Full wwPDB EM Validation Report ⓘ

Jan 15, 2025 – 11:35 am GMT

PDB ID	:	9H8B
EMDB ID	:	EMD-51935
Title	:	Ex vivo cannulae fiber structure of Pyrodictium abyssi
Authors	:	Sleutel, M.; Remaut, H.
Deposited on	:	2024-10-28
Resolution	:	2.30 Å(reported)

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

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

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

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

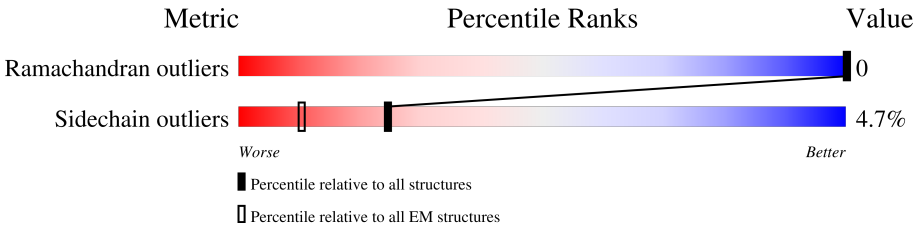
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	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 <=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	A0	174	7% 82% • • 14%
1	A1	174	8% 82% • • 14%
1	A2	174	7% 82% • • 14%
1	A3	174	8% 82% • • 14%
1	A4	174	8% 82% • • 14%
1	A5	174	8% 82% • • 14%
1	A6	174	8% 82% • • 14%
1	A7	174	7% 82% • • 14%
1	A8	174	8% 82% • • 14%

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Mol	Chain	Length	Quality of chain
1	A9	174	8% 82% 14%
1	Au	174	7% 82% 14%
1	Av	174	9% 82% 14%
1	Aw	174	7% 82% 14%
1	Ax	174	8% 82% 14%
1	Ay	174	9% 82% 14%
1	Az	174	8% 82% 14%
1	B1	174	9% 82% 14%
1	BA	174	8% 82% 14%
1	BB	174	8% 82% 14%
1	BC	174	8% 82% 14%
1	BD	174	7% 82% 14%
1	BE	174	8% 82% 14%
1	BF	174	8% 82% 14%
1	BG	174	9% 82% 14%
1	BH	174	8% 82% 14%
1	BI	174	8% 82% 14%
1	BJ	174	9% 82% 14%
1	BK	174	9% 82% 14%
1	BL	174	9% 82% 14%
1	BM	174	9% 82% 14%
1	BN	174	10% 82% 14%
1	BO	174	11% 82% 14%
1	BP	174	12% 82% 14%
1	BQ	174	7% 82% 14%

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Mol	Chain	Length	Quality of chain
1	BR	174	8% 82% 14%
1	BS	174	7% 82% 14%
1	BT	174	8% 82% 14%
1	BU	174	8% 82% 14%
1	BV	174	8% 82% 14%
1	BW	174	8% 82% 14%
1	BX	174	7% 82% 14%
1	BY	174	8% 82% 14%
1	BZ	174	8% 82% 14%
1	Ba	174	8% 82% 14%
1	Bb	174	8% 82% 14%
1	Bc	174	7% 82% 14%
1	Bd	174	8% 82% 14%
1	Be	174	8% 82% 14%
1	Bf	174	7% 82% 14%
1	Bg	174	8% 82% 14%
1	Bh	174	8% 82% 14%
1	Bi	174	8% 82% 14%
1	Bj	174	7% 82% 14%
1	Bk	174	8% 82% 14%
1	Bl	174	8% 82% 14%
1	Bm	174	9% 82% 14%
1	Bn	174	9% 82% 14%
1	Bo	174	8% 82% 14%
1	Bp	174	9% 82% 14%

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Mol	Chain	Length	Quality of chain
1	Bq	174	9% 82% 14%
1	Br	174	9% 82% 14%
1	Bs	174	9% 82% 14%
1	Bt	174	10% 82% 14%
1	Bu	174	11% 82% 14%
1	Bv	174	12% 82% 14%
1	Bw	174	17% 82% 14%
1	Bx	174	13% 82% 14%
1	By	174	11% 82% 14%
1	Bz	174	10% 82% 14%
1	C9	174	7% 82% 14%
1	D1	174	7% 82% 14%
1	D3	174	8% 82% 14%
1	D5	174	8% 82% 14%
1	D7	174	8% 82% 14%
1	D9	174	8% 82% 14%
1	DA	174	8% 82% 14%
1	DC	174	8% 82% 14%
1	DE	174	7% 82% 14%
1	DG	174	9% 82% 14%
1	DI	174	7% 82% 14%
1	DK	174	7% 82% 14%
1	DM	174	8% 82% 14%
1	DO	174	7% 82% 14%
1	DQ	174	7% 82% 14%

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Mol	Chain	Length	Quality of chain
1	DS	174	9% 82% 14%
1	DU	174	7% 82% 14%
1	DW	174	9% 82% 14%
1	DY	174	8% 82% 14%
1	Da	174	9% 82% 14%
1	Dc	174	7% 82% 14%
1	De	174	9% 82% 14%
1	Dg	174	7% 82% 14%
1	Di	174	8% 82% 14%
1	Dk	174	7% 82% 14%
1	Dm	174	7% 82% 14%
1	Do	174	8% 82% 14%
1	Dq	174	8% 82% 14%
1	Ds	174	7% 82% 14%
1	Du	174	8% 82% 14%
1	Dw	174	8% 82% 14%
1	Dy	174	8% 82% 14%
1	E1	174	8% 82% 14%
1	E3	174	8% 82% 14%
1	E5	174	7% 82% 14%
1	E7	174	8% 82% 14%
1	E9	174	7% 82% 14%
1	EA	174	7% 82% 14%
1	EC	174	9% 82% 14%
1	EE	174	7% 82% 14%

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Mol	Chain	Length	Quality of chain
1	EG	174	7% 82% 14%
1	EI	174	8% 82% 14%
1	EK	174	8% 82% 14%
1	EM	174	8% 82% 14%
1	EO	174	8% 82% 14%
1	EQ	174	17% 82% 14%
1	ES	174	13% 82% 14%
1	EU	174	12% 82% 14%
1	EW	174	10% 82% 14%
1	EY	174	9% 82% 14%
1	Ea	174	8% 82% 14%
1	Ec	174	8% 82% 14%
1	Ee	174	8% 82% 14%
1	Eg	174	7% 82% 14%
1	Ei	174	9% 82% 14%
1	Ek	174	7% 82% 14%
1	Em	174	7% 82% 14%
1	Eo	174	8% 82% 14%
1	Eq	174	7% 82% 14%
1	Es	174	7% 82% 14%
1	Eu	174	9% 82% 14%
1	Ew	174	7% 82% 14%
1	Ey	174	9% 82% 14%
1	FA	174	8% 82% 14%
1	FC	174	7% 82% 14%

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Mol	Chain	Length	Quality of chain
1	FE	174	7% 82% 14%
1	FG	174	7% 82% 14%
1	FI	174	8% 82% 14%
1	FK	174	7% 82% 14%
1	FM	174	8% 82% 14%
1	FO	174	8% 82% 14%
1	FQ	174	8% 82% 14%
1	FS	174	7% 82% 14%
1	FU	174	8% 82% 14%
1	FW	174	8% 82% 14%
1	FY	174	8% 82% 14%
1	Fa	174	8% 82% 14%
1	Fc	174	7% 82% 14%
1	Fe	174	9% 82% 14%
1	Fg	174	7% 82% 14%
1	Fi	174	8% 82% 14%
1	Fk	174	8% 82% 14%
1	Fm	174	8% 82% 14%
1	Fo	174	7% 82% 14%
1	Fq	174	8% 82% 14%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 179410 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 CanX.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Au	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Av	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Aw	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Ax	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Ay	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Az	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	A1	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	A2	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	A3	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	A4	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	A5	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	A6	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	A7	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	A8	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	A9	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	A0	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	BA	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	BB	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	BC	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	BD	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	BE	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	BF	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	BG	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	BH	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	BI	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	BJ	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	BK	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	BL	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	BM	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	BN	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	BO	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	BP	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	BQ	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	BR	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	BS	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	BT	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	BU	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	BV	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	BW	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	BX	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	BY	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	BZ	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Ba	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Bb	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Bc	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Bd	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Be	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Bf	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Bg	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Bh	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Bi	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Bj	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Bk	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Bl	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Bm	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Bn	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Bo	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Bp	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Bq	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Br	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Bs	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Bt	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Bu	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Bv	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Bw	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Bx	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	By	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Bz	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	B1	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	C9	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	DA	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	DC	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	DE	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	DG	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	DI	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	DK	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	DM	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	DO	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	DQ	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	DS	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	DU	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	DW	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	DY	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Da	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Dc	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	De	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Dg	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Di	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Dk	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Dm	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Do	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Dq	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Ds	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Du	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Dw	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Dy	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	D1	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	D3	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	D5	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	D7	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	D9	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	EA	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	EC	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	EE	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	EG	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	EI	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	EK	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	EM	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	EO	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	EQ	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	ES	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	EU	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	EW	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	EY	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Ea	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Ec	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Ee	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Eg	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Ei	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Ek	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Em	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Eo	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Eq	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Es	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Eu	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Ew	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Ey	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	E1	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	E3	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	E5	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	E7	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	E9	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	FA	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	FC	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	FE	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	FG	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	FI	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	FK	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	FM	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	FO	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	FQ	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	FS	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	FU	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	FW	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	FY	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Fa	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Fc	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Fe	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Fg	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Fi	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Fk	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Fm	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Fo	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		
1	Fq	149	Total	C	N	O	S	0	0
			1148	735	182	229	2		

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
2	Au	4	Total	Ca	0
			4	4	
2	Av	4	Total	Ca	0
			4	4	
2	Aw	4	Total	Ca	0
			4	4	
2	Ax	4	Total	Ca	0
			4	4	
2	Ay	4	Total	Ca	0
			4	4	
2	Az	4	Total	Ca	0
			4	4	
2	A1	4	Total	Ca	0
			4	4	
2	A2	4	Total	Ca	0
			4	4	

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Mol	Chain	Residues	Atoms	AltConf
2	A3	4	Total Ca 4 4	0
2	A4	4	Total Ca 4 4	0
2	A5	4	Total Ca 4 4	0
2	A6	4	Total Ca 4 4	0
2	A7	4	Total Ca 4 4	0
2	A8	4	Total Ca 4 4	0
2	A9	4	Total Ca 4 4	0
2	A0	4	Total Ca 4 4	0
2	BA	4	Total Ca 4 4	0
2	BB	5	Total Ca 5 5	0
2	BC	5	Total Ca 5 5	0
2	BD	5	Total Ca 5 5	0
2	BE	5	Total Ca 5 5	0
2	BF	5	Total Ca 5 5	0
2	BG	5	Total Ca 5 5	0
2	BH	5	Total Ca 5 5	0
2	BI	5	Total Ca 5 5	0
2	BJ	5	Total Ca 5 5	0
2	BK	5	Total Ca 5 5	0
2	BL	5	Total Ca 5 5	0
2	BM	5	Total Ca 5 5	0

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Mol	Chain	Residues	Atoms	AltConf
2	BN	5	Total Ca 5 5	0
2	BO	5	Total Ca 5 5	0
2	BP	5	Total Ca 5 5	0
2	BQ	3	Total Ca 3 3	0
2	BR	3	Total Ca 3 3	0
2	BS	3	Total Ca 3 3	0
2	BT	3	Total Ca 3 3	0
2	BU	3	Total Ca 3 3	0
2	BV	3	Total Ca 3 3	0
2	BW	3	Total Ca 3 3	0
2	BX	3	Total Ca 3 3	0
2	BY	3	Total Ca 3 3	0
2	BZ	3	Total Ca 3 3	0
2	Ba	3	Total Ca 3 3	0
2	Bb	3	Total Ca 3 3	0
2	Bc	3	Total Ca 3 3	0
2	Bd	3	Total Ca 3 3	0
2	Be	2	Total Ca 2 2	0
2	Bf	2	Total Ca 2 2	0
2	Bg	2	Total Ca 2 2	0
2	Bh	3	Total Ca 3 3	0

