)-3')



- Molecule 4: DNA (5'-D(P*AP*AP*AP*AP*A)-3')



- Molecule 4: DNA (5'-D(P*AP*AP*AP*AP*A)-3')



There are no outlier residues recorded for this chain.

- Molecule 4: DNA (5'-D(P*AP*AP*AP*AP*A)-3')



There are no outlier residues recorded for this chain.

- Molecule 4: DNA (5'-D(P*AP*AP*AP*AP*A)-3')



There are no outlier residues recorded for this chain.

- Molecule 4: DNA (5'-D(P*AP*AP*AP*AP*A)-3')



- Molecule 4: DNA (5'-D(P*AP*AP*AP*AP*A)-3')



- Molecule 4: DNA (5'-D(P*AP*AP*AP*AP*A)-3')



There are no outlier residues recorded for this chain.

- Molecule 4: DNA (5'-D(P*AP*AP*AP*AP*A)-3')

Chain MH:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: DNA (5'-D(P*AP*AP*AP*AP*A)-3')

Chain QH:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: DNA (5'-D(P*AP*AP*AP*AP*A)-3')

Chain UH:  20% 100%



- Molecule 4: DNA (5'-D(P*AP*AP*AP*AP*A)-3')

Chain YH:  20% 100%



- Molecule 4: DNA (5'-D(P*AP*AP*AP*AP*A)-3')

Chain CI:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: DNA (5'-D(P*AP*AP*AP*AP*A)-3')

Chain GI:  100%

There are no outlier residues recorded for this chain.

- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')

Chain U:  25% 75%



- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')

Chain a:  25% 75%



- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')

Chain b:  25% 75%

A8
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- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')

Chain c:  25% 75%

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A9
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A11

- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')

Chain d:  25% 75%

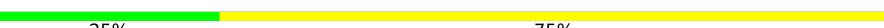
A8
A9
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A11

- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')

Chain e:  25% 75%

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A9
A10
A11

- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')

Chain f:  25% 75%

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A11

- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')

Chain g:  25% 75%

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A11

- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')

Chain h:  25% 75%

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A10
A11

- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')

Chain i:  25% 75%



- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')



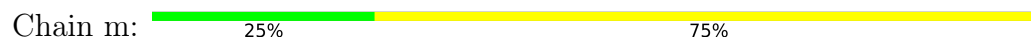
- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')



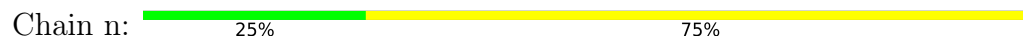
- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')



- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')



- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')



- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')



- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')



- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')

Chain q:  25% 75%

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- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')

Chain r:  25% 75%

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A11

- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')

Chain s:  25% 75%

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A11

- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')

Chain t:  25% 75%

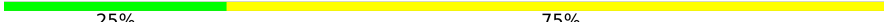
A8
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- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')

Chain u:  25% 75%

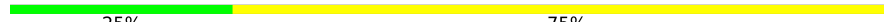
A8
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A11

- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')

Chain v:  25% 75%

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A11

- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')

Chain w:  25% 75%

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A9
A10
A11

- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')

Chain x:  25% 75%

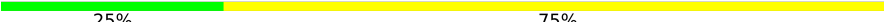
A8
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- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')

Chain y:  25% 75%

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- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')

Chain z:  25% 75%

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- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')

Chain 0:  25% 75%

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A9
A10
A11

- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')

Chain 1:  25% 75%

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A11

- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')

Chain 2:  25% 75%

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A10
A11

- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')

Chain 3:  25% 75%

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A9
A10
A11

- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')

Chain 4:  25% 75%

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A9
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A11

- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')

Chain 5:  25% 75%

A8
A9
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- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')

Chain 6:  25% 75%



- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')

Chain 7:  25% 75%



- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')

Chain 8:  25% 75%




- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')

Chain 9:  25% 75%



- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')

Chain aA:  25% 75%



- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')

Chain bA:  25% 75%



- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')

Chain cA:  25% 75%



- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')

Chain dA:  25% 75%



- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')

Chain eA:  25% 75%

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- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')

Chain fA:  25% 75%

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A11

- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')

Chain gA:  25% 75%

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A11

- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')

Chain hA:  25% 75%

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A11

- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')

Chain iA:  25% 75%

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A11

- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')

Chain jA:  25% 75%

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A11

- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')

Chain kA:  25% 75%

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A11

- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')

Chain lA:  25% 75%

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A11

- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')

Chain mA:  25% 75%



- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')

Chain nA:  25% 75%




- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')

Chain oA:  25% 75%




- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')

Chain pA:  25% 75%



- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')

Chain qA:  25% 75%

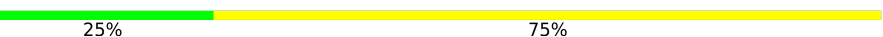


- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')

Chain rA:  25% 75%

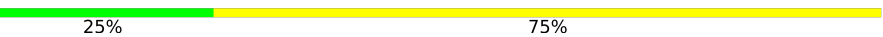


- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')

Chain sA:  25% 75%



- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')

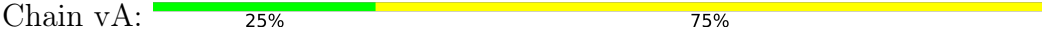
Chain tA:  25% 75%



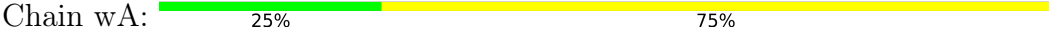
- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')



- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')



- Molecule 5: DNA (5'-D(P*AP*AP*AP*A)-3')



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	86486	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	22500	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.040	Depositor
Minimum map value	-2.448	Depositor
Average map value	0.036	Depositor
Map value standard deviation	0.255	Depositor
Recommended contour level	0.65	Depositor
Map size (Å)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	B	0.21	1/3495 (0.0%)	0.31	1/4753 (0.0%)
1	BB	0.21	1/3495 (0.0%)	0.31	1/4753 (0.0%)
1	BD	0.21	0/3495	0.31	1/4753 (0.0%)
1	BF	0.21	1/3495 (0.0%)	0.31	1/4753 (0.0%)
1	BH	0.21	0/3495	0.31	1/4753 (0.0%)
1	DA	0.21	1/3495 (0.0%)	0.31	1/4753 (0.0%)
1	DC	0.21	1/3495 (0.0%)	0.31	1/4753 (0.0%)
1	DE	0.21	1/3495 (0.0%)	0.31	1/4753 (0.0%)
1	DG	0.21	0/3495	0.31	1/4753 (0.0%)
1	DI	0.21	1/3495 (0.0%)	0.31	1/4753 (0.0%)
1	F	0.21	1/3495 (0.0%)	0.31	1/4753 (0.0%)
1	FB	0.21	1/3495 (0.0%)	0.31	1/4753 (0.0%)
1	FD	0.21	0/3495	0.31	1/4753 (0.0%)
1	FF	0.21	1/3495 (0.0%)	0.31	1/4753 (0.0%)
1	FH	0.21	1/3495 (0.0%)	0.31	1/4753 (0.0%)
1	H	0.21	1/3495 (0.0%)	0.31	1/4753 (0.0%)
1	HA	0.21	1/3495 (0.0%)	0.31	1/4753 (0.0%)
1	HC	0.21	1/3495 (0.0%)	0.31	1/4753 (0.0%)
1	HE	0.21	0/3495	0.31	1/4753 (0.0%)
1	HG	0.21	0/3495	0.31	1/4753 (0.0%)
1	JB	0.21	1/3495 (0.0%)	0.31	1/4753 (0.0%)
1	JD	0.21	0/3495	0.31	1/4753 (0.0%)
1	JF	0.21	1/3495 (0.0%)	0.31	1/4753 (0.0%)
1	JH	0.21	1/3495 (0.0%)	0.31	1/4753 (0.0%)
1	LA	0.21	1/3495 (0.0%)	0.31	1/4753 (0.0%)
1	LC	0.21	1/3495 (0.0%)	0.31	1/4753 (0.0%)
1	LE	0.21	1/3495 (0.0%)	0.31	1/4753 (0.0%)
1	LG	0.21	0/3495	0.31	1/4753 (0.0%)
1	M	0.21	1/3495 (0.0%)	0.31	1/4753 (0.0%)
1	NB	0.21	1/3495 (0.0%)	0.31	1/4753 (0.0%)
1	ND	0.21	1/3495 (0.0%)	0.31	1/4753 (0.0%)
1	NF	0.21	1/3495 (0.0%)	0.31	1/4753 (0.0%)
1	NH	0.21	1/3495 (0.0%)	0.31	1/4753 (0.0%)
1	PA	0.21	1/3495 (0.0%)	0.31	1/4753 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	PC	0.21	1/3495 (0.0%)	0.31	1/4753 (0.0%)
1	PE	0.21	1/3495 (0.0%)	0.31	1/4753 (0.0%)
1	PG	0.21	1/3495 (0.0%)	0.31	1/4753 (0.0%)
1	Q	0.21	1/3495 (0.0%)	0.31	1/4753 (0.0%)
1	RB	0.21	0/3495	0.31	1/4753 (0.0%)
1	RD	0.21	1/3495 (0.0%)	0.31	1/4753 (0.0%)
1	RF	0.21	1/3495 (0.0%)	0.31	1/4753 (0.0%)
1	RH	0.21	0/3495	0.31	1/4753 (0.0%)
1	TA	0.21	1/3495 (0.0%)	0.31	1/4753 (0.0%)
1	TC	0.21	1/3495 (0.0%)	0.31	1/4753 (0.0%)
1	TE	0.21	1/3495 (0.0%)	0.31	1/4753 (0.0%)
1	TG	0.21	1/3495 (0.0%)	0.31	1/4753 (0.0%)
1	V	0.21	1/3495 (0.0%)	0.31	1/4753 (0.0%)
1	VB	0.21	1/3495 (0.0%)	0.31	1/4753 (0.0%)
1	VD	0.21	0/3495	0.31	1/4753 (0.0%)
1	VF	0.21	1/3495 (0.0%)	0.31	1/4753 (0.0%)
1	VH	0.21	0/3495	0.31	1/4753 (0.0%)
1	XA	0.21	0/3495	0.31	1/4753 (0.0%)
1	XC	0.21	1/3495 (0.0%)	0.31	1/4753 (0.0%)
1	XE	0.21	0/3495	0.31	1/4753 (0.0%)
1	XG	0.21	0/3495	0.31	1/4753 (0.0%)
1	Z	0.21	1/3495 (0.0%)	0.31	1/4753 (0.0%)
1	ZB	0.21	1/3495 (0.0%)	0.31	1/4753 (0.0%)
1	ZD	0.21	1/3495 (0.0%)	0.31	1/4753 (0.0%)
1	ZF	0.21	1/3495 (0.0%)	0.31	1/4753 (0.0%)
1	ZH	0.21	1/3495 (0.0%)	0.31	1/4753 (0.0%)
2	AA	0.16	0/1357	0.34	0/1859
2	AC	0.16	0/1357	0.34	0/1859
2	AE	0.16	0/1357	0.34	0/1859
2	AG	0.16	0/1357	0.34	0/1859
2	AI	0.16	0/1357	0.34	0/1859
2	C	0.16	0/1357	0.34	0/1859
2	CB	0.16	0/1357	0.34	0/1859
2	CD	0.16	0/1357	0.34	0/1859
2	CF	0.16	0/1357	0.34	0/1859
2	CH	0.16	0/1357	0.34	0/1859
2	EA	0.16	0/1357	0.34	0/1859
2	EC	0.16	0/1357	0.34	0/1859
2	EE	0.16	0/1357	0.34	0/1859
2	EG	0.16	0/1357	0.34	0/1859
2	EI	0.16	0/1357	0.34	0/1859
2	G	0.16	0/1357	0.34	0/1859
2	GB	0.16	0/1357	0.34	0/1859

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	GD	0.16	0/1357	0.34	0/1859
2	GF	0.16	0/1357	0.34	0/1859
2	GH	0.16	0/1357	0.34	0/1859
2	I	0.16	0/1357	0.34	0/1859
2	IA	0.16	0/1357	0.34	0/1859
2	IC	0.16	0/1357	0.34	0/1859
2	IE	0.16	0/1357	0.34	0/1859
2	IG	0.16	0/1357	0.34	0/1859
2	KB	0.16	0/1357	0.34	0/1859
2	KD	0.16	0/1357	0.34	0/1859
2	KF	0.16	0/1357	0.34	0/1859
2	KH	0.16	0/1357	0.34	0/1859
2	MA	0.16	0/1357	0.34	0/1859
2	MC	0.16	0/1357	0.34	0/1859
2	ME	0.16	0/1357	0.34	0/1859
2	MG	0.16	0/1357	0.34	0/1859
2	N	0.16	0/1357	0.34	0/1859
2	OB	0.16	0/1357	0.34	0/1859
2	OD	0.16	0/1357	0.34	0/1859
2	OF	0.16	0/1357	0.34	0/1859
2	OH	0.16	0/1357	0.34	0/1859
2	QA	0.16	0/1357	0.34	0/1859
2	QC	0.16	0/1357	0.34	0/1859
2	QE	0.16	0/1357	0.34	0/1859
2	QG	0.16	0/1357	0.34	0/1859
2	R	0.16	0/1357	0.34	0/1859
2	SB	0.16	0/1357	0.34	0/1859
2	SD	0.16	0/1357	0.34	0/1859
2	SF	0.16	0/1357	0.34	0/1859
2	SH	0.16	0/1357	0.34	0/1859
2	UA	0.16	0/1357	0.34	0/1859
2	UC	0.16	0/1357	0.34	0/1859
2	UE	0.16	0/1357	0.34	0/1859
2	UG	0.16	0/1357	0.34	0/1859
2	W	0.16	0/1357	0.34	0/1859
2	WB	0.16	0/1357	0.34	0/1859
2	WD	0.16	0/1357	0.34	0/1859
2	WF	0.16	0/1357	0.34	0/1859
2	WH	0.16	0/1357	0.34	0/1859
2	YA	0.16	0/1357	0.34	0/1859
2	YC	0.16	0/1357	0.34	0/1859
2	YE	0.16	0/1357	0.34	0/1859
2	YG	0.16	0/1357	0.34	0/1859

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
3	BA	0.12	0/209	0.26	0/273
3	BC	0.12	0/209	0.26	0/273
3	BE	0.12	0/209	0.27	0/273
3	BG	0.11	0/209	0.26	0/273
3	BI	0.12	0/209	0.27	0/273
3	D	0.12	0/209	0.27	0/273
3	DB	0.12	0/209	0.26	0/273
3	DD	0.12	0/209	0.26	0/273
3	DF	0.12	0/209	0.26	0/273
3	DH	0.12	0/209	0.26	0/273
3	FA	0.12	0/209	0.26	0/273
3	FC	0.11	0/209	0.26	0/273
3	FE	0.12	0/209	0.26	0/273
3	FG	0.12	0/209	0.26	0/273
3	FI	0.12	0/209	0.27	0/273
3	HB	0.12	0/209	0.26	0/273
3	HD	0.12	0/209	0.27	0/273
3	HF	0.11	0/209	0.26	0/273
3	HH	0.12	0/209	0.26	0/273
3	J	0.11	0/209	0.26	0/273
3	JA	0.12	0/209	0.27	0/273
3	JC	0.12	0/209	0.27	0/273
3	JE	0.12	0/209	0.26	0/273
3	JG	0.12	0/209	0.26	0/273
3	K	0.12	0/209	0.27	0/273
3	LB	0.11	0/209	0.26	0/273
3	LD	0.12	0/209	0.26	0/273
3	LF	0.12	0/209	0.26	0/273
3	LH	0.12	0/209	0.26	0/273
3	NA	0.12	0/209	0.26	0/273
3	NC	0.12	0/209	0.27	0/273
3	NE	0.11	0/209	0.26	0/273
3	NG	0.12	0/209	0.26	0/273
3	O	0.12	0/209	0.27	0/273
3	PB	0.12	0/209	0.27	0/273
3	PD	0.12	0/209	0.27	0/273
3	PF	0.12	0/209	0.27	0/273
3	PH	0.11	0/209	0.26	0/273
3	RA	0.11	0/209	0.26	0/273
3	RC	0.12	0/209	0.26	0/273
3	RE	0.12	0/209	0.26	0/273
3	RG	0.12	0/209	0.26	0/273
3	S	0.12	0/209	0.26	0/273

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	TB	0.12	0/209	0.26	0/273
3	TD	0.11	0/209	0.26	0/273
3	TF	0.12	0/209	0.27	0/273
3	TH	0.12	0/209	0.27	0/273
3	VA	0.12	0/209	0.26	0/273
3	VC	0.12	0/209	0.26	0/273
3	VE	0.12	0/209	0.26	0/273
3	VG	0.11	0/209	0.26	0/273
3	X	0.11	0/209	0.26	0/273
3	XB	0.12	0/209	0.27	0/273
3	XD	0.12	0/209	0.26	0/273
3	XF	0.12	0/209	0.26	0/273
3	XH	0.12	0/209	0.26	0/273
3	ZA	0.12	0/209	0.26	0/273
3	ZC	0.11	0/209	0.26	0/273
3	ZE	0.12	0/209	0.26	0/273
3	ZG	0.12	0/209	0.27	0/273
4	A	0.19	0/119	0.33	0/181
4	AB	0.19	0/119	0.33	0/181
4	AD	0.19	0/119	0.33	0/181
4	AF	0.19	0/119	0.33	0/181
4	AH	0.19	0/119	0.33	0/181
4	CA	0.19	0/119	0.33	0/181
4	CC	0.18	0/119	0.33	0/181
4	CE	0.19	0/119	0.33	0/181
4	CG	0.19	0/119	0.33	0/181
4	CI	0.19	0/119	0.33	0/181
4	E	0.19	0/119	0.33	0/181
4	EB	0.19	0/119	0.33	0/181
4	ED	0.19	0/119	0.33	0/181
4	EF	0.19	0/119	0.33	0/181
4	EH	0.19	0/119	0.33	0/181
4	GA	0.19	0/119	0.33	0/181
4	GC	0.19	0/119	0.33	0/181
4	GE	0.19	0/119	0.33	0/181
4	GG	0.19	0/119	0.33	0/181
4	GI	0.19	0/119	0.33	0/181
4	IB	0.18	0/119	0.33	0/181
4	ID	0.19	0/119	0.33	0/181
4	IF	0.19	0/119	0.33	0/181
4	IH	0.19	0/119	0.33	0/181
4	KA	0.19	0/119	0.33	0/181
4	KC	0.19	0/119	0.33	0/181

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	KE	0.19	0/119	0.33	0/181
4	KG	0.19	0/119	0.33	0/181
4	L	0.18	0/119	0.33	0/181
4	MB	0.19	0/119	0.33	0/181
4	MD	0.19	0/119	0.33	0/181
4	MF	0.19	0/119	0.33	0/181
4	MH	0.18	0/119	0.33	0/181
4	OA	0.19	0/119	0.33	0/181
4	OC	0.19	0/119	0.33	0/181
4	OE	0.19	0/119	0.33	0/181
4	OG	0.19	0/119	0.33	0/181
4	P	0.19	0/119	0.33	0/181
4	QB	0.18	0/119	0.33	0/181
4	QD	0.19	0/119	0.33	0/181
4	QF	0.19	0/119	0.33	0/181
4	QH	0.19	0/119	0.33	0/181
4	SA	0.19	0/119	0.33	0/181
4	SC	0.18	0/119	0.33	0/181
4	SE	0.19	0/119	0.33	0/181
4	SG	0.19	0/119	0.33	0/181
4	T	0.19	0/119	0.33	0/181
4	UB	0.19	0/119	0.33	0/181
4	UD	0.19	0/119	0.33	0/181
4	UF	0.19	0/119	0.33	0/181
4	UH	0.19	0/119	0.33	0/181
4	WA	0.19	0/119	0.33	0/181
4	WC	0.19	0/119	0.33	0/181
4	WE	0.19	0/119	0.33	0/181
4	WG	0.19	0/119	0.33	0/181
4	Y	0.19	0/119	0.33	0/181
4	YB	0.19	0/119	0.33	0/181
4	YD	0.19	0/119	0.33	0/181
4	YF	0.19	0/119	0.33	0/181
4	YH	0.18	0/119	0.33	0/181
5	0	0.24	0/95	0.57	0/144
5	1	0.24	0/95	0.57	0/144
5	2	0.24	0/95	0.57	0/144
5	3	0.24	0/95	0.57	0/144
5	4	0.24	0/95	0.57	0/144
5	5	0.24	0/95	0.57	0/144
5	6	0.24	0/95	0.56	0/144
5	7	0.24	0/95	0.57	0/144
5	8	0.24	0/95	0.57	0/144

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	9	0.24	0/95	0.57	0/144
5	U	0.24	0/95	0.57	0/144
5	a	0.24	0/95	0.57	0/144
5	aA	0.24	0/95	0.57	0/144
5	b	0.24	0/95	0.57	0/144
5	bA	0.24	0/95	0.57	0/144
5	c	0.24	0/95	0.57	0/144
5	cA	0.24	0/95	0.57	0/144
5	d	0.24	0/95	0.57	0/144
5	dA	0.24	0/95	0.57	0/144
5	e	0.24	0/95	0.57	0/144
5	eA	0.24	0/95	0.57	0/144
5	f	0.24	0/95	0.57	0/144
5	fA	0.24	0/95	0.57	0/144
5	g	0.24	0/95	0.57	0/144
5	gA	0.24	0/95	0.57	0/144
5	h	0.24	0/95	0.57	0/144
5	hA	0.24	0/95	0.57	0/144
5	i	0.24	0/95	0.57	0/144
5	iA	0.24	0/95	0.57	0/144
5	j	0.24	0/95	0.57	0/144
5	jA	0.24	0/95	0.57	0/144
5	k	0.24	0/95	0.56	0/144
5	kA	0.24	0/95	0.57	0/144
5	l	0.24	0/95	0.57	0/144
5	lA	0.24	0/95	0.57	0/144
5	m	0.24	0/95	0.56	0/144
5	mA	0.24	0/95	0.57	0/144
5	n	0.24	0/95	0.57	0/144
5	nA	0.24	0/95	0.57	0/144
5	o	0.24	0/95	0.57	0/144
5	oA	0.24	0/95	0.57	0/144
5	p	0.24	0/95	0.57	0/144
5	pA	0.24	0/95	0.57	0/144
5	q	0.24	0/95	0.57	0/144
5	qA	0.24	0/95	0.57	0/144
5	r	0.24	0/95	0.56	0/144
5	rA	0.24	0/95	0.57	0/144
5	s	0.24	0/95	0.56	0/144
5	sA	0.24	0/95	0.57	0/144
5	t	0.24	0/95	0.57	0/144
5	tA	0.24	0/95	0.57	0/144
5	u	0.24	0/95	0.57	0/144

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	uA	0.24	0/95	0.57	0/144
5	v	0.24	0/95	0.57	0/144
5	vA	0.24	0/95	0.57	0/144
5	w	0.24	0/95	0.57	0/144
5	wA	0.24	0/95	0.57	0/144
5	x	0.24	0/95	0.57	0/144
5	y	0.24	0/95	0.57	0/144
5	z	0.24	0/95	0.57	0/144
All	All	0.19	45/316500 (0.0%)	0.33	60/432600 (0.0%)

The worst 5 of 45 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	192	ASP	C-O	-5.10	1.17	1.24
1	TE	192	ASP	C-O	-5.10	1.17	1.24
1	LC	192	ASP	C-O	-5.10	1.17	1.24
1	NF	192	ASP	C-O	-5.10	1.17	1.24
1	HA	192	ASP	C-O	-5.09	1.17	1.24

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	VB	194	MET	N-CA-C	-8.01	101.32	112.45
1	BF	194	MET	N-CA-C	-8.00	101.33	112.45
1	PG	194	MET	N-CA-C	-8.00	101.33	112.45
1	DI	194	MET	N-CA-C	-8.00	101.33	112.45
1	TA	194	MET	N-CA-C	-8.00	101.33	112.45