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Mol	Chain	Residues	Atoms	AltConf
2	Bi	4	Total Ca 4 4	0
2	Bj	4	Total Ca 4 4	0
2	Bk	4	Total Ca 4 4	0
2	Bl	4	Total Ca 4 4	0
2	Bm	4	Total Ca 4 4	0
2	Bn	4	Total Ca 4 4	0
2	Bo	4	Total Ca 4 4	0
2	Bp	4	Total Ca 4 4	0
2	Bq	4	Total Ca 4 4	0
2	Br	4	Total Ca 4 4	0
2	Bs	4	Total Ca 4 4	0
2	Bt	4	Total Ca 4 4	0
2	Bu	4	Total Ca 4 4	0
2	Bv	4	Total Ca 4 4	0
2	Bw	2	Total Ca 2 2	0
2	Bx	2	Total Ca 2 2	0
2	By	2	Total Ca 2 2	0
2	Bz	2	Total Ca 2 2	0
2	B1	2	Total Ca 2 2	0
2	C9	2	Total Ca 2 2	0
2	DA	2	Total Ca 2 2	0

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Mol	Chain	Residues	Atoms	AltConf
2	DC	2	Total Ca 2 2	0
2	DE	2	Total Ca 2 2	0
2	DG	2	Total Ca 2 2	0
2	DI	2	Total Ca 2 2	0
2	DK	2	Total Ca 2 2	0
2	DM	2	Total Ca 2 2	0
2	DO	2	Total Ca 2 2	0
2	DQ	3	Total Ca 3 3	0
2	DS	4	Total Ca 4 4	0
2	DU	4	Total Ca 4 4	0
2	DW	4	Total Ca 4 4	0
2	DY	4	Total Ca 4 4	0
2	Da	4	Total Ca 4 4	0
2	Dc	4	Total Ca 4 4	0
2	De	4	Total Ca 4 4	0
2	Dg	4	Total Ca 4 4	0
2	Di	4	Total Ca 4 4	0
2	Dk	4	Total Ca 4 4	0
2	Dm	4	Total Ca 4 4	0
2	Do	4	Total Ca 4 4	0
2	Dq	4	Total Ca 4 4	0

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Mol	Chain	Residues	Atoms	AltConf
2	Ds	4	Total Ca 4 4	0
2	Du	4	Total Ca 4 4	0
2	Dw	4	Total Ca 4 4	0
2	Dy	3	Total Ca 3 3	0
2	D1	3	Total Ca 3 3	0
2	D3	3	Total Ca 3 3	0
2	D5	3	Total Ca 3 3	0
2	D7	3	Total Ca 3 3	0
2	D9	3	Total Ca 3 3	0
2	EA	3	Total Ca 3 3	0
2	EC	3	Total Ca 3 3	0
2	EE	3	Total Ca 3 3	0
2	EG	3	Total Ca 3 3	0
2	EI	3	Total Ca 3 3	0
2	EK	3	Total Ca 3 3	0
2	EM	3	Total Ca 3 3	0
2	EO	3	Total Ca 3 3	0
2	EQ	1	Total Ca 1 1	0
2	ES	1	Total Ca 1 1	0
2	EU	1	Total Ca 1 1	0
2	EW	1	Total Ca 1 1	0

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Mol	Chain	Residues	Atoms	AltConf
2	EY	1	Total Ca 1 1	0
2	Ea	1	Total Ca 1 1	0
2	Ec	1	Total Ca 1 1	0
2	Ee	1	Total Ca 1 1	0
2	Eg	1	Total Ca 1 1	0
2	Ei	1	Total Ca 1 1	0
2	Ek	1	Total Ca 1 1	0
2	Em	1	Total Ca 1 1	0
2	Eo	1	Total Ca 1 1	0
2	Eq	1	Total Ca 1 1	0
2	Es	1	Total Ca 1 1	0
2	Eu	2	Total Ca 2 2	0
2	Ew	2	Total Ca 2 2	0
2	Ey	2	Total Ca 2 2	0
2	E1	2	Total Ca 2 2	0
2	E3	2	Total Ca 2 2	0
2	E5	2	Total Ca 2 2	0
2	E7	2	Total Ca 2 2	0
2	E9	2	Total Ca 2 2	0
2	FA	2	Total Ca 2 2	0
2	FC	2	Total Ca 2 2	0

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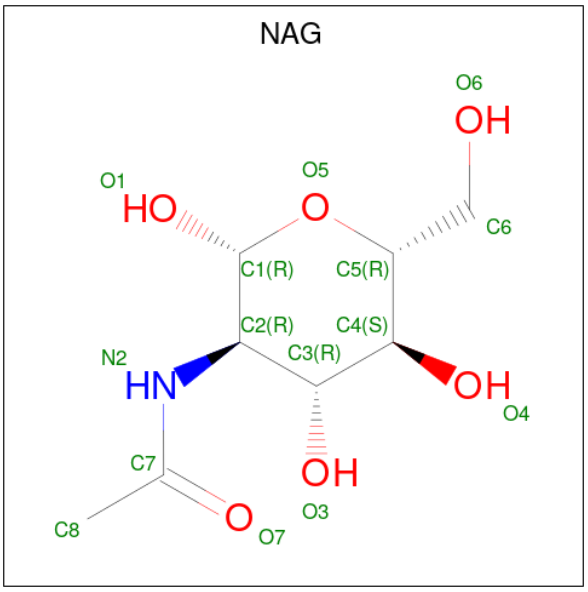
Mol	Chain	Residues	Atoms	AltConf
2	FE	2	Total Ca 2 2	0
2	FG	2	Total Ca 2 2	0
2	FI	2	Total Ca 2 2	0
2	FK	2	Total Ca 2 2	0
2	FM	2	Total Ca 2 2	0
2	FO	2	Total Ca 2 2	0
2	FQ	2	Total Ca 2 2	0
2	FS	2	Total Ca 2 2	0
2	FU	2	Total Ca 2 2	0
2	FW	2	Total Ca 2 2	0
2	FY	2	Total Ca 2 2	0
2	Fa	2	Total Ca 2 2	0
2	Fc	2	Total Ca 2 2	0
2	Fe	2	Total Ca 2 2	0
2	Fg	2	Total Ca 2 2	0
2	Fi	2	Total Ca 2 2	0
2	Fk	2	Total Ca 2 2	0
2	Fm	2	Total Ca 2 2	0
2	Fo	2	Total Ca 2 2	0
2	Fq	2	Total Ca 2 2	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
3	Au	1	Total	C	N	O	0
			14	8	1	5	
3	Av	1	Total	C	N	O	0
			14	8	1	5	
3	Aw	1	Total	C	N	O	0
			14	8	1	5	
3	Ax	1	Total	C	N	O	0
			14	8	1	5	
3	Ay	1	Total	C	N	O	0
			14	8	1	5	
3	Az	1	Total	C	N	O	0
			14	8	1	5	
3	A1	1	Total	C	N	O	0
			14	8	1	5	
3	A2	1	Total	C	N	O	0
			14	8	1	5	
3	A3	1	Total	C	N	O	0
			14	8	1	5	
3	A4	1	Total	C	N	O	0
			14	8	1	5	
3	A5	1	Total	C	N	O	0
			14	8	1	5	
3	A6	1	Total	C	N	O	0
			14	8	1	5	
3	A7	1	Total	C	N	O	0
			14	8	1	5	
3	A8	1	Total	C	N	O	0
			14	8	1	5	

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Mol	Chain	Residues	Atoms				AltConf
3	A9	1	Total	C	N	O	0
			14	8	1	5	
3	A0	1	Total	C	N	O	0
			14	8	1	5	
3	BA	1	Total	C	N	O	0
			14	8	1	5	
3	BB	1	Total	C	N	O	0
			14	8	1	5	
3	BC	1	Total	C	N	O	0
			14	8	1	5	
3	BD	1	Total	C	N	O	0
			14	8	1	5	
3	BE	1	Total	C	N	O	0
			14	8	1	5	
3	BF	1	Total	C	N	O	0
			14	8	1	5	
3	BG	1	Total	C	N	O	0
			14	8	1	5	
3	BH	1	Total	C	N	O	0
			14	8	1	5	
3	BI	1	Total	C	N	O	0
			14	8	1	5	
3	BJ	1	Total	C	N	O	0
			14	8	1	5	
3	BK	1	Total	C	N	O	0
			14	8	1	5	
3	BL	1	Total	C	N	O	0
			14	8	1	5	
3	BM	1	Total	C	N	O	0
			14	8	1	5	
3	BN	1	Total	C	N	O	0
			14	8	1	5	
3	BO	1	Total	C	N	O	0
			14	8	1	5	
3	BP	1	Total	C	N	O	0
			14	8	1	5	
3	BQ	1	Total	C	N	O	0
			14	8	1	5	
3	BR	1	Total	C	N	O	0
			14	8	1	5	
3	BS	1	Total	C	N	O	0
			14	8	1	5	

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Mol	Chain	Residues	Atoms				AltConf
3	BT	1	Total	C	N	O	0
			14	8	1	5	
3	BU	1	Total	C	N	O	0
			14	8	1	5	
3	BV	1	Total	C	N	O	0
			14	8	1	5	
3	BW	1	Total	C	N	O	0
			14	8	1	5	
3	BX	1	Total	C	N	O	0
			14	8	1	5	
3	BY	1	Total	C	N	O	0
			14	8	1	5	
3	BZ	1	Total	C	N	O	0
			14	8	1	5	
3	Ba	1	Total	C	N	O	0
			14	8	1	5	
3	Bb	1	Total	C	N	O	0
			14	8	1	5	
3	Bc	1	Total	C	N	O	0
			14	8	1	5	
3	Bd	1	Total	C	N	O	0
			14	8	1	5	
3	Be	1	Total	C	N	O	0
			14	8	1	5	
3	Bf	1	Total	C	N	O	0
			14	8	1	5	
3	Bg	1	Total	C	N	O	0
			14	8	1	5	
3	Bh	1	Total	C	N	O	0
			14	8	1	5	
3	Bi	1	Total	C	N	O	0
			14	8	1	5	
3	Bj	1	Total	C	N	O	0
			14	8	1	5	
3	Bk	1	Total	C	N	O	0
			14	8	1	5	
3	Bl	1	Total	C	N	O	0
			14	8	1	5	
3	Bm	1	Total	C	N	O	0
			14	8	1	5	
3	Bn	1	Total	C	N	O	0
			14	8	1	5	

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Mol	Chain	Residues	Atoms				AltConf
3	Bo	1	Total	C	N	O	0
			14	8	1	5	
3	Bp	1	Total	C	N	O	0
			14	8	1	5	
3	Bq	1	Total	C	N	O	0
			14	8	1	5	
3	Br	1	Total	C	N	O	0
			14	8	1	5	
3	Bs	1	Total	C	N	O	0
			14	8	1	5	
3	Bt	1	Total	C	N	O	0
			14	8	1	5	
3	Bu	1	Total	C	N	O	0
			14	8	1	5	
3	Bv	1	Total	C	N	O	0
			14	8	1	5	
3	Bw	1	Total	C	N	O	0
			14	8	1	5	
3	Bx	1	Total	C	N	O	0
			14	8	1	5	
3	By	1	Total	C	N	O	0
			14	8	1	5	
3	Bz	1	Total	C	N	O	0
			14	8	1	5	
3	B1	1	Total	C	N	O	0
			14	8	1	5	
3	C9	1	Total	C	N	O	0
			14	8	1	5	
3	DA	1	Total	C	N	O	0
			14	8	1	5	
3	DC	1	Total	C	N	O	0
			14	8	1	5	
3	DE	1	Total	C	N	O	0
			14	8	1	5	
3	DG	1	Total	C	N	O	0
			14	8	1	5	
3	DI	1	Total	C	N	O	0
			14	8	1	5	
3	DK	1	Total	C	N	O	0
			14	8	1	5	
3	DM	1	Total	C	N	O	0
			14	8	1	5	