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3402	0	3280	37	0
1	BB	3402	0	3280	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BD	3402	0	3280	39	0
1	BF	3402	0	3280	37	0
1	BH	3402	0	3280	38	0
1	DA	3402	0	3280	38	0
1	DC	3402	0	3280	39	0
1	DE	3402	0	3280	39	0
1	DG	3402	0	3280	36	0
1	DI	3402	0	3280	35	0
1	F	3402	0	3280	38	0
1	FB	3402	0	3280	38	0
1	FD	3402	0	3280	39	0
1	FF	3402	0	3280	38	0
1	FH	3402	0	3280	38	0
1	H	3402	0	3280	39	0
1	HA	3402	0	3280	37	0
1	HC	3402	0	3280	40	0
1	HE	3402	0	3280	36	0
1	HG	3402	0	3280	36	0
1	JB	3402	0	3280	38	0
1	JD	3402	0	3280	38	0
1	JF	3402	0	3280	38	0
1	JH	3402	0	3280	39	0
1	LA	3402	0	3280	36	0
1	LC	3402	0	3280	38	0
1	LE	3402	0	3280	39	0
1	LG	3402	0	3280	39	0
1	M	3402	0	3280	38	0
1	NB	3402	0	3280	37	0
1	ND	3402	0	3280	38	0
1	NF	3402	0	3280	38	0
1	NH	3402	0	3280	37	0
1	PA	3402	0	3280	38	0
1	PC	3402	0	3280	37	0
1	PE	3402	0	3280	35	0
1	PG	3402	0	3280	35	0
1	Q	3402	0	3280	40	0
1	RB	3402	0	3280	39	0
1	RD	3402	0	3280	40	0
1	RF	3402	0	3280	37	0
1	RH	3402	0	3280	36	0
1	TA	3402	0	3280	37	0
1	TC	3402	0	3280	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	TE	3402	0	3280	36	0
1	TG	3402	0	3280	38	0
1	V	3402	0	3280	38	0
1	VB	3402	0	3280	38	0
1	VD	3402	0	3280	36	0
1	VF	3402	0	3280	40	0
1	VH	3402	0	3280	36	0
1	XA	3402	0	3280	37	0
1	XC	3402	0	3280	37	0
1	XE	3402	0	3280	39	0
1	XG	3402	0	3280	38	0
1	Z	3402	0	3280	37	0
1	ZB	3402	0	3280	40	0
1	ZD	3402	0	3280	36	0
1	ZF	3402	0	3280	36	0
1	ZH	3402	0	3280	38	0
2	AA	1327	0	1347	20	0
2	AC	1327	0	1347	21	0
2	AE	1327	0	1347	22	0
2	AG	1327	0	1347	22	0
2	AI	1327	0	1347	20	0
2	C	1327	0	1347	21	0
2	CB	1327	0	1347	20	0
2	CD	1327	0	1347	21	0
2	CF	1327	0	1347	22	0
2	CH	1327	0	1347	22	0
2	EA	1327	0	1347	20	0
2	EC	1327	0	1347	22	0
2	EE	1327	0	1347	21	0
2	EG	1327	0	1347	22	0
2	EI	1327	0	1347	21	0
2	G	1327	0	1347	21	0
2	GB	1327	0	1347	22	0
2	GD	1327	0	1347	21	0
2	GF	1327	0	1347	22	0
2	GH	1327	0	1347	21	0
2	I	1327	0	1347	20	0
2	IA	1327	0	1347	20	0
2	IC	1327	0	1347	21	0
2	IE	1327	0	1347	22	0
2	IG	1327	0	1347	20	0
2	KB	1327	0	1347	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	KD	1327	0	1347	22	0
2	KF	1327	0	1347	21	0
2	KH	1327	0	1347	21	0
2	MA	1327	0	1347	22	0
2	MC	1327	0	1347	21	0
2	ME	1327	0	1347	20	0
2	MG	1327	0	1347	20	0
2	N	1327	0	1347	20	0
2	OB	1327	0	1347	21	0
2	OD	1327	0	1347	20	0
2	OF	1327	0	1347	22	0
2	OH	1327	0	1347	22	0
2	QA	1327	0	1347	22	0
2	QC	1327	0	1347	22	0
2	QE	1327	0	1347	21	0
2	QG	1327	0	1347	21	0
2	R	1327	0	1347	21	0
2	SB	1327	0	1347	21	0
2	SD	1327	0	1347	21	0
2	SF	1327	0	1347	22	0
2	SH	1327	0	1347	22	0
2	UA	1327	0	1347	20	0
2	UC	1327	0	1347	20	0
2	UE	1327	0	1347	22	0
2	UG	1327	0	1347	22	0
2	W	1327	0	1347	22	0
2	WB	1327	0	1347	20	0
2	WD	1327	0	1347	21	0
2	WF	1327	0	1347	22	0
2	WH	1327	0	1347	20	0
2	YA	1327	0	1347	20	0
2	YC	1327	0	1347	22	0
2	YE	1327	0	1347	21	0
2	YG	1327	0	1347	21	0
3	BA	205	0	212	4	0
3	BC	205	0	212	4	0
3	BE	205	0	212	5	0
3	BG	205	0	212	5	0
3	BI	205	0	212	5	0
3	D	205	0	212	5	0
3	DB	205	0	212	5	0
3	DD	205	0	212	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	DF	205	0	212	3	0
3	DH	205	0	212	5	0
3	FA	205	0	212	4	0
3	FC	205	0	212	4	0
3	FE	205	0	212	4	0
3	FG	205	0	212	6	0
3	FI	205	0	212	3	0
3	HB	205	0	212	4	0
3	HD	205	0	212	4	0
3	HF	205	0	212	4	0
3	HH	205	0	212	4	0
3	J	205	0	212	4	0
3	JA	205	0	212	5	0
3	JC	205	0	212	4	0
3	JE	205	0	212	4	0
3	JG	205	0	212	4	0
3	K	205	0	212	5	0
3	LB	205	0	212	5	0
3	LD	205	0	212	4	0
3	LF	205	0	212	5	0
3	LH	205	0	212	5	0
3	NA	205	0	212	4	0
3	NC	205	0	212	4	0
3	NE	205	0	212	3	0
3	NG	205	0	212	5	0
3	O	205	0	212	4	0
3	PB	205	0	212	5	0
3	PD	205	0	212	4	0
3	PF	205	0	212	4	0
3	PH	205	0	212	5	0
3	RA	205	0	212	4	0
3	RC	205	0	212	4	0
3	RE	205	0	212	5	0
3	RG	205	0	212	3	0
3	S	205	0	212	4	0
3	TB	205	0	212	5	0
3	TD	205	0	212	3	0
3	TF	205	0	212	4	0
3	TH	205	0	212	5	0
3	VA	205	0	212	4	0
3	VC	205	0	212	4	0
3	VE	205	0	212	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	VG	205	0	212	4	0
3	X	205	0	212	3	0
3	XB	205	0	212	4	0
3	XD	205	0	212	5	0
3	XF	205	0	212	5	0
3	XH	205	0	212	4	0
3	ZA	205	0	212	4	0
3	ZC	205	0	212	4	0
3	ZE	205	0	212	5	0
3	ZG	205	0	212	5	0
4	A	105	0	56	0	0
4	AB	105	0	56	0	0
4	AD	105	0	56	0	0
4	AF	105	0	56	0	0
4	AH	105	0	56	0	0
4	CA	105	0	56	0	0
4	CC	105	0	56	0	0
4	CE	105	0	56	0	0
4	CG	105	0	56	0	0
4	CI	105	0	56	0	0
4	E	105	0	56	0	0
4	EB	105	0	56	0	0
4	ED	105	0	56	0	0
4	EF	105	0	56	0	0
4	EH	105	0	56	0	0
4	GA	105	0	56	0	0
4	GC	105	0	56	0	0
4	GE	105	0	56	0	0
4	GG	105	0	56	0	0
4	GI	105	0	56	0	0
4	IB	105	0	56	0	0
4	ID	105	0	56	0	0
4	IF	105	0	56	0	0
4	IH	105	0	56	0	0
4	KA	105	0	56	0	0
4	KC	105	0	56	0	0
4	KE	105	0	56	0	0
4	KG	105	0	56	0	0
4	L	105	0	56	0	0
4	MB	105	0	56	0	0
4	MD	105	0	56	0	0
4	MF	105	0	56	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	MH	105	0	56	0	0
4	OA	105	0	56	0	0
4	OC	105	0	56	0	0
4	OE	105	0	56	0	0
4	OG	105	0	56	0	0
4	P	105	0	56	0	0
4	QB	105	0	56	0	0
4	QD	105	0	56	0	0
4	QF	105	0	56	0	0
4	QH	105	0	56	0	0
4	SA	105	0	56	0	0
4	SC	105	0	56	0	0
4	SE	105	0	56	0	0
4	SG	105	0	56	0	0
4	T	105	0	56	0	0
4	UB	105	0	56	0	0
4	UD	105	0	56	0	0
4	UF	105	0	56	0	0
4	UH	105	0	56	0	0
4	WA	105	0	56	0	0
4	WC	105	0	56	0	0
4	WE	105	0	56	0	0
4	WG	105	0	56	0	0
4	Y	105	0	56	0	0
4	YB	105	0	56	0	0
4	YD	105	0	56	0	0
4	YF	105	0	56	0	0
4	YH	105	0	56	0	0
5	0	84	0	45	4	0
5	1	84	0	45	4	0
5	2	84	0	45	4	0
5	3	84	0	45	4	0
5	4	84	0	45	4	0
5	5	84	0	45	4	0
5	6	84	0	45	4	0
5	7	84	0	45	4	0
5	8	84	0	45	4	0
5	9	84	0	45	4	0
5	U	84	0	45	4	0
5	a	84	0	45	4	0
5	aA	84	0	45	4	0
5	b	84	0	45	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	bA	84	0	45	4	0
5	c	84	0	45	4	0
5	cA	84	0	45	4	0
5	d	84	0	45	4	0
5	dA	84	0	45	4	0
5	e	84	0	45	4	0
5	eA	84	0	45	4	0
5	f	84	0	45	4	0
5	fA	84	0	45	4	0
5	g	84	0	45	4	0
5	gA	84	0	45	4	0
5	h	84	0	45	4	0
5	hA	84	0	45	4	0
5	i	84	0	45	4	0
5	iA	84	0	45	4	0
5	j	84	0	45	4	0
5	jA	84	0	45	4	0
5	k	84	0	45	4	0
5	kA	84	0	45	4	0
5	l	84	0	45	4	0
5	lA	84	0	45	4	0
5	m	84	0	45	4	0
5	mA	84	0	45	4	0
5	n	84	0	45	4	0
5	nA	84	0	45	4	0
5	o	84	0	45	4	0
5	oA	84	0	45	4	0
5	p	84	0	45	4	0
5	pA	84	0	45	4	0
5	q	84	0	45	4	0
5	qA	84	0	45	4	0
5	r	84	0	45	4	0
5	rA	84	0	45	4	0
5	s	84	0	45	4	0
5	sA	84	0	45	4	0
5	t	84	0	45	4	0
5	tA	84	0	45	4	0
5	u	84	0	45	4	0
5	uA	84	0	45	4	0
5	v	84	0	45	4	0
5	vA	84	0	45	4	0
5	w	84	0	45	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	wA	84	0	45	4	0
5	x	84	0	45	4	0
5	y	84	0	45	4	0
5	z	84	0	45	4	0
All	All	307380	0	296400	2885	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 2885 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:k:11:DA:H62	1:LG:423:ARG:HH21	1.22	0.88
5:f:11:DA:H62	1:ZH:423:ARG:HH21	1.22	0.88
1:HC:423:ARG:HH21	5:pA:11:DA:H62	1.23	0.87
1:BH:423:ARG:HH21	5:wA:11:DA:H62	1.22	0.87
1:Q:423:ARG:HH21	5:dA:11:DA:H62	1.22	0.87

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	426/429 (99%)	419 (98%)	7 (2%)	0	100	100
1	BB	426/429 (99%)	419 (98%)	7 (2%)	0	100	100
1	BD	426/429 (99%)	419 (98%)	7 (2%)	0	100	100
1	BF	426/429 (99%)	419 (98%)	7 (2%)	0	100	100
1	BH	426/429 (99%)	419 (98%)	7 (2%)	0	100	100
1	DA	426/429 (99%)	419 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	DC	426/429 (99%)	419 (98%)	7 (2%)	0	100	100
1	DE	426/429 (99%)	419 (98%)	7 (2%)	0	100	100
1	DG	426/429 (99%)	419 (98%)	7 (2%)	0	100	100
1	DI	426/429 (99%)	419 (98%)	7 (2%)	0	100	100
1	F	426/429 (99%)	419 (98%)	7 (2%)	0	100	100
1	FB	426/429 (99%)	419 (98%)	7 (2%)	0	100	100
1	FD	426/429 (99%)	419 (98%)	7 (2%)	0	100	100
1	FF	426/429 (99%)	419 (98%)	7 (2%)	0	100	100
1	FH	426/429 (99%)	419 (98%)	7 (2%)	0	100	100
1	H	426/429 (99%)	419 (98%)	7 (2%)	0	100	100
1	HA	426/429 (99%)	419 (98%)	7 (2%)	0	100	100
1	HC	426/429 (99%)	419 (98%)	7 (2%)	0	100	100
1	HE	426/429 (99%)	419 (98%)	7 (2%)	0	100	100
1	HG	426/429 (99%)	419 (98%)	7 (2%)	0	100	100
1	JB	426/429 (99%)	419 (98%)	7 (2%)	0	100	100
1	JD	426/429 (99%)	419 (98%)	7 (2%)	0	100	100
1	JF	426/429 (99%)	419 (98%)	7 (2%)	0	100	100
1	JH	426/429 (99%)	419 (98%)	7 (2%)	0	100	100
1	LA	426/429 (99%)	419 (98%)	7 (2%)	0	100	100
1	LC	426/429 (99%)	419 (98%)	7 (2%)	0	100	100
1	LE	426/429 (99%)	419 (98%)	7 (2%)	0	100	100
1	LG	426/429 (99%)	419 (98%)	7 (2%)	0	100	100
1	M	426/429 (99%)	419 (98%)	7 (2%)	0	100	100
1	NB	426/429 (99%)	419 (98%)	7 (2%)	0	100	100
1	ND	426/429 (99%)	419 (98%)	7 (2%)	0	100	100
1	NF	426/429 (99%)	419 (98%)	7 (2%)	0	100	100
1	NH	426/429 (99%)	419 (98%)	7 (2%)	0	100	100
1	PA	426/429 (99%)	419 (98%)	7 (2%)	0	100	100
1	PC	426/429 (99%)	419 (98%)	7 (2%)	0	100	100
1	PE	426/429 (99%)	419 (98%)	7 (2%)	0	100	100
1	PG	426/429 (99%)	419 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	426/429 (99%)	419 (98%)	7 (2%)	0	100	100
1	RB	426/429 (99%)	419 (98%)	7 (2%)	0	100	100
1	RD	426/429 (99%)	419 (98%)	7 (2%)	0	100	100
1	RF	426/429 (99%)	419 (98%)	7 (2%)	0	100	100
1	RH	426/429 (99%)	419 (98%)	7 (2%)	0	100	100
1	TA	426/429 (99%)	419 (98%)	7 (2%)	0	100	100
1	TC	426/429 (99%)	419 (98%)	7 (2%)	0	100	100
1	TE	426/429 (99%)	419 (98%)	7 (2%)	0	100	100
1	TG	426/429 (99%)	419 (98%)	7 (2%)	0	100	100
1	V	426/429 (99%)	419 (98%)	7 (2%)	0	100	100
1	VB	426/429 (99%)	419 (98%)	7 (2%)	0	100	100
1	VD	426/429 (99%)	419 (98%)	7 (2%)	0	100	100
1	VF	426/429 (99%)	419 (98%)	7 (2%)	0	100	100
1	VH	426/429 (99%)	419 (98%)	7 (2%)	0	100	100
1	XA	426/429 (99%)	419 (98%)	7 (2%)	0	100	100
1	XC	426/429 (99%)	419 (98%)	7 (2%)	0	100	100
1	XE	426/429 (99%)	419 (98%)	7 (2%)	0	100	100
1	XG	426/429 (99%)	419 (98%)	7 (2%)	0	100	100
1	Z	426/429 (99%)	419 (98%)	7 (2%)	0	100	100
1	ZB	426/429 (99%)	419 (98%)	7 (2%)	0	100	100
1	ZD	426/429 (99%)	419 (98%)	7 (2%)	0	100	100
1	ZF	426/429 (99%)	419 (98%)	7 (2%)	0	100	100
1	ZH	426/429 (99%)	419 (98%)	7 (2%)	0	100	100
2	AA	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
2	AC	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
2	AE	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
2	AG	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
2	AI	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
2	C	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
2	CB	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
2	CD	175/177 (99%)	164 (94%)	11 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	CF	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
2	CH	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
2	EA	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
2	EC	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
2	EE	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
2	EG	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
2	EI	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
2	G	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
2	GB	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
2	GD	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
2	GF	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
2	GH	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
2	I	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
2	IA	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
2	IC	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
2	IE	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
2	IG	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
2	KB	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
2	KD	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
2	KF	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
2	KH	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
2	MA	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
2	MC	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
2	ME	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
2	MG	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
2	N	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
2	OB	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
2	OD	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
2	OF	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
2	OH	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
2	QA	175/177 (99%)	164 (94%)	11 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	QC	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
2	QE	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
2	QG	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
2	R	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
2	SB	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
2	SD	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
2	SF	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
2	SH	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
2	UA	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
2	UC	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
2	UE	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
2	UG	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
2	W	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
2	WB	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
2	WD	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
2	WF	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
2	WH	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
2	YA	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
2	YC	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
2	YE	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
2	YG	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
3	BA	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
3	BC	24/26 (92%)	22 (92%)	2 (8%)	0	100	100
3	BE	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
3	BG	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
3	BI	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
3	D	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
3	DB	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
3	DD	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
3	DF	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
3	DH	24/26 (92%)	21 (88%)	3 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	FA	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
3	FC	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
3	FE	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
3	FG	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
3	FI	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
3	HB	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
3	HD	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
3	HF	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
3	HH	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
3	J	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
3	JA	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
3	JC	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
3	JE	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
3	JG	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
3	K	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
3	LB	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
3	LD	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
3	LF	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
3	LH	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
3	NA	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
3	NC	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
3	NE	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
3	NG	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
3	O	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
3	PB	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
3	PD	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
3	PF	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
3	PH	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
3	RA	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
3	RC	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
3	RE	24/26 (92%)	21 (88%)	3 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	RG	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
3	S	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
3	TB	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
3	TD	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
3	TF	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
3	TH	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
3	VA	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
3	VC	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
3	VE	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
3	VG	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
3	X	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
3	XB	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
3	XD	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
3	XF	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
3	XH	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
3	ZA	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
3	ZC	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
3	ZE	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
3	ZG	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
All	All	37500/37920 (99%)	36241 (97%)	1259 (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	B	371/372 (100%)	371 (100%)	0	100	100
1	BB	371/372 (100%)	371 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BD	371/372 (100%)	371 (100%)	0	100	100
1	BF	371/372 (100%)	371 (100%)	0	100	100
1	BH	371/372 (100%)	371 (100%)	0	100	100
1	DA	371/372 (100%)	371 (100%)	0	100	100
1	DC	371/372 (100%)	371 (100%)	0	100	100
1	DE	371/372 (100%)	371 (100%)	0	100	100
1	DG	371/372 (100%)	371 (100%)	0	100	100
1	DI	371/372 (100%)	371 (100%)	0	100	100
1	F	371/372 (100%)	371 (100%)	0	100	100
1	FB	371/372 (100%)	371 (100%)	0	100	100
1	FD	371/372 (100%)	371 (100%)	0	100	100
1	FF	371/372 (100%)	371 (100%)	0	100	100
1	FH	371/372 (100%)	371 (100%)	0	100	100
1	H	371/372 (100%)	371 (100%)	0	100	100
1	HA	371/372 (100%)	371 (100%)	0	100	100
1	HC	371/372 (100%)	371 (100%)	0	100	100
1	HE	371/372 (100%)	371 (100%)	0	100	100
1	HG	371/372 (100%)	371 (100%)	0	100	100
1	JB	371/372 (100%)	371 (100%)	0	100	100
1	JD	371/372 (100%)	371 (100%)	0	100	100
1	JF	371/372 (100%)	371 (100%)	0	100	100
1	JH	371/372 (100%)	371 (100%)	0	100	100
1	LA	371/372 (100%)	371 (100%)	0	100	100
1	LC	371/372 (100%)	371 (100%)	0	100	100
1	LE	371/372 (100%)	371 (100%)	0	100	100
1	LG	371/372 (100%)	371 (100%)	0	100	100
1	M	371/372 (100%)	371 (100%)	0	100	100
1	NB	371/372 (100%)	371 (100%)	0	100	100
1	ND	371/372 (100%)	371 (100%)	0	100	100
1	NF	371/372 (100%)	371 (100%)	0	100	100
1	NH	371/372 (100%)	371 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	PA	371/372 (100%)	371 (100%)	0	100	100
1	PC	371/372 (100%)	371 (100%)	0	100	100
1	PE	371/372 (100%)	371 (100%)	0	100	100
1	PG	371/372 (100%)	371 (100%)	0	100	100
1	Q	371/372 (100%)	371 (100%)	0	100	100
1	RB	371/372 (100%)	371 (100%)	0	100	100
1	RD	371/372 (100%)	371 (100%)	0	100	100
1	RF	371/372 (100%)	371 (100%)	0	100	100
1	RH	371/372 (100%)	371 (100%)	0	100	100
1	TA	371/372 (100%)	371 (100%)	0	100	100
1	TC	371/372 (100%)	371 (100%)	0	100	100
1	TE	371/372 (100%)	371 (100%)	0	100	100
1	TG	371/372 (100%)	371 (100%)	0	100	100
1	V	371/372 (100%)	371 (100%)	0	100	100
1	VB	371/372 (100%)	371 (100%)	0	100	100
1	VD	371/372 (100%)	371 (100%)	0	100	100
1	VF	371/372 (100%)	371 (100%)	0	100	100
1	VH	371/372 (100%)	371 (100%)	0	100	100
1	XA	371/372 (100%)	371 (100%)	0	100	100
1	XC	371/372 (100%)	371 (100%)	0	100	100
1	XE	371/372 (100%)	371 (100%)	0	100	100
1	XG	371/372 (100%)	371 (100%)	0	100	100
1	Z	371/372 (100%)	371 (100%)	0	100	100
1	ZB	371/372 (100%)	371 (100%)	0	100	100
1	ZD	371/372 (100%)	371 (100%)	0	100	100
1	ZF	371/372 (100%)	371 (100%)	0	100	100
1	ZH	371/372 (100%)	371 (100%)	0	100	100
2	AA	150/150 (100%)	149 (99%)	1 (1%)	81	93
2	AC	150/150 (100%)	149 (99%)	1 (1%)	81	93
2	AE	150/150 (100%)	149 (99%)	1 (1%)	81	93
2	AG	150/150 (100%)	149 (99%)	1 (1%)	81	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AI	150/150 (100%)	149 (99%)	1 (1%)	81	93
2	C	150/150 (100%)	149 (99%)	1 (1%)	81	93
2	CB	150/150 (100%)	149 (99%)	1 (1%)	81	93
2	CD	150/150 (100%)	149 (99%)	1 (1%)	81	93
2	CF	150/150 (100%)	149 (99%)	1 (1%)	81	93
2	CH	150/150 (100%)	149 (99%)	1 (1%)	81	93
2	EA	150/150 (100%)	149 (99%)	1 (1%)	81	93
2	EC	150/150 (100%)	149 (99%)	1 (1%)	81	93
2	EE	150/150 (100%)	149 (99%)	1 (1%)	81	93
2	EG	150/150 (100%)	149 (99%)	1 (1%)	81	93
2	EI	150/150 (100%)	149 (99%)	1 (1%)	81	93
2	G	150/150 (100%)	149 (99%)	1 (1%)	81	93
2	GB	150/150 (100%)	149 (99%)	1 (1%)	81	93
2	GD	150/150 (100%)	149 (99%)	1 (1%)	81	93
2	GF	150/150 (100%)	149 (99%)	1 (1%)	81	93
2	GH	150/150 (100%)	149 (99%)	1 (1%)	81	93
2	I	150/150 (100%)	149 (99%)	1 (1%)	81	93
2	IA	150/150 (100%)	149 (99%)	1 (1%)	81	93
2	IC	150/150 (100%)	149 (99%)	1 (1%)	81	93
2	IE	150/150 (100%)	149 (99%)	1 (1%)	81	93
2	IG	150/150 (100%)	149 (99%)	1 (1%)	81	93
2	KB	150/150 (100%)	149 (99%)	1 (1%)	81	93
2	KD	150/150 (100%)	149 (99%)	1 (1%)	81	93
2	KF	150/150 (100%)	149 (99%)	1 (1%)	81	93
2	KH	150/150 (100%)	149 (99%)	1 (1%)	81	93
2	MA	150/150 (100%)	149 (99%)	1 (1%)	81	93
2	MC	150/150 (100%)	149 (99%)	1 (1%)	81	93
2	ME	150/150 (100%)	149 (99%)	1 (1%)	81	93
2	MG	150/150 (100%)	149 (99%)	1 (1%)	81	93
2	N	150/150 (100%)	149 (99%)	1 (1%)	81	93
2	OB	150/150 (100%)	149 (99%)	1 (1%)	81	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	OD	150/150 (100%)	149 (99%)	1 (1%)	81	93
2	OF	150/150 (100%)	149 (99%)	1 (1%)	81	93
2	OH	150/150 (100%)	149 (99%)	1 (1%)	81	93
2	QA	150/150 (100%)	149 (99%)	1 (1%)	81	93
2	QC	150/150 (100%)	149 (99%)	1 (1%)	81	93
2	QE	150/150 (100%)	149 (99%)	1 (1%)	81	93
2	QG	150/150 (100%)	149 (99%)	1 (1%)	81	93
2	R	150/150 (100%)	149 (99%)	1 (1%)	81	93
2	SB	150/150 (100%)	149 (99%)	1 (1%)	81	93
2	SD	150/150 (100%)	149 (99%)	1 (1%)	81	93
2	SF	150/150 (100%)	149 (99%)	1 (1%)	81	93
2	SH	150/150 (100%)	149 (99%)	1 (1%)	81	93
2	UA	150/150 (100%)	149 (99%)	1 (1%)	81	93
2	UC	150/150 (100%)	149 (99%)	1 (1%)	81	93
2	UE	150/150 (100%)	149 (99%)	1 (1%)	81	93
2	UG	150/150 (100%)	149 (99%)	1 (1%)	81	93
2	W	150/150 (100%)	149 (99%)	1 (1%)	81	93
2	WB	150/150 (100%)	149 (99%)	1 (1%)	81	93
2	WD	150/150 (100%)	149 (99%)	1 (1%)	81	93
2	WF	150/150 (100%)	149 (99%)	1 (1%)	81	93
2	WH	150/150 (100%)	149 (99%)	1 (1%)	81	93
2	YA	150/150 (100%)	149 (99%)	1 (1%)	81	93
2	YC	150/150 (100%)	149 (99%)	1 (1%)	81	93
2	YE	150/150 (100%)	149 (99%)	1 (1%)	81	93
2	YG	150/150 (100%)	149 (99%)	1 (1%)	81	93
3	BA	20/20 (100%)	20 (100%)	0	100	100
3	BC	20/20 (100%)	20 (100%)	0	100	100
3	BE	20/20 (100%)	20 (100%)	0	100	100
3	BG	20/20 (100%)	20 (100%)	0	100	100
3	BI	20/20 (100%)	20 (100%)	0	100	100
3	D	20/20 (100%)	20 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	DB	20/20 (100%)	20 (100%)	0	100	100
3	DD	20/20 (100%)	20 (100%)	0	100	100
3	DF	20/20 (100%)	20 (100%)	0	100	100
3	DH	20/20 (100%)	20 (100%)	0	100	100
3	FA	20/20 (100%)	20 (100%)	0	100	100
3	FC	20/20 (100%)	20 (100%)	0	100	100
3	FE	20/20 (100%)	20 (100%)	0	100	100
3	FG	20/20 (100%)	20 (100%)	0	100	100
3	FI	20/20 (100%)	20 (100%)	0	100	100
3	HB	20/20 (100%)	20 (100%)	0	100	100
3	HD	20/20 (100%)	20 (100%)	0	100	100
3	HF	20/20 (100%)	20 (100%)	0	100	100
3	HH	20/20 (100%)	20 (100%)	0	100	100
3	J	20/20 (100%)	20 (100%)	0	100	100
3	JA	20/20 (100%)	20 (100%)	0	100	100
3	JC	20/20 (100%)	20 (100%)	0	100	100
3	JE	20/20 (100%)	20 (100%)	0	100	100
3	JG	20/20 (100%)	20 (100%)	0	100	100
3	K	20/20 (100%)	20 (100%)	0	100	100
3	LB	20/20 (100%)	20 (100%)	0	100	100
3	LD	20/20 (100%)	20 (100%)	0	100	100
3	LF	20/20 (100%)	20 (100%)	0	100	100
3	LH	20/20 (100%)	20 (100%)	0	100	100
3	NA	20/20 (100%)	20 (100%)	0	100	100
3	NC	20/20 (100%)	20 (100%)	0	100	100
3	NE	20/20 (100%)	20 (100%)	0	100	100
3	NG	20/20 (100%)	20 (100%)	0	100	100
3	O	20/20 (100%)	20 (100%)	0	100	100
3	PB	20/20 (100%)	20 (100%)	0	100	100
3	PD	20/20 (100%)	20 (100%)	0	100	100
3	PF	20/20 (100%)	20 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	PH	20/20 (100%)	20 (100%)	0	100	100
3	RA	20/20 (100%)	20 (100%)	0	100	100
3	RC	20/20 (100%)	20 (100%)	0	100	100
3	RE	20/20 (100%)	20 (100%)	0	100	100
3	RG	20/20 (100%)	20 (100%)	0	100	100
3	S	20/20 (100%)	20 (100%)	0	100	100
3	TB	20/20 (100%)	20 (100%)	0	100	100
3	TD	20/20 (100%)	20 (100%)	0	100	100
3	TF	20/20 (100%)	20 (100%)	0	100	100
3	TH	20/20 (100%)	20 (100%)	0	100	100
3	VA	20/20 (100%)	20 (100%)	0	100	100
3	VC	20/20 (100%)	20 (100%)	0	100	100
3	VE	20/20 (100%)	20 (100%)	0	100	100
3	VG	20/20 (100%)	20 (100%)	0	100	100
3	X	20/20 (100%)	20 (100%)	0	100	100
3	XB	20/20 (100%)	20 (100%)	0	100	100
3	XD	20/20 (100%)	20 (100%)	0	100	100
3	XF	20/20 (100%)	20 (100%)	0	100	100
3	XH	20/20 (100%)	20 (100%)	0	100	100
3	ZA	20/20 (100%)	20 (100%)	0	100	100
3	ZC	20/20 (100%)	20 (100%)	0	100	100
3	ZE	20/20 (100%)	20 (100%)	0	100	100
3	ZG	20/20 (100%)	20 (100%)	0	100	100
All	All	32460/32520 (100%)	32400 (100%)	60 (0%)	91	98

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	KD	136	VAL
2	OH	136	VAL
2	ME	136	VAL
2	KH	136	VAL
2	EI	136	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 184 such sidechains are listed below:

Mol	Chain	Res	Type
1	TE	401	GLN
1	DG	406	ASN
1	BF	214	GLN
1	NF	401	GLN
1	PG	214	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

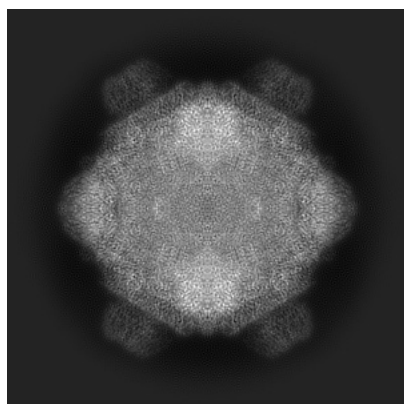
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62023. These allow visual inspection of the internal detail of the map and identification of artifacts.

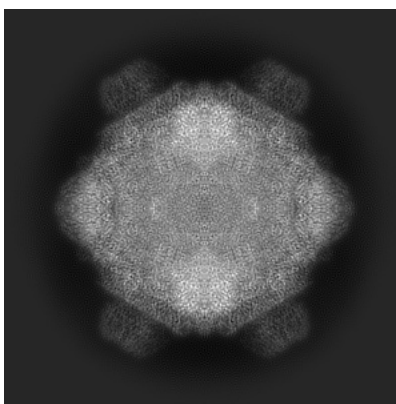
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

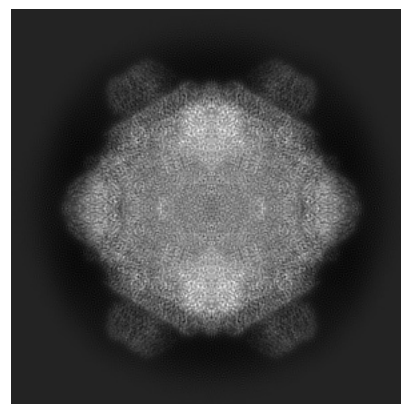
6.1.1 Primary map



X

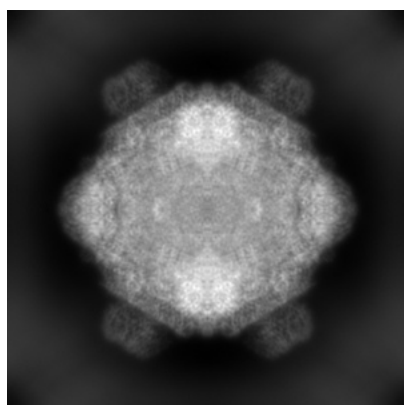


Y

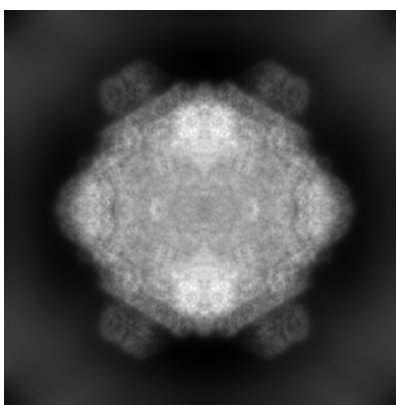


Z

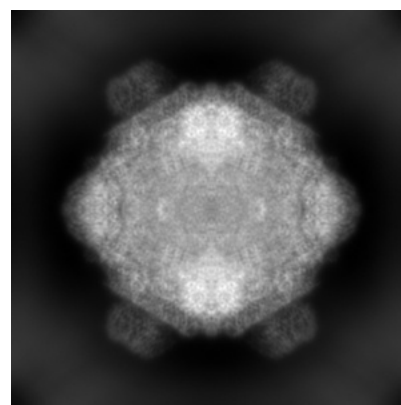
6.1.2 Raw map



X



Y

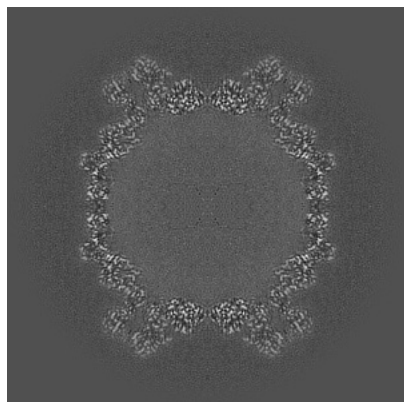


Z

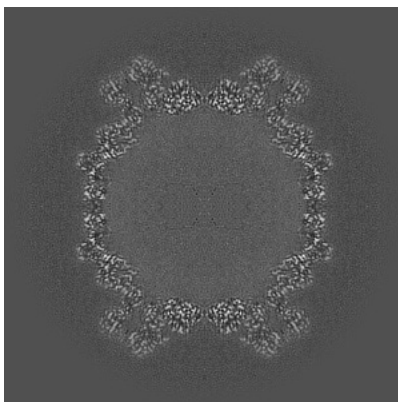
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

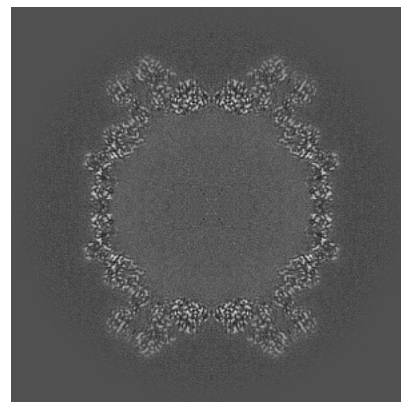
6.2.1 Primary map



X Index: 200

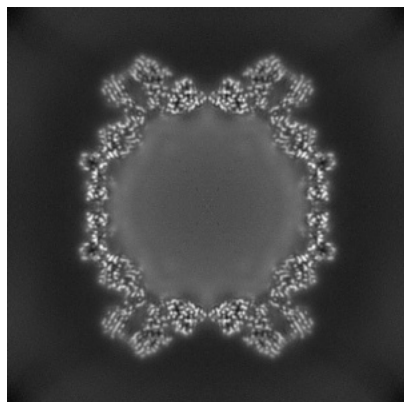


Y Index: 200

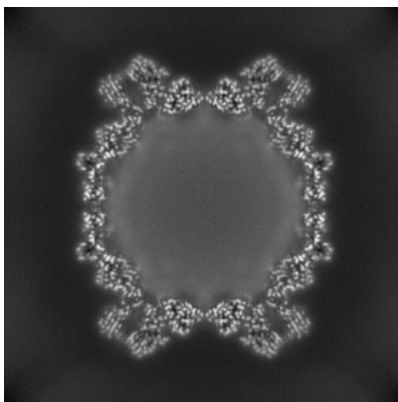


Z Index: 200

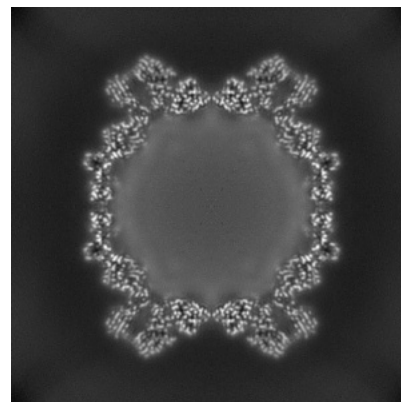
6.2.2 Raw map



X Index: 200



Y Index: 200

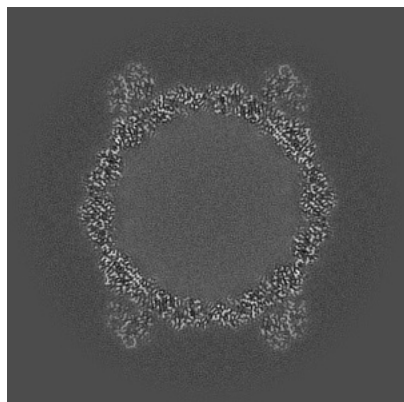


Z Index: 200

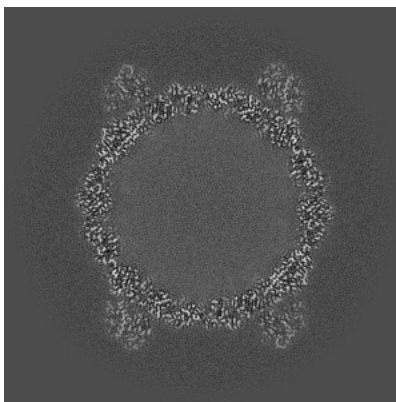
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

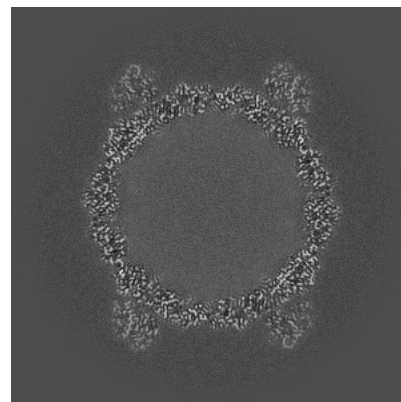
6.3.1 Primary map



X Index: 178

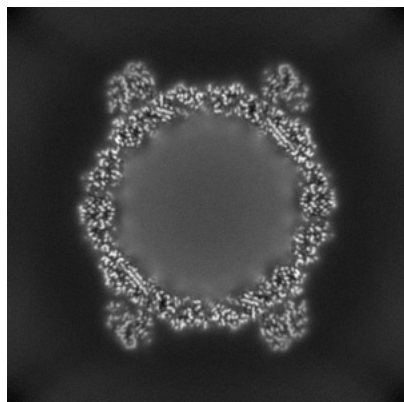


Y Index: 222

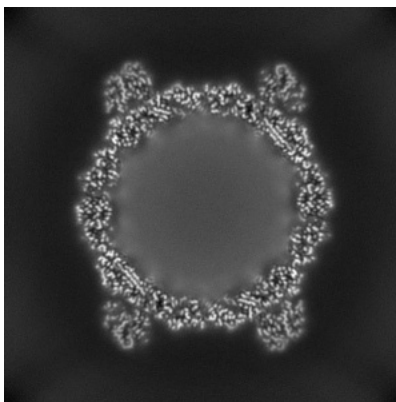


Z Index: 222

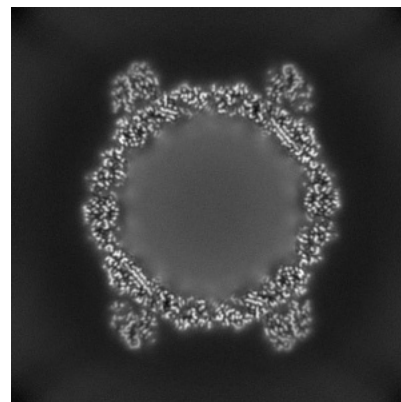
6.3.2 Raw map



X Index: 178



Y Index: 178

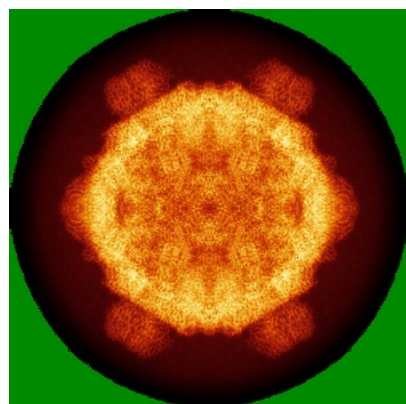


Z Index: 178

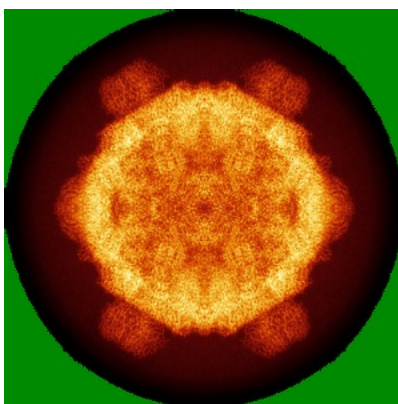
The images above show the largest variance slices of the map in three orthogonal directions.

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

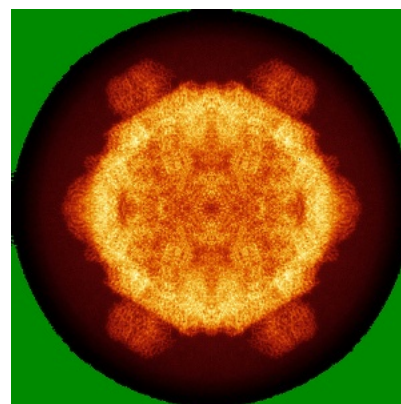
6.4.1 Primary map



X

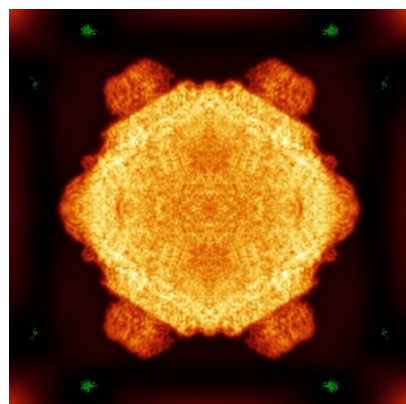


Y

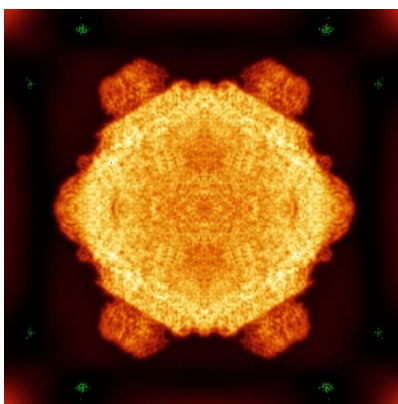


Z

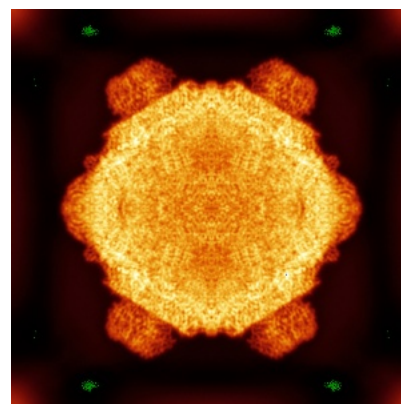
6.4.2 Raw map



X



Y

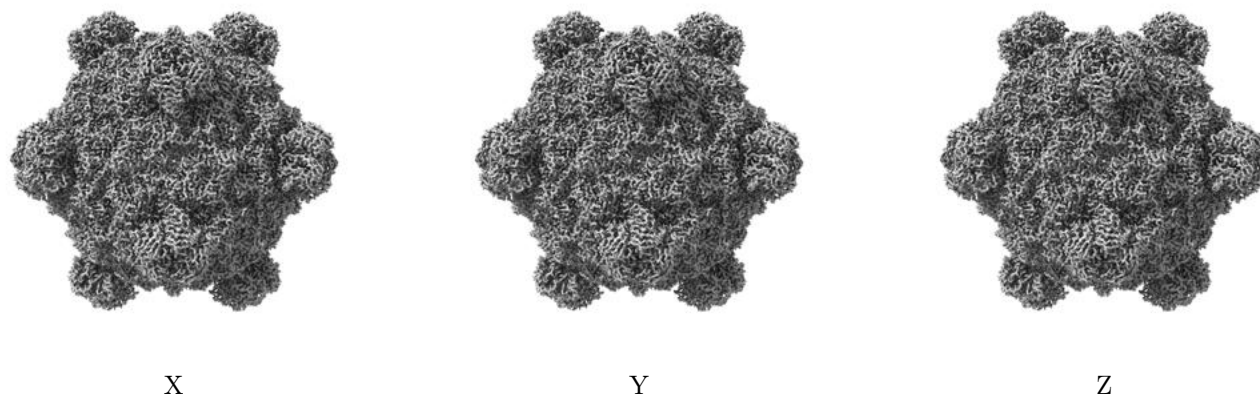


Z

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

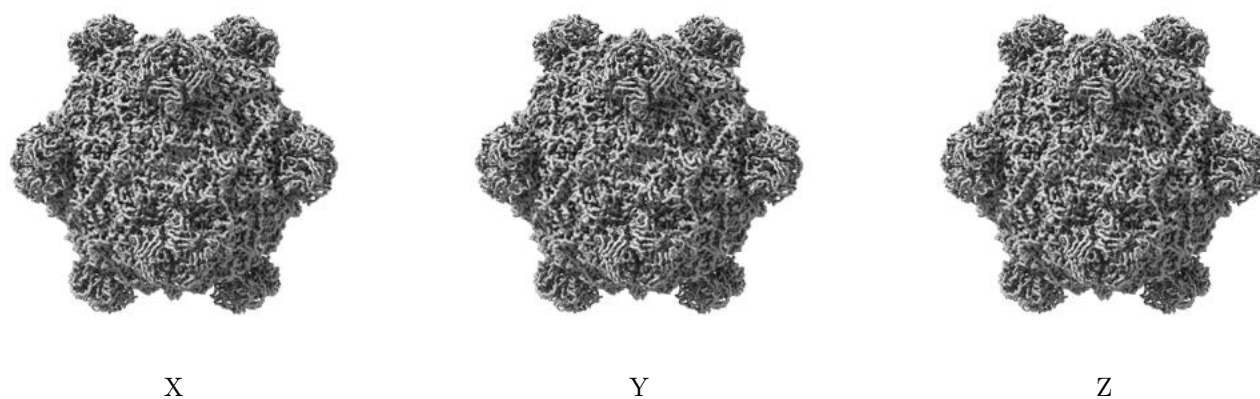
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.65. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

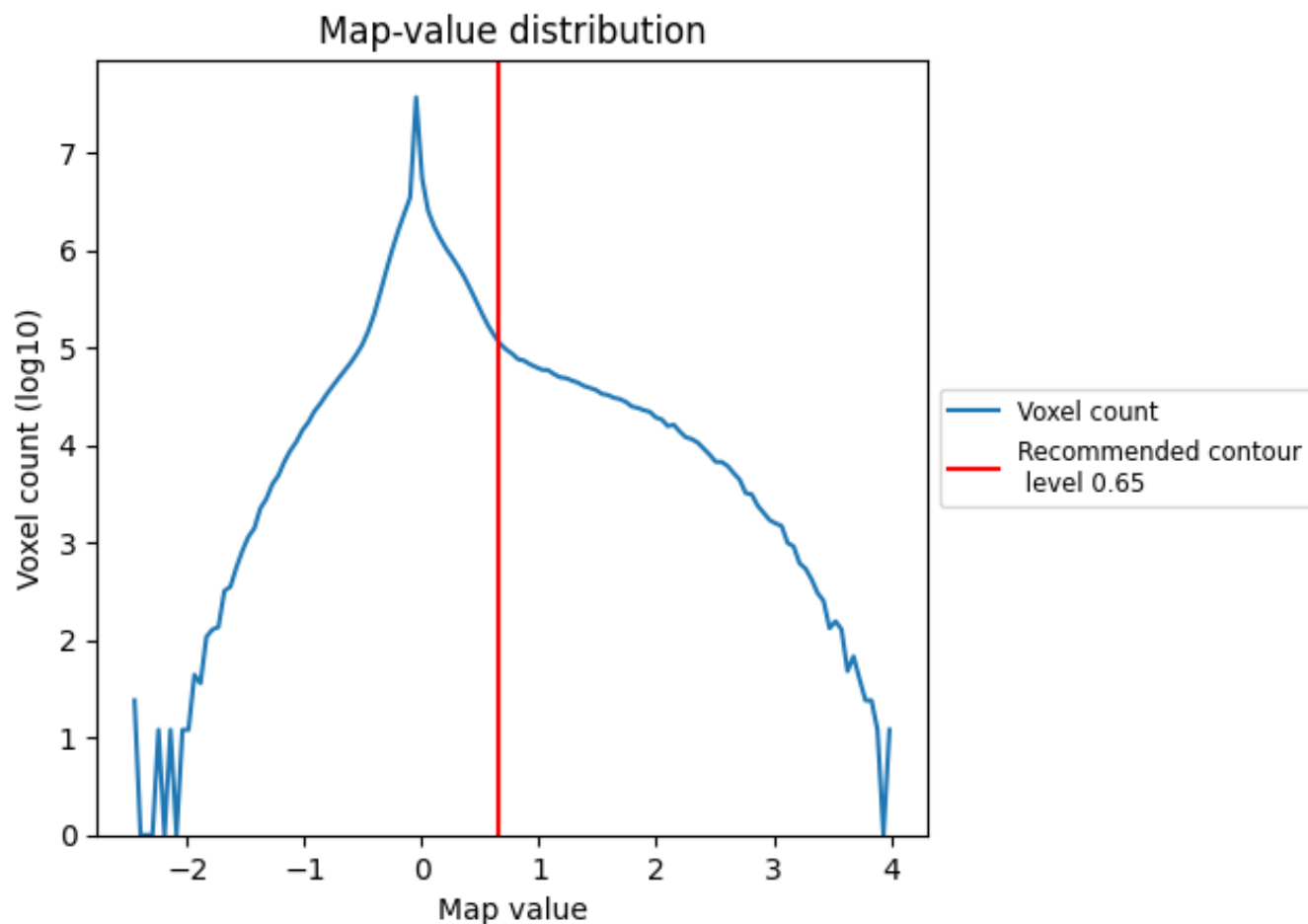
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

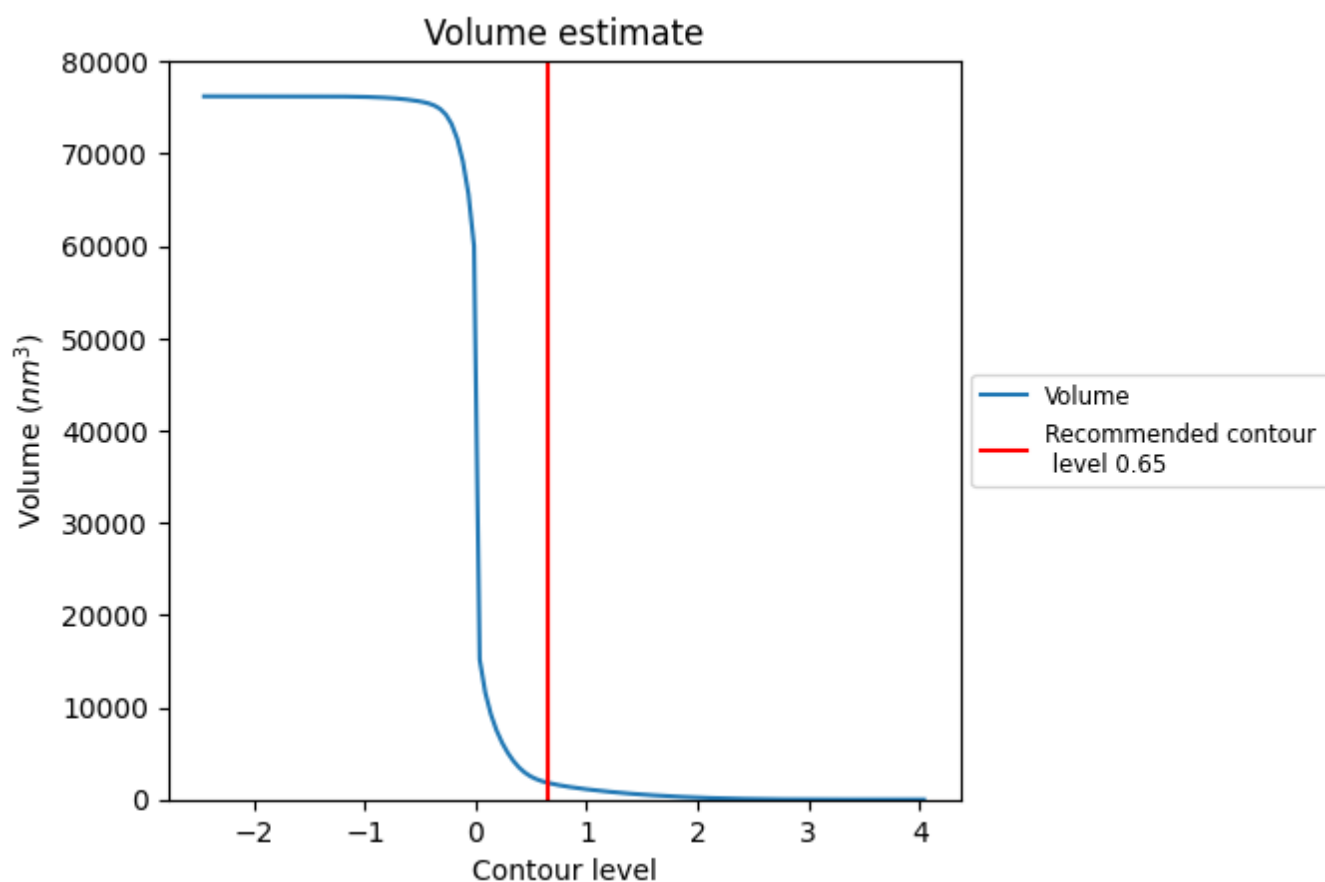
This section contains the results of statistical analysis of the map.

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.

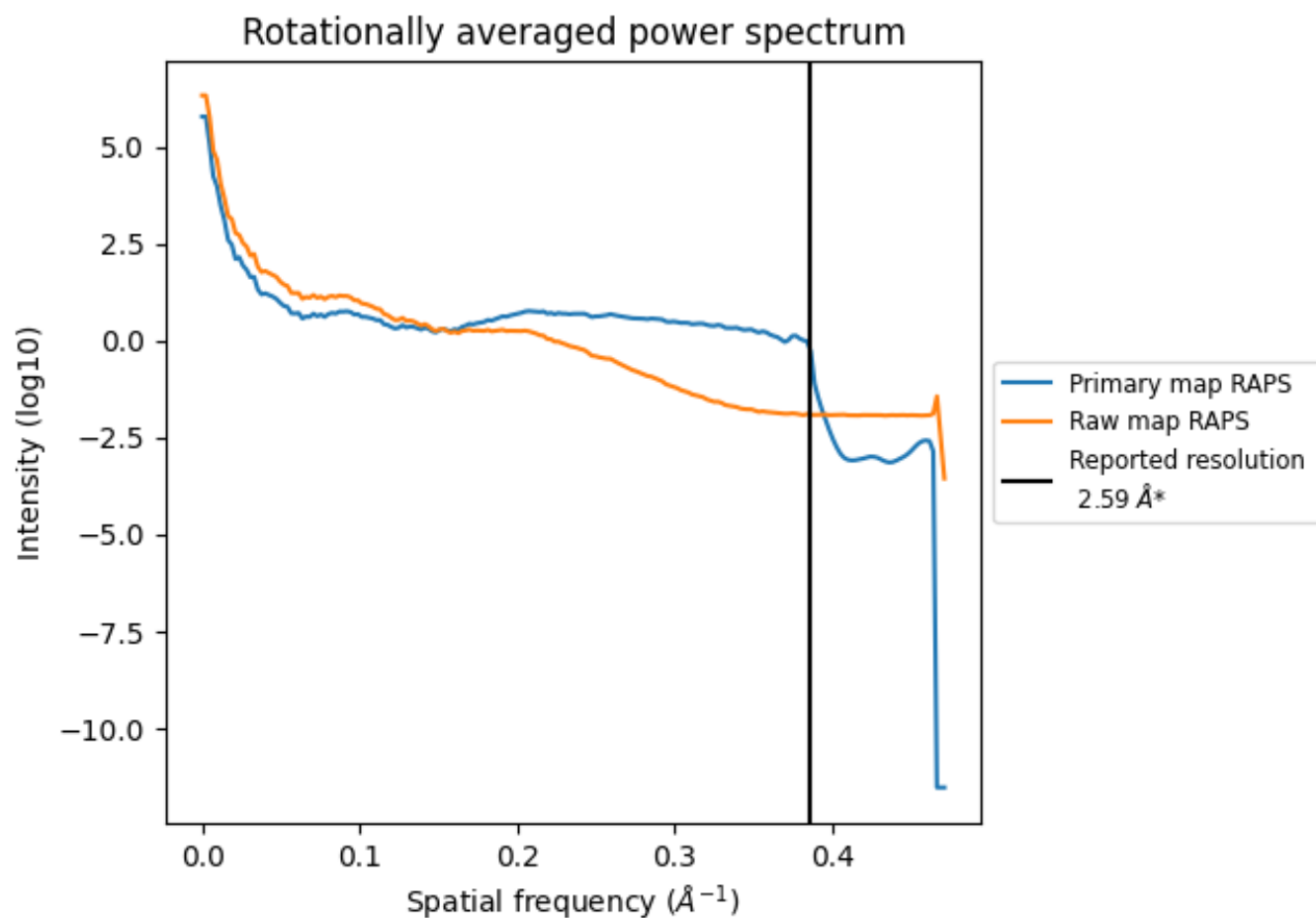
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1816 nm³; this corresponds to an approximate mass of 1640 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 ⓘ

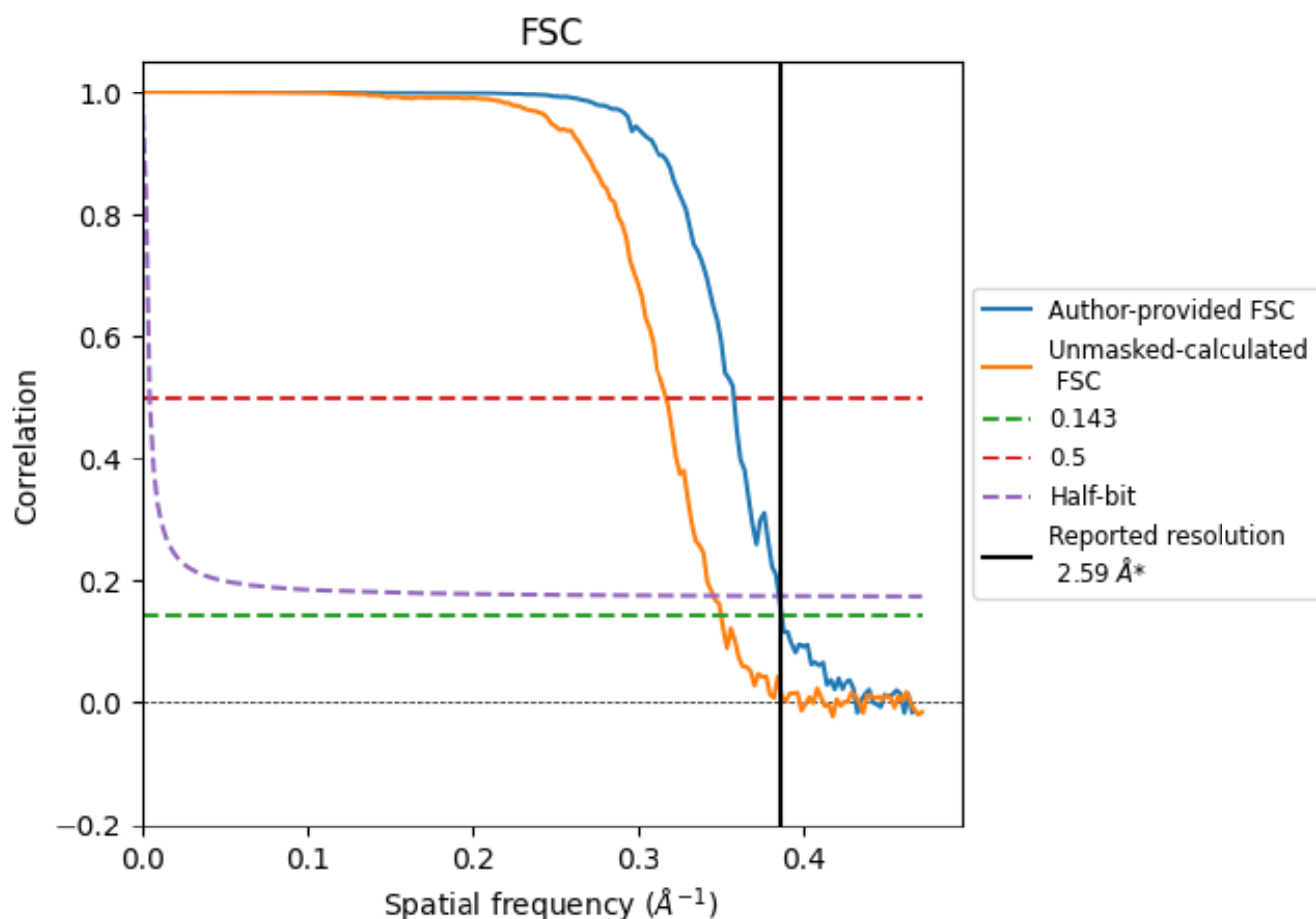


*Reported resolution corresponds to spatial frequency of 0.386 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.386 Å⁻¹

8.2 Resolution estimates [i](#)

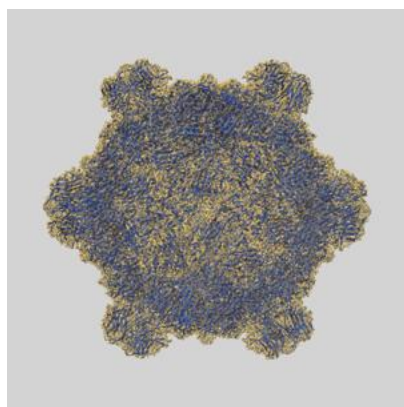
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.59	-	-
Author-provided FSC curve	2.59	2.79	2.60
Unmasked-calculated*	2.86	3.15	2.89

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.86 differs from the reported value 2.59 by more than 10 %

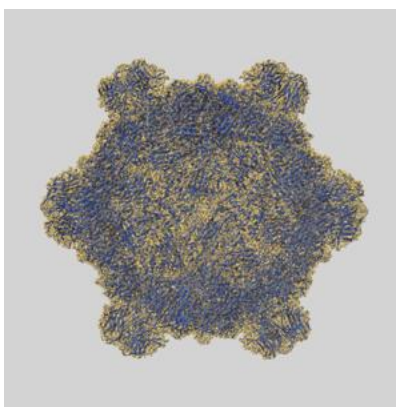
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-62023 and PDB model 9K3N. Per-residue inclusion information can be found in [section 3](#) on [page 30](#).

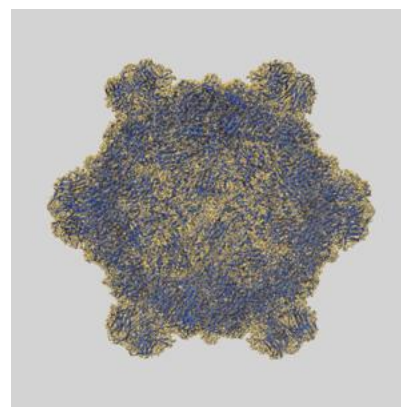
9.1 Map-model overlay [i](#)



X



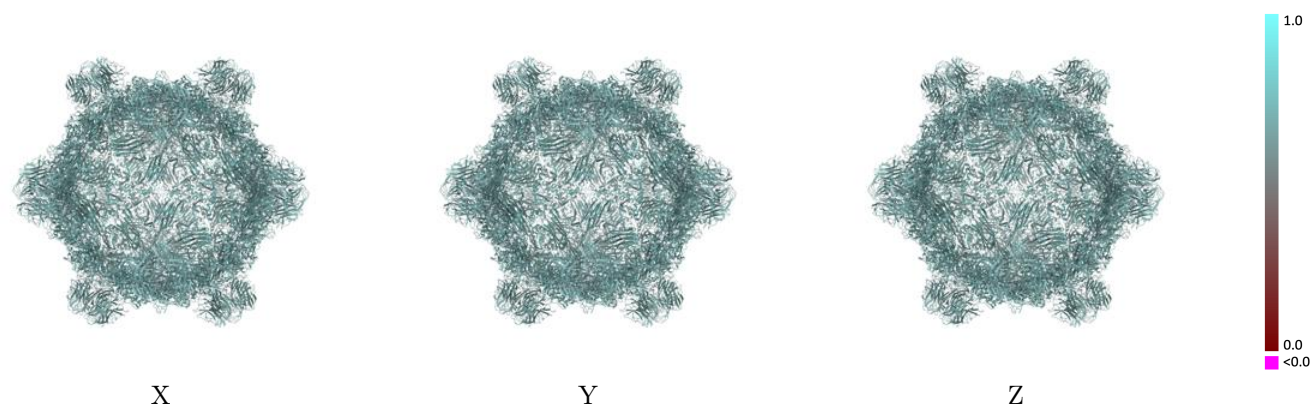
Y



Z

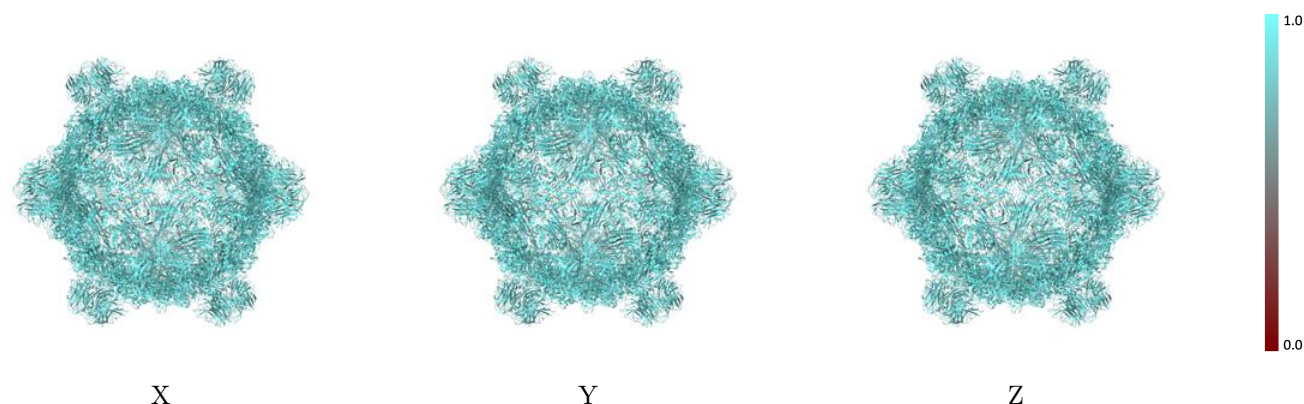
The images above show the 3D surface view of the map at the recommended contour level 0.65 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



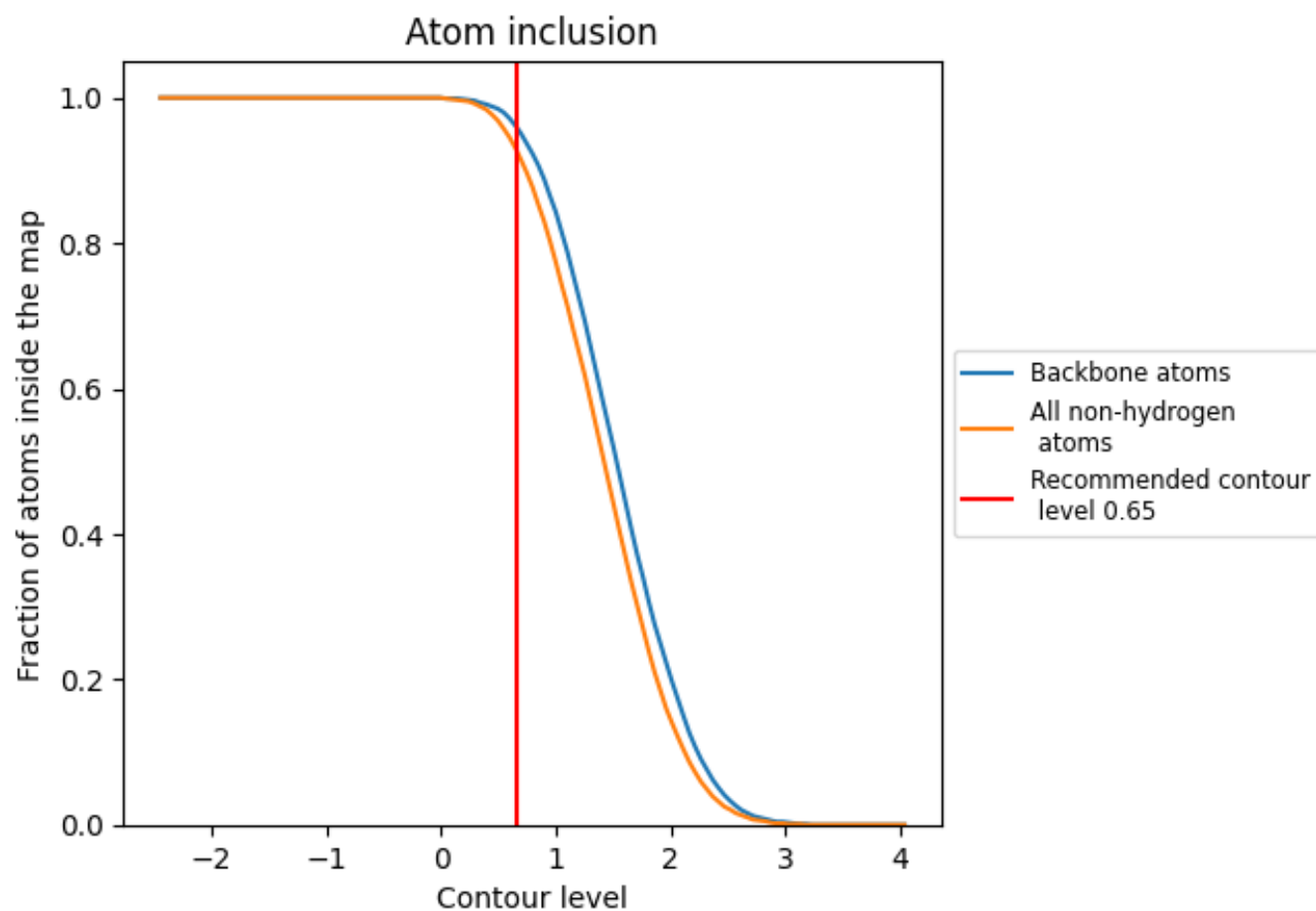
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.65).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 93% 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 (0.65) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9300	 0.6560
0	 0.8450	 0.5900
1	 0.8210	 0.5890
2	 0.8210	 0.6020
3	 0.8450	 0.6080
4	 0.8090	 0.6060
5	 0.8450	 0.5910
6	 0.8210	 0.5880
7	 0.8210	 0.5930
8	 0.8450	 0.6110
9	 0.8090	 0.5930
A	 0.7520	 0.5990
AA	 0.8700	 0.6360
AB	 0.7430	 0.5870
AC	 0.8700	 0.6360
AD	 0.7520	 0.6020
AE	 0.8780	 0.6380
AF	 0.7430	 0.6000
AG	 0.8710	 0.6410
AH	 0.7330	 0.5940
AI	 0.8720	 0.6370
B	 0.9670	 0.6690
BA	 0.8470	 0.6240
BB	 0.9650	 0.6670
BC	 0.8520	 0.6270
BD	 0.9670	 0.6660
BE	 0.8620	 0.6320
BF	 0.9660	 0.6670
BG	 0.8620	 0.6340
BH	 0.9660	 0.6680
BI	 0.8520	 0.6290
C	 0.8700	 0.6390
CA	 0.7330	 0.5910
CB	 0.8740	 0.6380
CC	 0.7430	 0.5900























































































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Chain	Atom inclusion	Q-score
CD	 0.8720	 0.6360
CE	 0.7430	 0.5900
CF	 0.8740	 0.6370
CG	 0.7520	 0.5990
CH	 0.8810	 0.6360
CI	 0.7430	 0.5910
D	 0.8470	 0.6290
DA	 0.9650	 0.6660
DB	 0.8520	 0.6280
DC	 0.9660	 0.6700
DD	 0.8470	 0.6210
DE	 0.9650	 0.6670
DF	 0.8520	 0.6300
DG	 0.9670	 0.6660
DH	 0.8620	 0.6290
DI	 0.9660	 0.6660
E	 0.7330	 0.5930
EA	 0.8770	 0.6360
EB	 0.7520	 0.5920
EC	 0.8780	 0.6390
ED	 0.7330	 0.5930
EE	 0.8690	 0.6390
EF	 0.7430	 0.5940
EG	 0.8670	 0.6360
EH	 0.7430	 0.5970
EI	 0.8750	 0.6350
F	 0.9660	 0.6720
FA	 0.8620	 0.6300
FB	 0.9650	 0.6660
FC	 0.8620	 0.6340
FD	 0.9660	 0.6660
FE	 0.8520	 0.6290
FF	 0.9650	 0.6720
FG	 0.8470	 0.6250
FH	 0.9650	 0.6680
FI	 0.8520	 0.6200
G	 0.8760	 0.6410
GA	 0.7430	 0.5880
GB	 0.8700	 0.6380
GC	 0.7520	 0.5980
GD	 0.8780	 0.6360
GE	 0.7430	 0.5940





















































































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Chain	Atom inclusion	Q-score
GF	 0.8710	 0.6400
GG	 0.7330	 0.5870
GH	 0.8720	 0.6370
GI	 0.7430	 0.5910
H	 0.9650	 0.6660
HA	 0.9650	 0.6660
HB	 0.8520	 0.6230
HC	 0.9670	 0.6680
HD	 0.8620	 0.6280
HE	 0.9660	 0.6670
HF	 0.8620	 0.6370
HG	 0.9660	 0.6660
HH	 0.8520	 0.6350
I	 0.8770	 0.6370
IA	 0.8750	 0.6360
IB	 0.7430	 0.5910
IC	 0.8720	 0.6350
ID	 0.7430	 0.5910
IE	 0.8740	 0.6380
IF	 0.7520	 0.5960
IG	 0.8790	 0.6340
IH	 0.7430	 0.5890
J	 0.8620	 0.6370
JA	 0.8520	 0.6280
JB	 0.9660	 0.6710
JC	 0.8470	 0.6280
JD	 0.9650	 0.6670
JE	 0.8520	 0.6260
JF	 0.9670	 0.6660
JG	 0.8620	 0.6330
JH	 0.9660	 0.6650
K	 0.8620	 0.6290
KA	 0.7520	 0.5980
KB	 0.8760	 0.6420
KC	 0.7330	 0.5970
KD	 0.8690	 0.6370
KE	 0.7430	 0.5870
KF	 0.8670	 0.6390
KG	 0.7430	 0.5930
KH	 0.8750	 0.6350
L	 0.7430	 0.5940
LA	 0.9650	 0.6680





















































































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Chain	Atom inclusion	Q-score
LB	 0.8620	 0.6320
LC	 0.9660	 0.6670
LD	 0.8520	 0.6260
LE	 0.9660	 0.6700
LF	 0.8470	 0.6240
LG	 0.9650	 0.6670
LH	 0.8520	 0.6240
M	 0.9650	 0.6660
MA	 0.8700	 0.6390
MB	 0.7520	 0.5940
MC	 0.8780	 0.6350
MD	 0.7430	 0.5930
ME	 0.8780	 0.6400
MF	 0.7330	 0.5880
MG	 0.8730	 0.6390
MH	 0.7430	 0.5920
N	 0.8740	 0.6370
NA	 0.8520	 0.6270
NB	 0.9670	 0.6680
NC	 0.8620	 0.6290
ND	 0.9660	 0.6680
NE	 0.8620	 0.6320
NF	 0.9660	 0.6680
NG	 0.8520	 0.6270
NH	 0.9660	 0.6720
O	 0.8520	 0.6290
OA	 0.7430	 0.5950
OB	 0.8700	 0.6390
OC	 0.7430	 0.5930
OD	 0.8740	 0.6380
OE	 0.7520	 0.5990
OF	 0.8800	 0.6370
OG	 0.7520	 0.5890
OH	 0.8710	 0.6400
P	 0.7520	 0.5970
PA	 0.9660	 0.6700
PB	 0.8470	 0.6290
PC	 0.9650	 0.6660
PD	 0.8520	 0.6240
PE	 0.9670	 0.6660
PF	 0.8620	 0.6340
PG	 0.9660	 0.6670





















































































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Chain	Atom inclusion	Q-score
PH	 0.8620	 0.6370
Q	 0.9650	 0.6660
QA	 0.8760	 0.6400
QB	 0.7330	 0.5950
QC	 0.8690	 0.6370
QD	 0.7430	 0.5930
QE	 0.8720	 0.6340
QF	 0.7430	 0.5960
QG	 0.8750	 0.6360
QH	 0.7520	 0.6020
R	 0.8700	 0.6370
RA	 0.8620	 0.6300
RB	 0.9650	 0.6670
RC	 0.8520	 0.6290
RD	 0.9660	 0.6700
RE	 0.8470	 0.6300
RF	 0.9650	 0.6670
RG	 0.8520	 0.6270
RH	 0.9670	 0.6670
S	 0.8520	 0.6250
SA	 0.7520	 0.6000
SB	 0.8760	 0.6370
SC	 0.7430	 0.5990
SD	 0.8780	 0.6380
SE	 0.7330	 0.5910
SF	 0.8720	 0.6370
SG	 0.7430	 0.5910
SH	 0.8670	 0.6390
T	 0.7430	 0.5920
TA	 0.9670	 0.6660
TB	 0.8620	 0.6270
TC	 0.9660	 0.6670
TD	 0.8620	 0.6300
TE	 0.9660	 0.6670
TF	 0.8520	 0.6290
TG	 0.9660	 0.6710
TH	 0.8470	 0.6300
U	 0.8450	 0.6090
UA	 0.8700	 0.6370
UB	 0.7430	 0.5890
UC	 0.8740	 0.6380
UD	 0.7520	 0.6050





















































































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Chain	Atom inclusion	Q-score
UE	 0.8780	 0.6370
UF	 0.7430	 0.5970
UG	 0.8710	 0.6400
UH	 0.7330	 0.5840
V	 0.9660	 0.6710
VA	 0.8470	 0.6220
VB	 0.9650	 0.6660
VC	 0.8520	 0.6250
VD	 0.9670	 0.6660
VE	 0.8620	 0.6300
VF	 0.9660	 0.6650
VG	 0.8620	 0.6370
VH	 0.9660	 0.6640
W	 0.8760	 0.6420
WA	 0.7330	 0.5870
WB	 0.8750	 0.6350
WC	 0.7430	 0.6000
WD	 0.8720	 0.6340
WE	 0.7430	 0.5890
WF	 0.8750	 0.6340
WG	 0.7520	 0.6060
WH	 0.8800	 0.6340
X	 0.8620	 0.6310
XA	 0.9650	 0.6660
XB	 0.8520	 0.6240
XC	 0.9660	 0.6720
XD	 0.8470	 0.6280
XE	 0.9650	 0.6660
XF	 0.8520	 0.6270
XG	 0.9670	 0.6650
XH	 0.8620	 0.6290
Y	 0.7520	 0.5930
YA	 0.8770	 0.6370
YB	 0.7520	 0.6000
YC	 0.8780	 0.6400
YD	 0.7330	 0.5910
YE	 0.8690	 0.6360
YF	 0.7430	 0.5940
YG	 0.8670	 0.6370
YH	 0.7430	 0.5980
Z	 0.9670	 0.6650
ZA	 0.8620	 0.6300





























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Chain	Atom inclusion	Q-score
ZB	 0.9650	 0.6660
ZC	 0.8620	 0.6350
ZD	 0.9660	 0.6670
ZE	 0.8520	 0.6260
ZF	 0.9650	 0.6730
ZG	 0.8470	 0.6260
ZH	 0.9650	 0.6660
a	 0.8090	 0.5960
aA	 0.8450	 0.5860
b	 0.8450	 0.6030
bA	 0.8210	 0.5940
c	 0.8210	 0.5990
cA	 0.8210	 0.5960
d	 0.8210	 0.6000
dA	 0.8450	 0.6040
e	 0.8450	 0.6060
eA	 0.8090	 0.6070
f	 0.8090	 0.5960
fA	 0.8450	 0.5990
g	 0.8450	 0.5910
gA	 0.8210	 0.5910
h	 0.8210	 0.5970
hA	 0.8210	 0.6000
i	 0.8210	 0.6100
iA	 0.8450	 0.6030
j	 0.8450	 0.6070
jA	 0.8090	 0.6020
k	 0.8090	 0.5980
kA	 0.8450	 0.5910
l	 0.8450	 0.5980
lA	 0.8210	 0.5890
m	 0.8210	 0.6010
mA	 0.8210	 0.6040
n	 0.8210	 0.6050
nA	 0.8450	 0.6050
o	 0.8450	 0.6080
oA	 0.8090	 0.5960
p	 0.8090	 0.5930
pA	 0.8450	 0.5980
q	 0.8450	 0.5920
qA	 0.8210	 0.5990
r	 0.8210	 0.5930

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Chain	Atom inclusion	Q-score
rA	 0.8210	 0.6050
s	 0.8210	 0.6110
sA	 0.8450	 0.6040
t	 0.8450	 0.6100
tA	 0.8090	 0.5970
u	 0.8090	 0.5980
uA	 0.8450	 0.5920
v	 0.8450	 0.5900
vA	 0.8210	 0.5900
w	 0.8210	 0.5970
wA	 0.8210	 0.6010
x	 0.8210	 0.6050
y	 0.8450	 0.6160
z	 0.8090	 0.6110