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Mol	Chain	Residues	Atoms				AltConf
3	DO	1	Total	C	N	O	0
			14	8	1	5	
3	DQ	1	Total	C	N	O	0
			14	8	1	5	
3	DS	1	Total	C	N	O	0
			14	8	1	5	
3	DU	1	Total	C	N	O	0
			14	8	1	5	
3	DW	1	Total	C	N	O	0
			14	8	1	5	
3	DY	1	Total	C	N	O	0
			14	8	1	5	
3	Da	1	Total	C	N	O	0
			14	8	1	5	
3	Dc	1	Total	C	N	O	0
			14	8	1	5	
3	De	1	Total	C	N	O	0
			14	8	1	5	
3	Dg	1	Total	C	N	O	0
			14	8	1	5	
3	Di	1	Total	C	N	O	0
			14	8	1	5	
3	Dk	1	Total	C	N	O	0
			14	8	1	5	
3	Dm	1	Total	C	N	O	0
			14	8	1	5	
3	Do	1	Total	C	N	O	0
			14	8	1	5	
3	Dq	1	Total	C	N	O	0
			14	8	1	5	
3	Ds	1	Total	C	N	O	0
			14	8	1	5	
3	Du	1	Total	C	N	O	0
			14	8	1	5	
3	Dw	1	Total	C	N	O	0
			14	8	1	5	
3	Dy	1	Total	C	N	O	0
			14	8	1	5	
3	D1	1	Total	C	N	O	0
			14	8	1	5	
3	D3	1	Total	C	N	O	0
			14	8	1	5	

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Mol	Chain	Residues	Atoms				AltConf
3	D5	1	Total	C	N	O	0
			14	8	1	5	
3	D7	1	Total	C	N	O	0
			14	8	1	5	
3	D9	1	Total	C	N	O	0
			14	8	1	5	
3	EA	1	Total	C	N	O	0
			14	8	1	5	
3	EC	1	Total	C	N	O	0
			14	8	1	5	
3	EE	1	Total	C	N	O	0
			14	8	1	5	
3	EG	1	Total	C	N	O	0
			14	8	1	5	
3	EI	1	Total	C	N	O	0
			14	8	1	5	
3	EK	1	Total	C	N	O	0
			14	8	1	5	
3	EM	1	Total	C	N	O	0
			14	8	1	5	
3	EO	1	Total	C	N	O	0
			14	8	1	5	
3	EQ	1	Total	C	N	O	0
			14	8	1	5	
3	ES	1	Total	C	N	O	0
			14	8	1	5	
3	EU	1	Total	C	N	O	0
			14	8	1	5	
3	EW	1	Total	C	N	O	0
			14	8	1	5	
3	EY	1	Total	C	N	O	0
			14	8	1	5	
3	Ea	1	Total	C	N	O	0
			14	8	1	5	
3	Ec	1	Total	C	N	O	0
			14	8	1	5	
3	Ee	1	Total	C	N	O	0
			14	8	1	5	
3	Eg	1	Total	C	N	O	0
			14	8	1	5	
3	Ei	1	Total	C	N	O	0
			14	8	1	5	

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Mol	Chain	Residues	Atoms				AltConf
3	Ek	1	Total	C	N	O	0
			14	8	1	5	
3	Em	1	Total	C	N	O	0
			14	8	1	5	
3	Eo	1	Total	C	N	O	0
			14	8	1	5	
3	Eq	1	Total	C	N	O	0
			14	8	1	5	
3	Es	1	Total	C	N	O	0
			14	8	1	5	
3	Eu	1	Total	C	N	O	0
			14	8	1	5	
3	Ew	1	Total	C	N	O	0
			14	8	1	5	
3	Ey	1	Total	C	N	O	0
			14	8	1	5	
3	E1	1	Total	C	N	O	0
			14	8	1	5	
3	E3	1	Total	C	N	O	0
			14	8	1	5	
3	E5	1	Total	C	N	O	0
			14	8	1	5	
3	E7	1	Total	C	N	O	0
			14	8	1	5	
3	E9	1	Total	C	N	O	0
			14	8	1	5	
3	FA	1	Total	C	N	O	0
			14	8	1	5	
3	FC	1	Total	C	N	O	0
			14	8	1	5	
3	FE	1	Total	C	N	O	0
			14	8	1	5	
3	FG	1	Total	C	N	O	0
			14	8	1	5	
3	FI	1	Total	C	N	O	0
			14	8	1	5	
3	FK	1	Total	C	N	O	0
			14	8	1	5	
3	FM	1	Total	C	N	O	0
			14	8	1	5	
3	FO	1	Total	C	N	O	0
			14	8	1	5	

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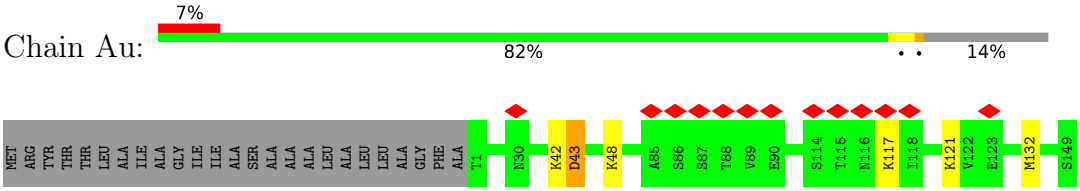
Mol	Chain	Residues	Atoms				AltConf
3	FQ	1	Total	C	N	O	0
			14	8	1	5	
3	FS	1	Total	C	N	O	0
			14	8	1	5	
3	FU	1	Total	C	N	O	0
			14	8	1	5	
3	FW	1	Total	C	N	O	0
			14	8	1	5	
3	FY	1	Total	C	N	O	0
			14	8	1	5	
3	Fa	1	Total	C	N	O	0
			14	8	1	5	
3	Fc	1	Total	C	N	O	0
			14	8	1	5	
3	Fe	1	Total	C	N	O	0
			14	8	1	5	
3	Fg	1	Total	C	N	O	0
			14	8	1	5	
3	Fi	1	Total	C	N	O	0
			14	8	1	5	
3	Fk	1	Total	C	N	O	0
			14	8	1	5	
3	Fm	1	Total	C	N	O	0
			14	8	1	5	
3	Fo	1	Total	C	N	O	0
			14	8	1	5	
3	Fq	1	Total	C	N	O	0
			14	8	1	5	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

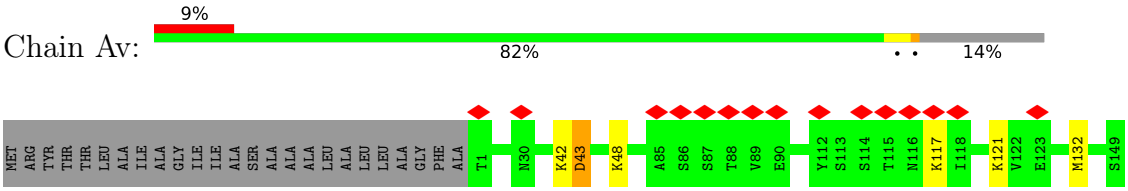
• Molecule 1: CanX

Chain Au:



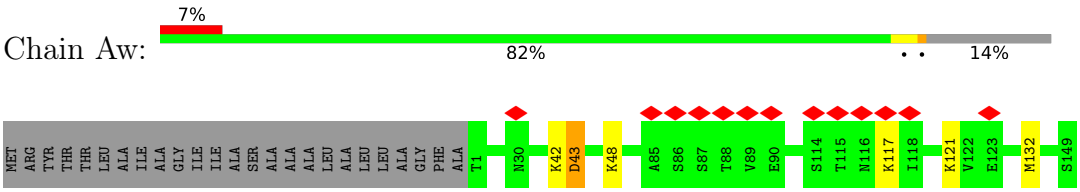
• Molecule 1: CanX

Chain Av:



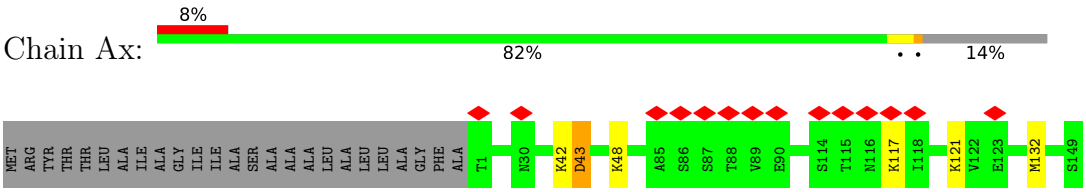
• Molecule 1: CanX

Chain Aw:



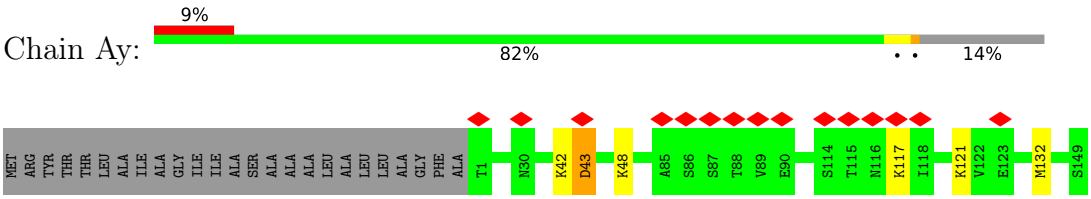
• Molecule 1: CanX

Chain Ax:



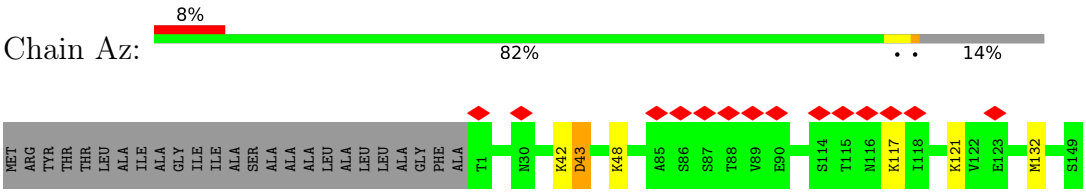
• Molecule 1: CanX

Chain Ay:



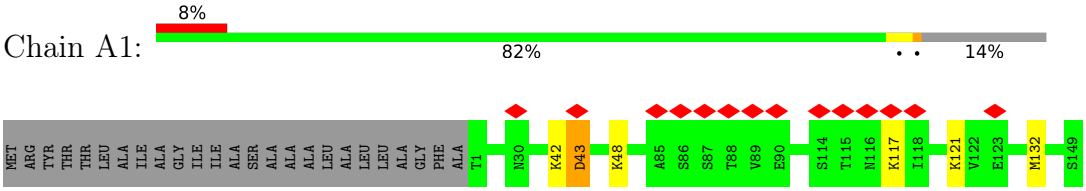
• Molecule 1: CanX

Chain Az:



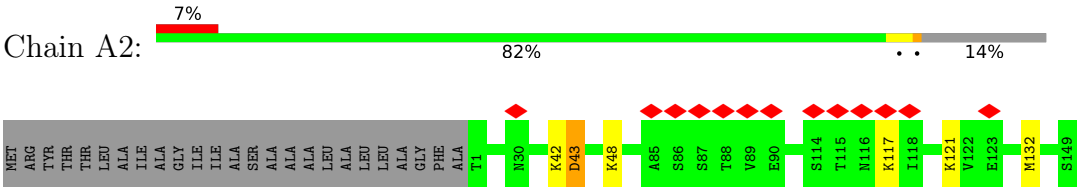
• Molecule 1: CanX

Chain A1:



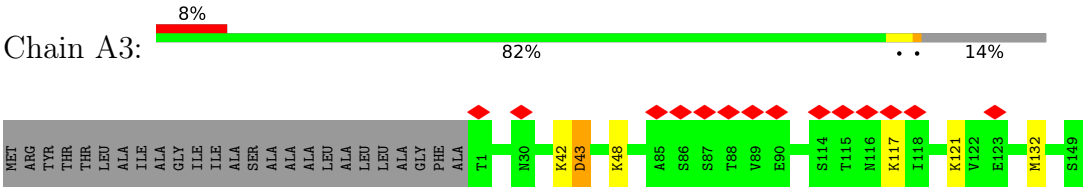
• Molecule 1: CanX

Chain A2:



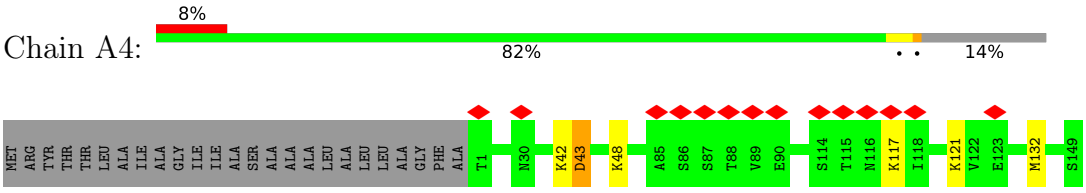
• Molecule 1: CanX

Chain A3:



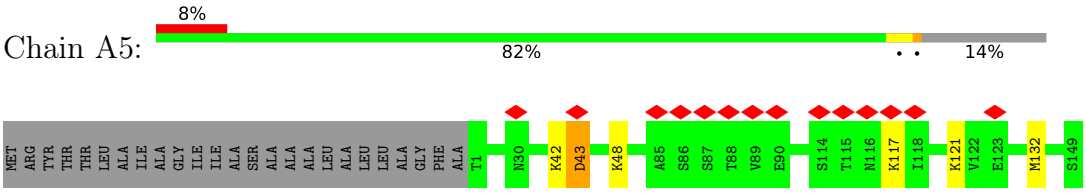
• Molecule 1: CanX

Chain A4:



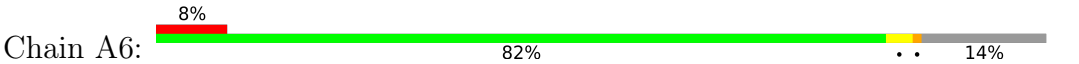
• Molecule 1: CanX

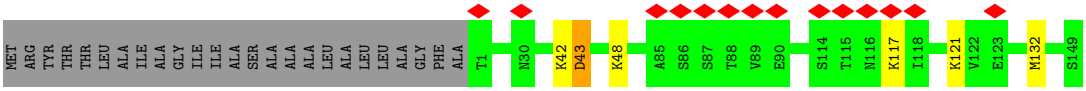
Chain A5:



• Molecule 1: CanX

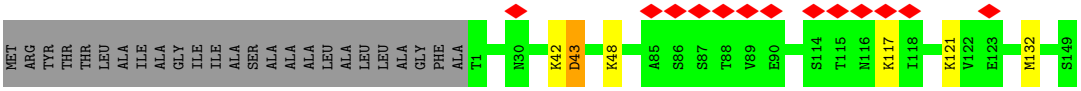
Chain A6:





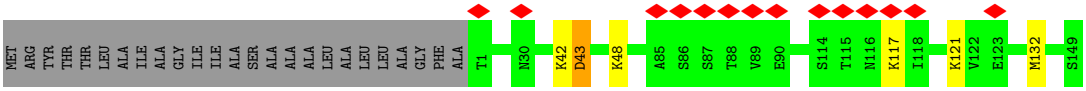
• Molecule 1: CanX

Chain A7:



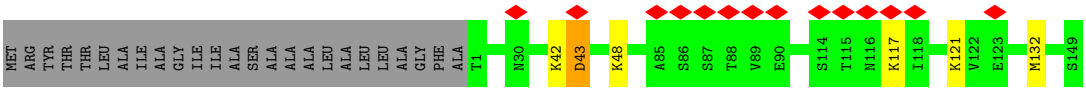
• Molecule 1: CanX

Chain A8:



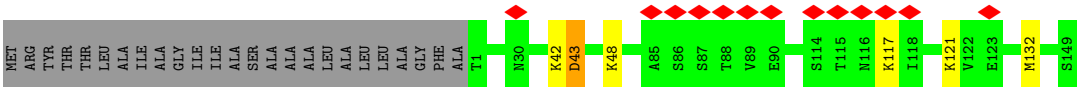
• Molecule 1: CanX

Chain A9:



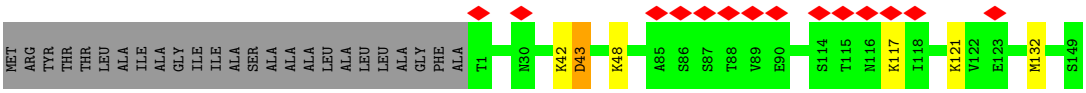
• Molecule 1: CanX

Chain A0:



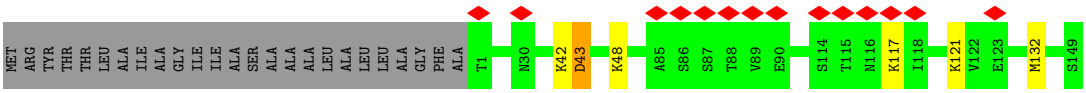
• Molecule 1: CanX

Chain BA:



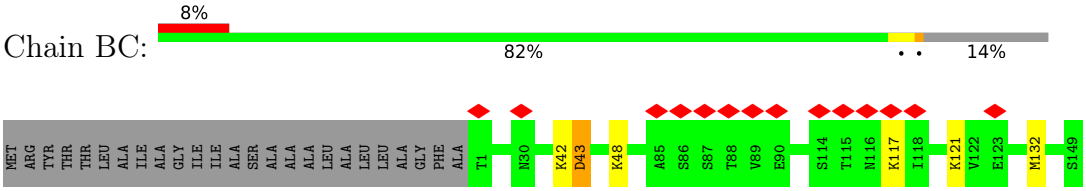
• Molecule 1: CanX

Chain BB:



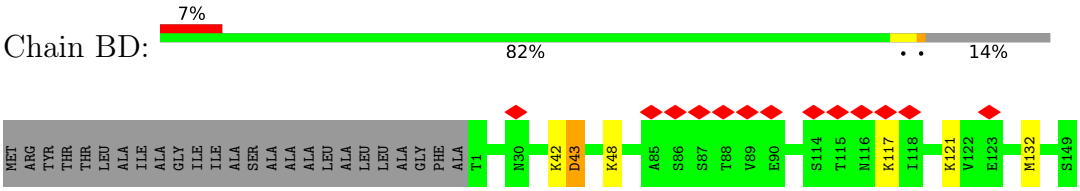
• Molecule 1: CanX

Chain BC:



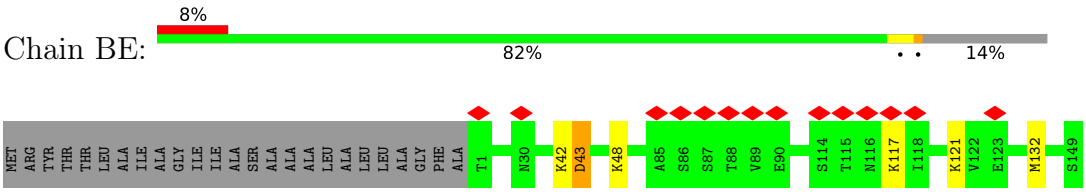
• Molecule 1: CanX

Chain BD:



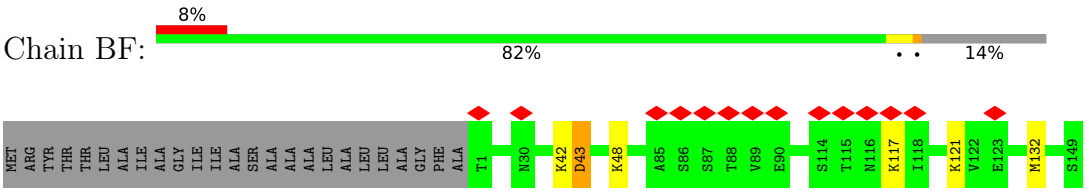
• Molecule 1: CanX

Chain BE:



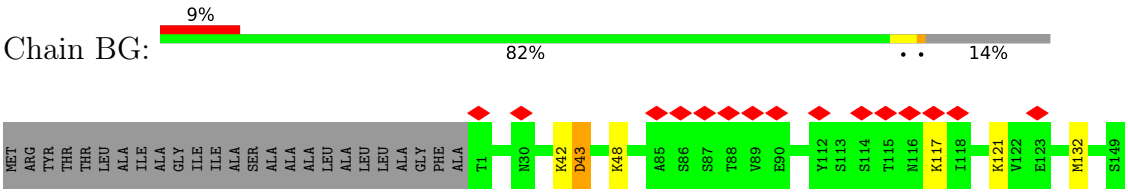
• Molecule 1: CanX

Chain BF:



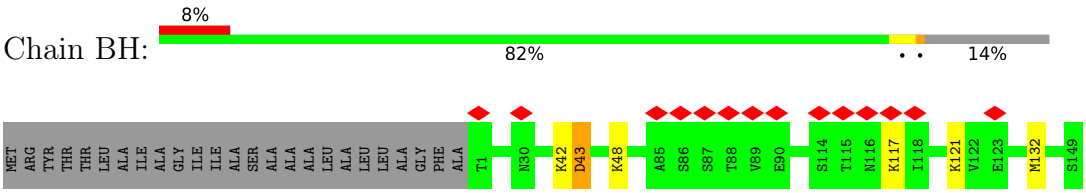
• Molecule 1: CanX

Chain BG:



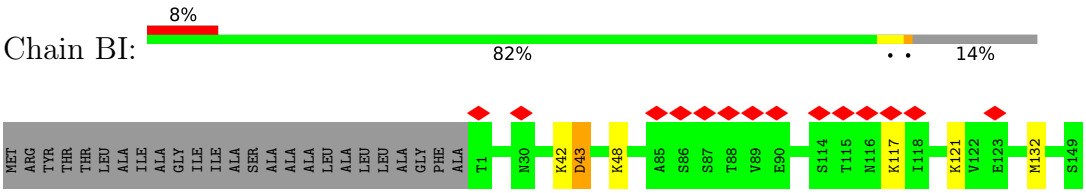
• Molecule 1: CanX

Chain BH:



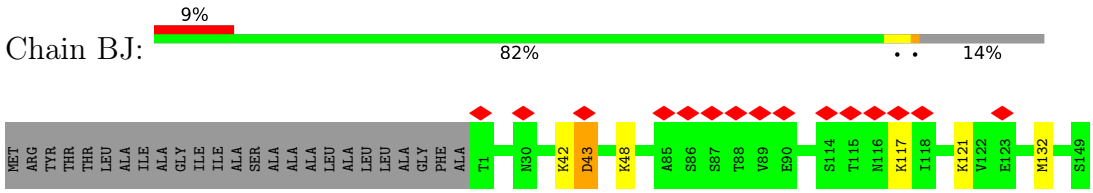
• Molecule 1: CanX

Chain BI:



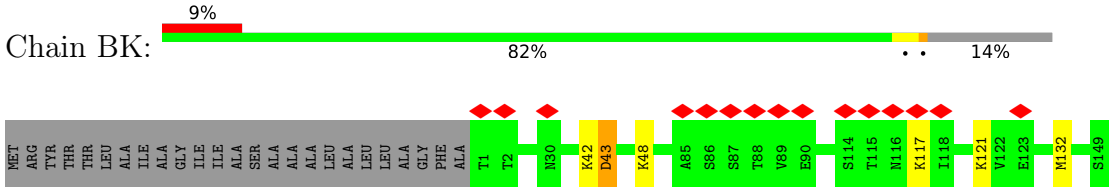
• Molecule 1: CanX

Chain BJ:



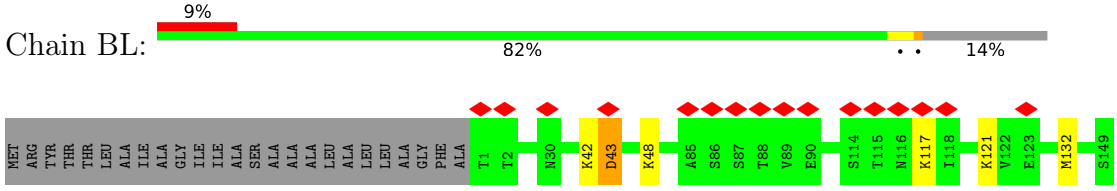
• Molecule 1: CanX

Chain BK:



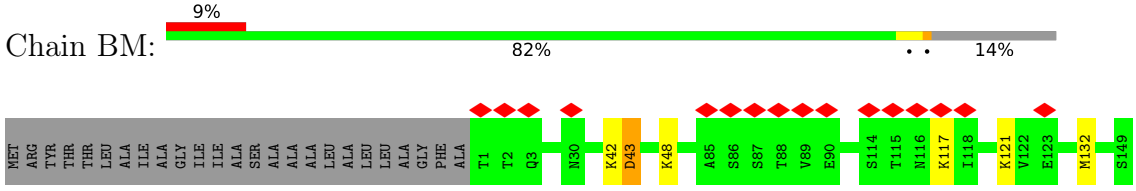
• Molecule 1: CanX

Chain BL:



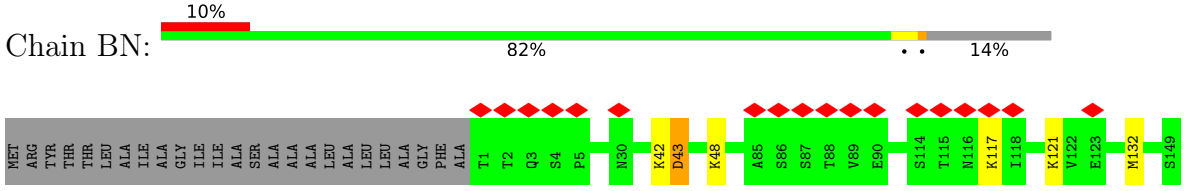
• Molecule 1: CanX

Chain BM:



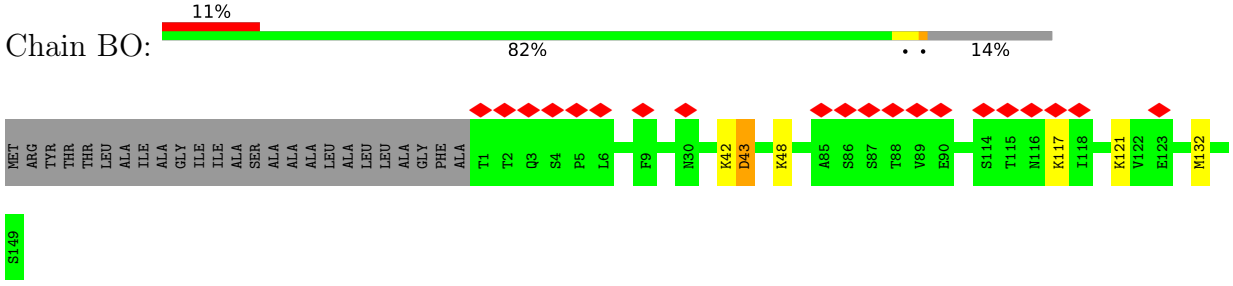
• Molecule 1: CanX

Chain BN:



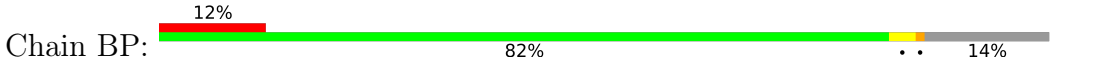
• Molecule 1: CanX

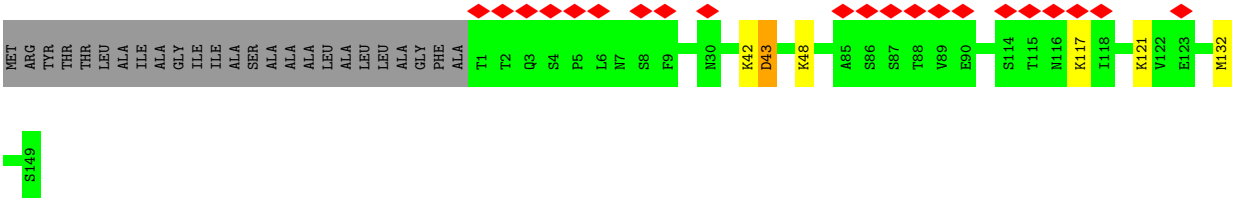
Chain BO:



• Molecule 1: CanX

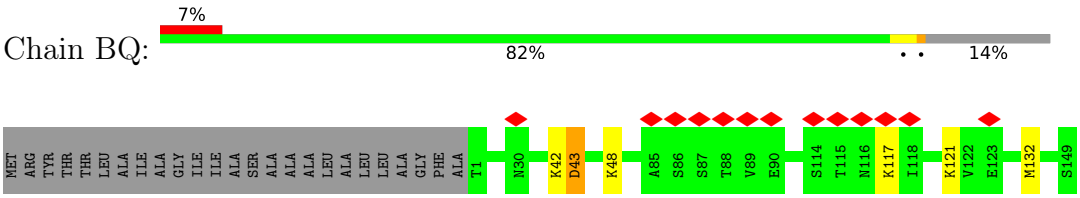
Chain BP:





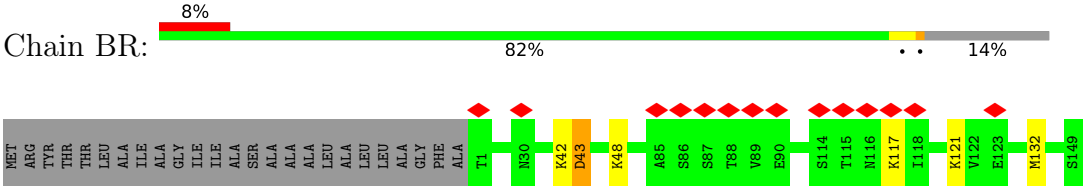
• Molecule 1: CanX

Chain BQ:



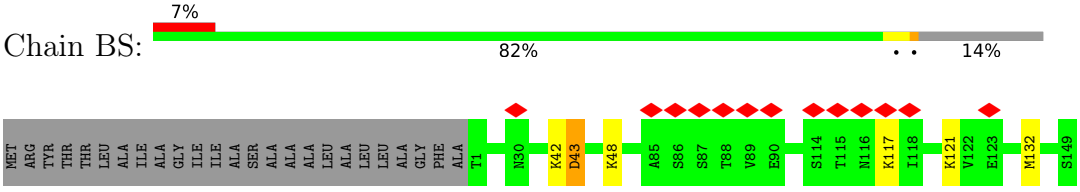
• Molecule 1: CanX

Chain BR:



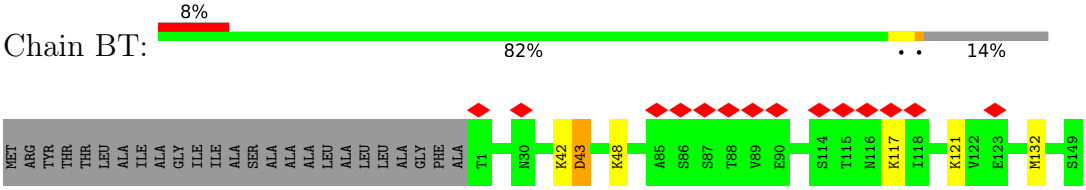
• Molecule 1: CanX

Chain BS:



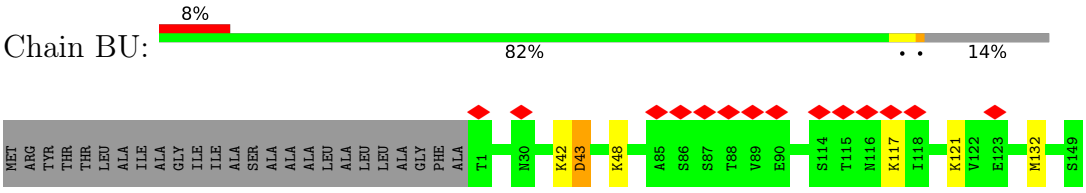
• Molecule 1: CanX

Chain BT:



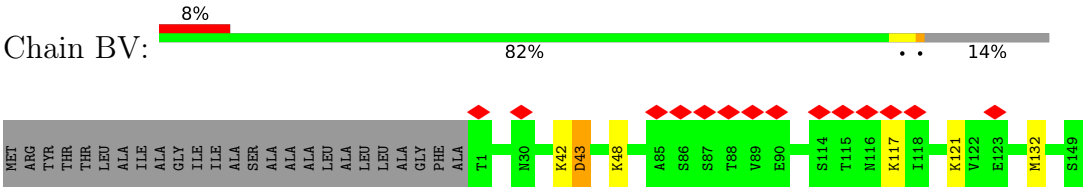
• Molecule 1: CanX

Chain BU:



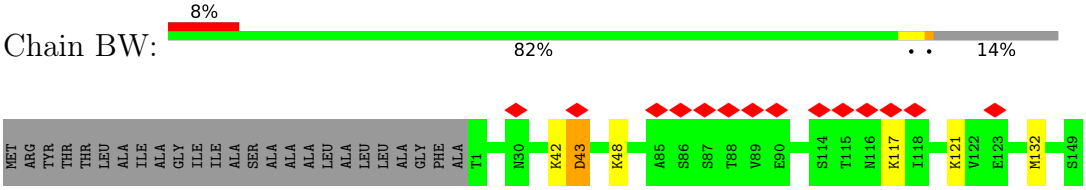
• Molecule 1: CanX

Chain BV:



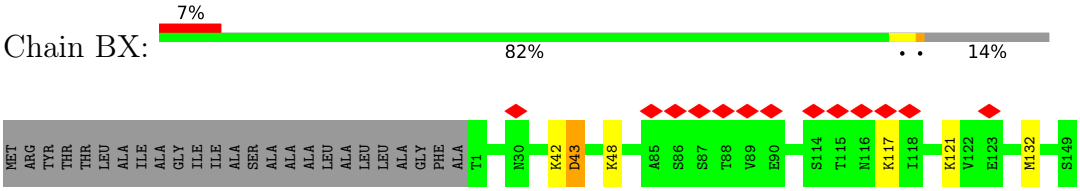
• Molecule 1: CanX

Chain BW:



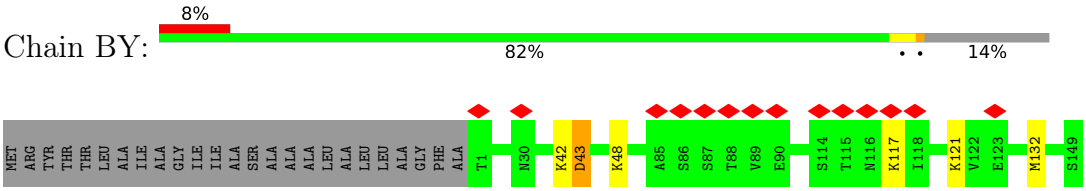
• Molecule 1: CanX

Chain BX:



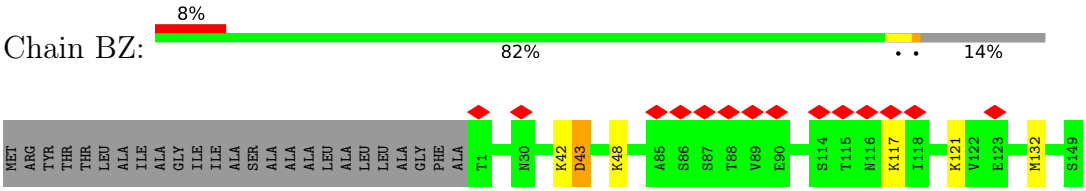
• Molecule 1: CanX

Chain BY:



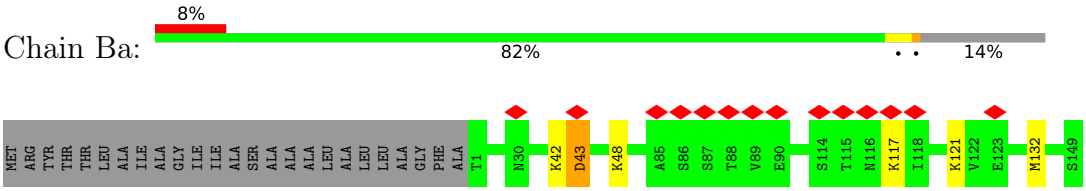
• Molecule 1: CanX

Chain BZ:



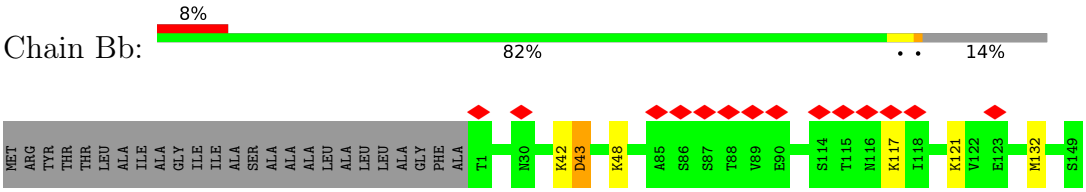
• Molecule 1: CanX

Chain Ba:



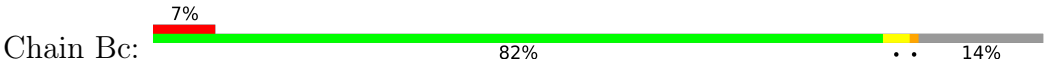
• Molecule 1: CanX

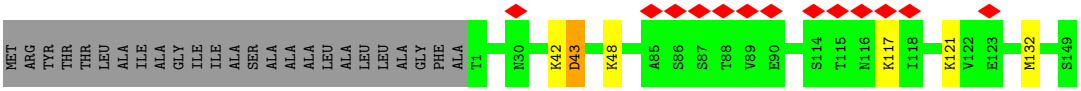
Chain Bb:



• Molecule 1: CanX

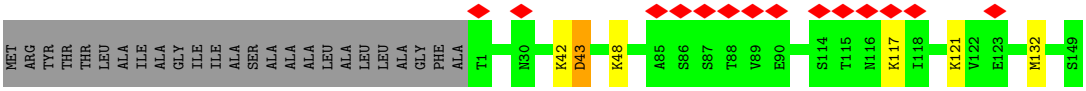
Chain Bc:





• Molecule 1: CanX

Chain Bd:



• Molecule 1: CanX

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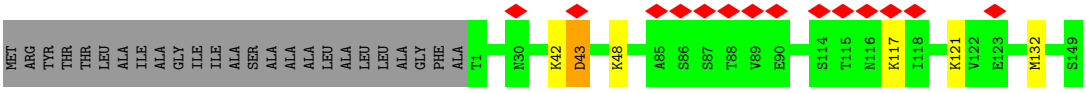
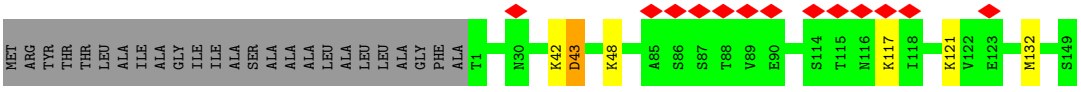


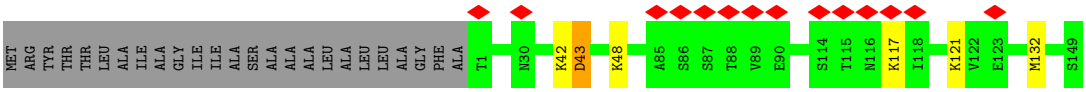
• Molecule 1: CanX

Chain Bf:



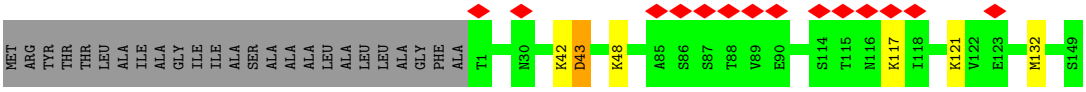
• Molecule 1: CanX

Chain Bg:



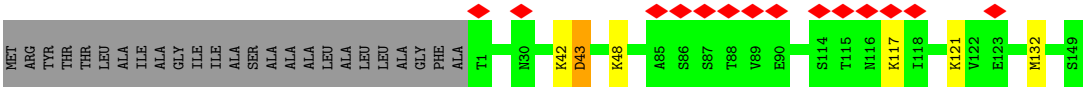
• Molecule 1: CanX

Chain Bh:



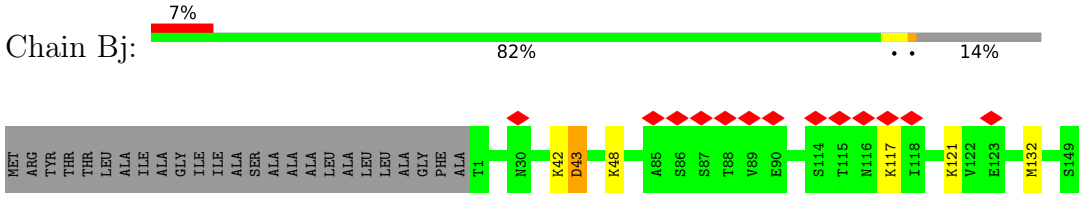
• Molecule 1: CanX

Chain Bi:



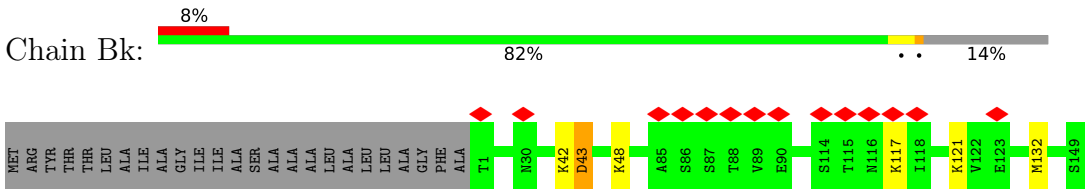
• Molecule 1: CanX

Chain Bj:



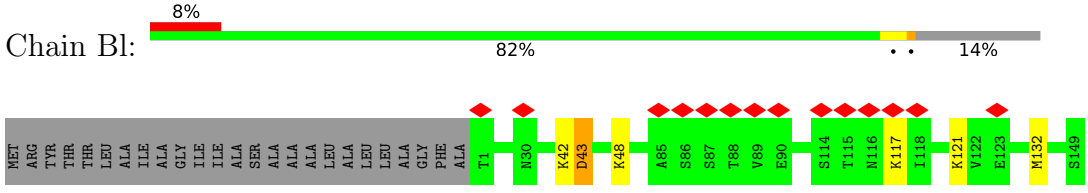
• Molecule 1: CanX

Chain Bk:



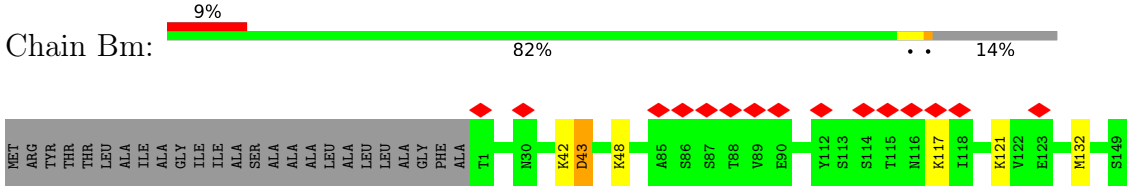
• Molecule 1: CanX

Chain Bl:



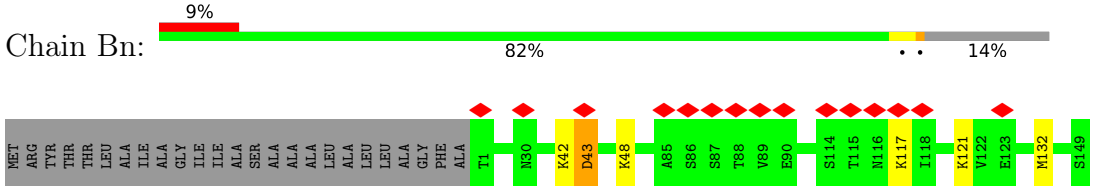
• Molecule 1: CanX

Chain Bm:



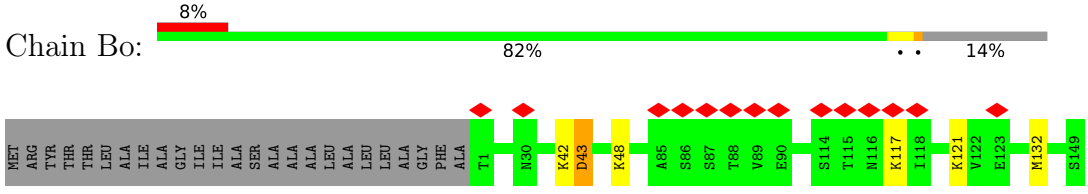
• Molecule 1: CanX

Chain Bn:



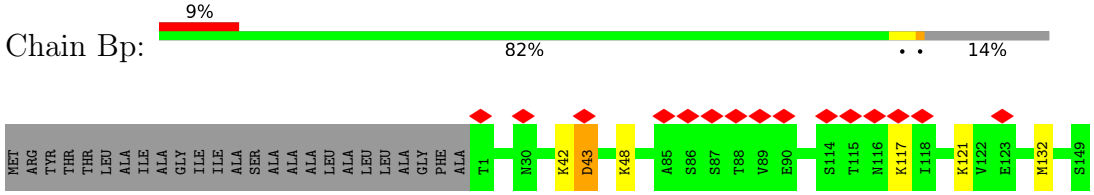
• Molecule 1: CanX

Chain Bo:



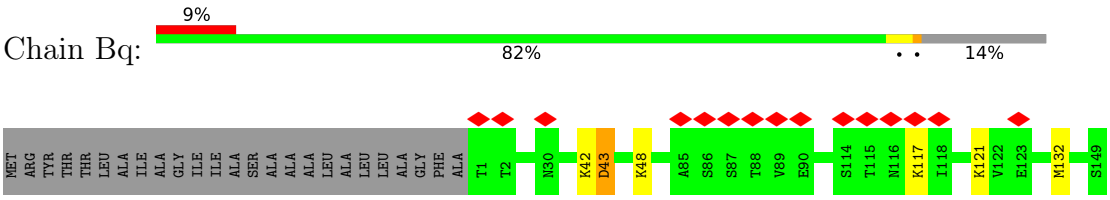
• Molecule 1: CanX

Chain Bp:



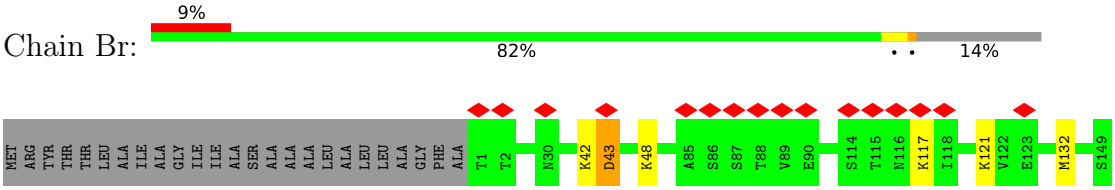
• Molecule 1: CanX

Chain Bq:



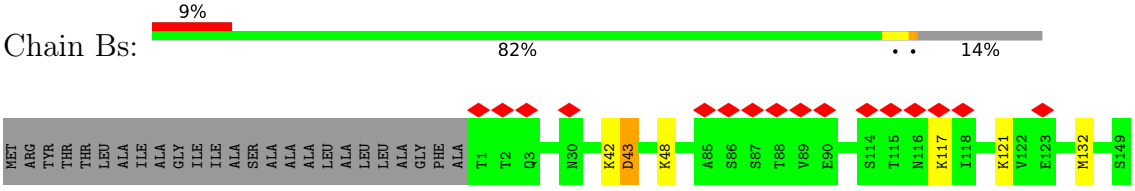
• Molecule 1: CanX

Chain Br:



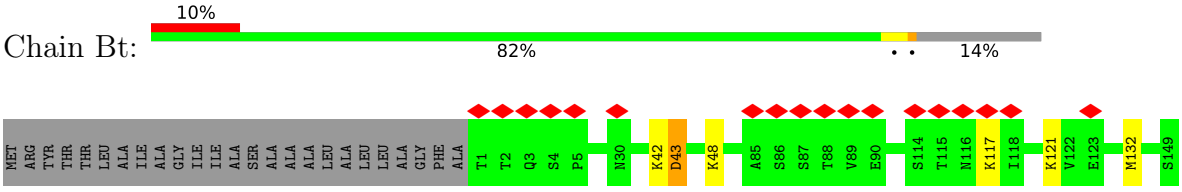
• Molecule 1: CanX

Chain Bs:



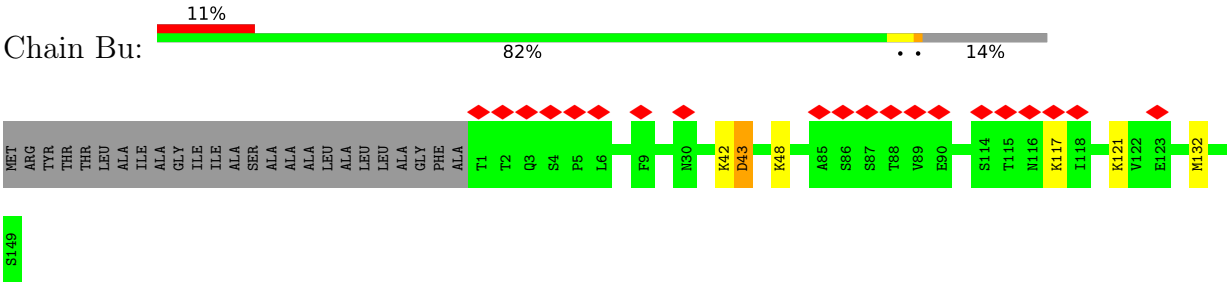
• Molecule 1: CanX

Chain Bt:



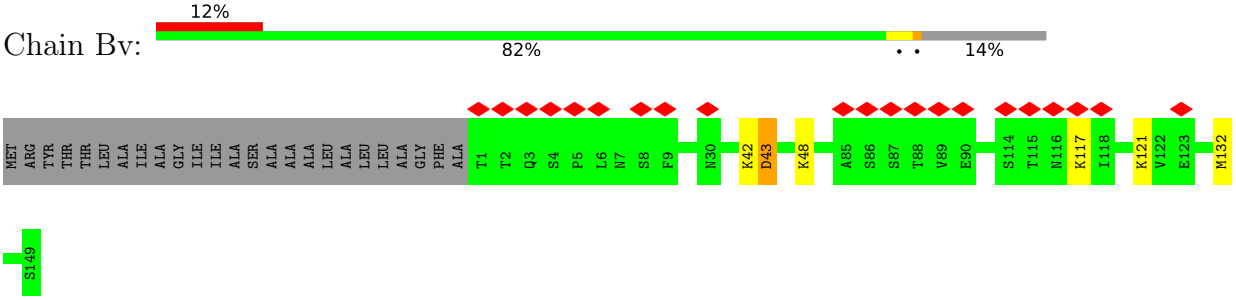
• Molecule 1: CanX

Chain Bu:



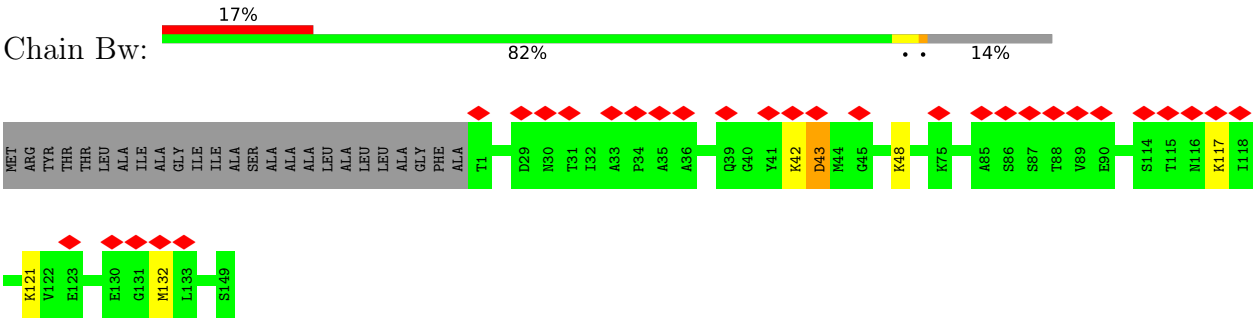
• Molecule 1: CanX

Chain Bv:



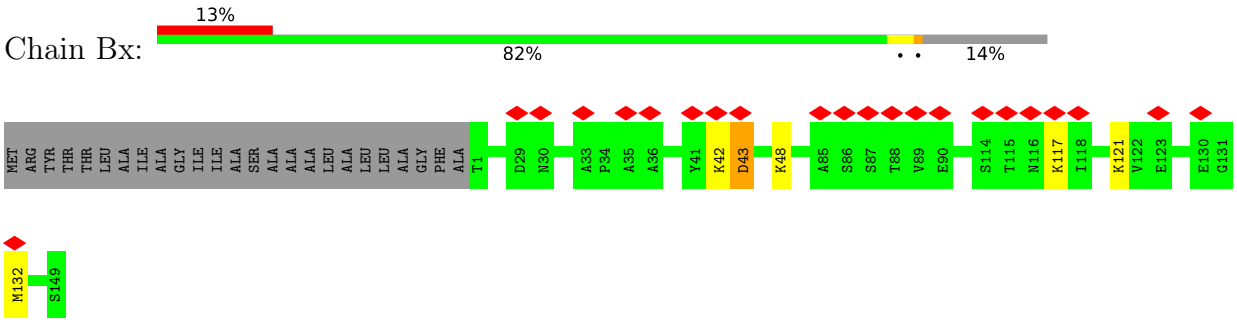
• Molecule 1: CanX

Chain Bw:



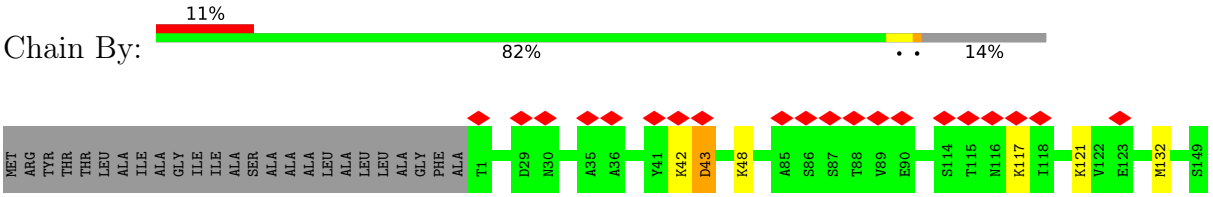
• Molecule 1: CanX

Chain Bx:



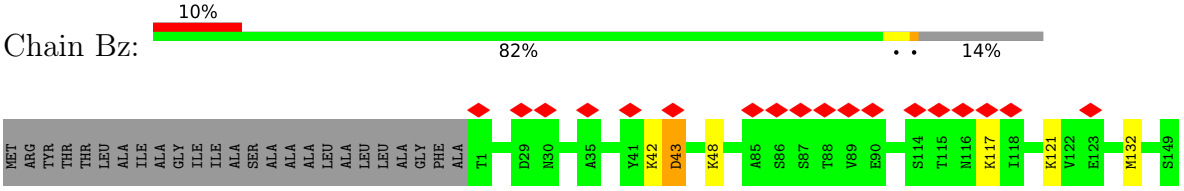
• Molecule 1: CanX

Chain By:



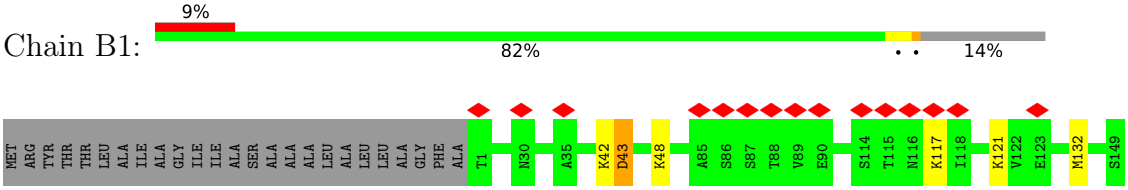
• Molecule 1: CanX

Chain Bz:



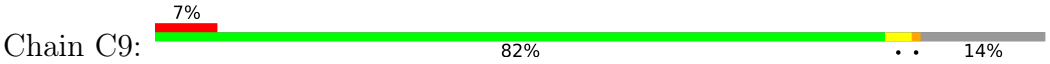
• Molecule 1: CanX

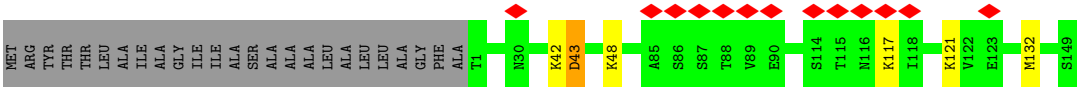
Chain B1:



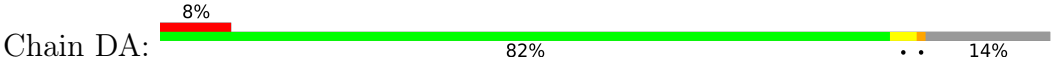
• Molecule 1: CanX

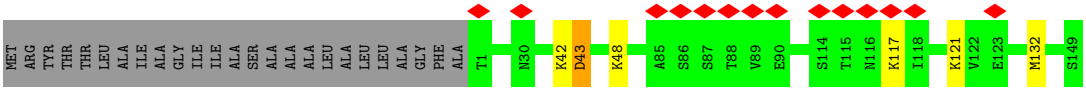
Chain C9:



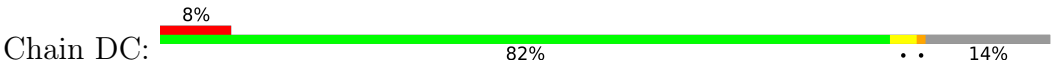


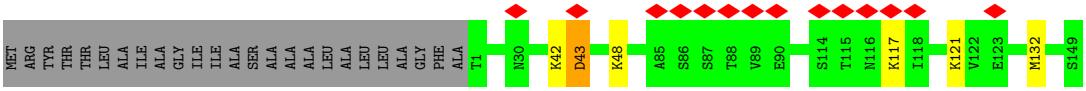
• Molecule 1: CanX



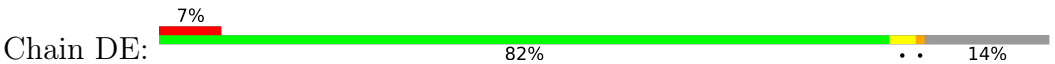


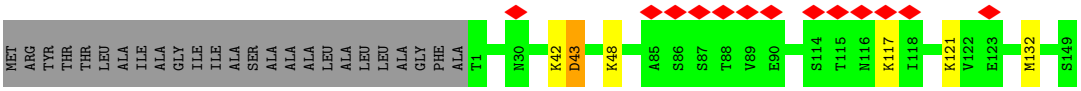
• Molecule 1: CanX



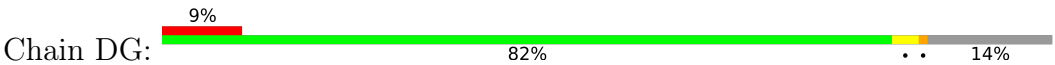


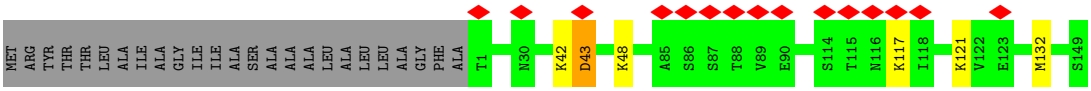
• Molecule 1: CanX



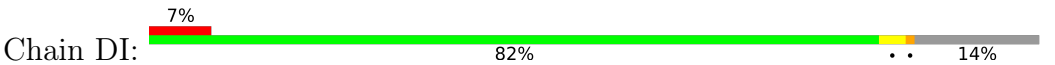


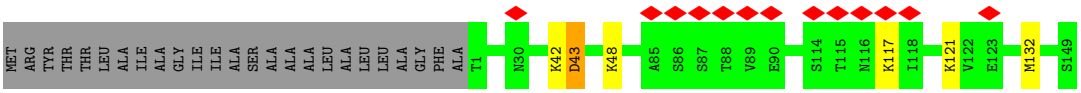
• Molecule 1: CanX



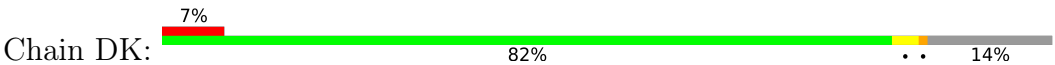


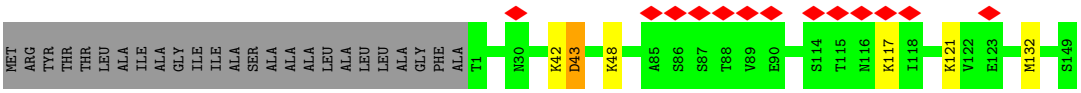
• Molecule 1: CanX





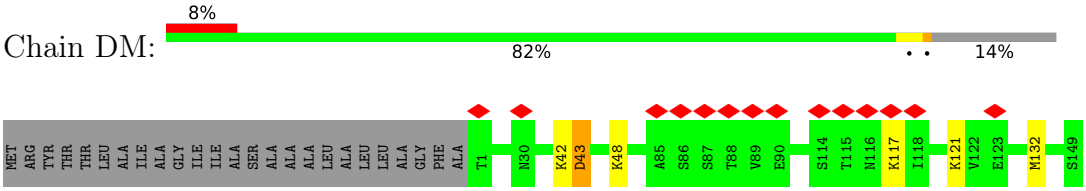
• Molecule 1: CanX





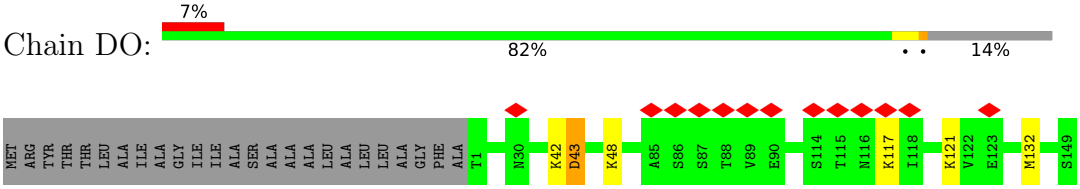
• Molecule 1: CanX

Chain DM:



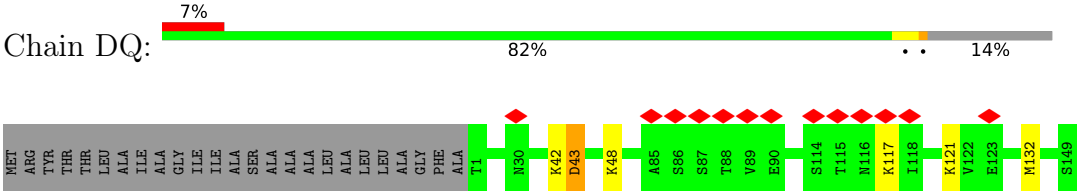
• Molecule 1: CanX

Chain DO:



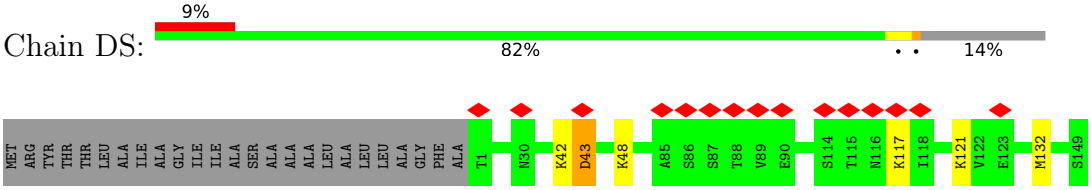
• Molecule 1: CanX

Chain DQ:



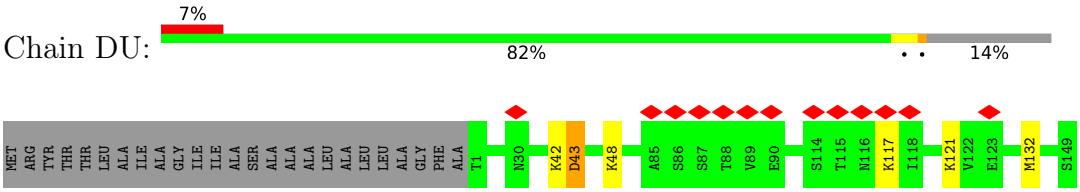
• Molecule 1: CanX

Chain DS:



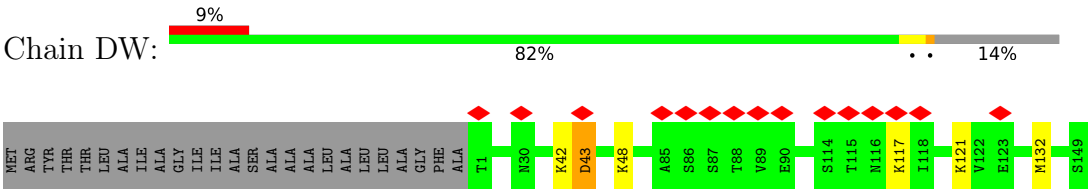
• Molecule 1: CanX

Chain DU:



• Molecule 1: CanX

Chain DW:



• Molecule 1: CanX

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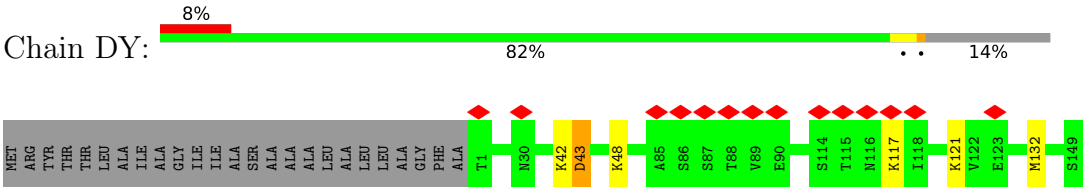
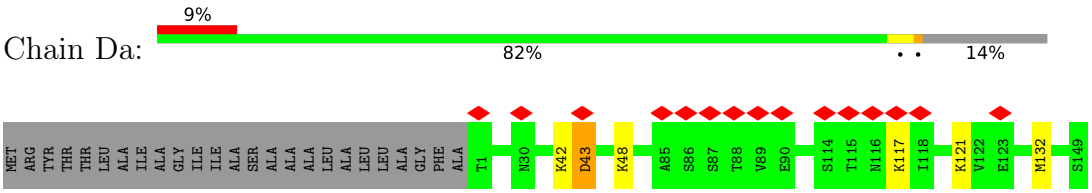


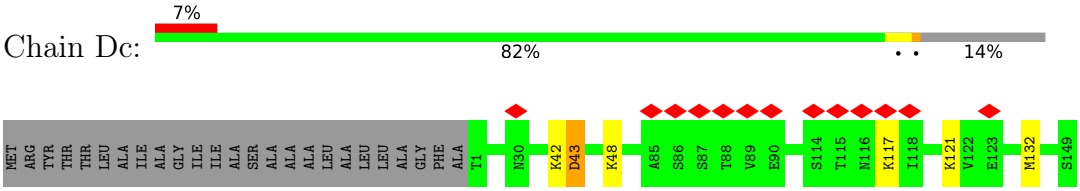
• Molecule 1: CanX

Chain Da:



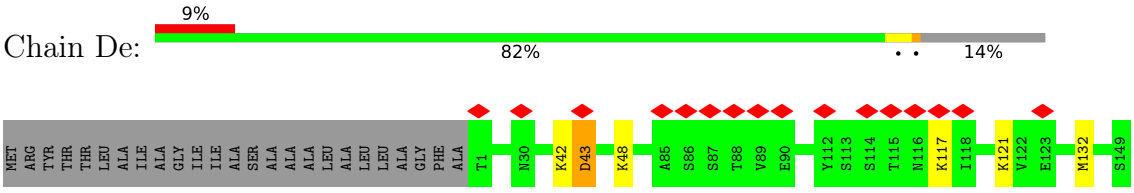
• Molecule 1: CanX

Chain Dc:



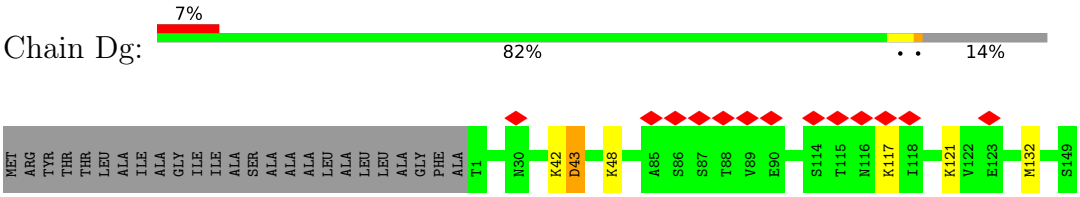
• Molecule 1: CanX

Chain De:



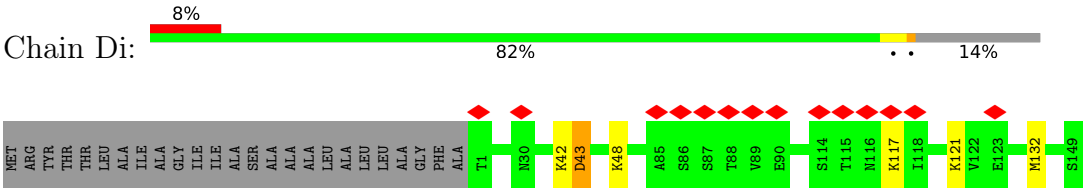
• Molecule 1: CanX

Chain Dg:



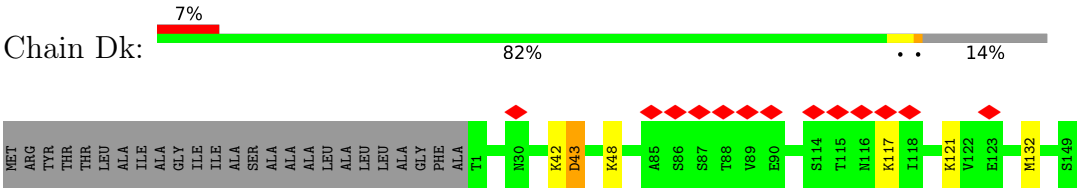
• Molecule 1: CanX

Chain Di:



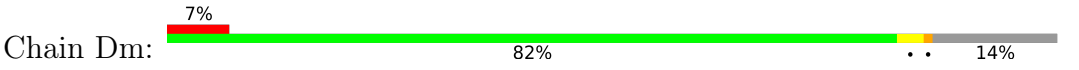
• Molecule 1: CanX

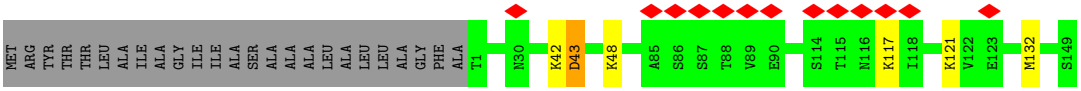
Chain Dk:



• Molecule 1: CanX

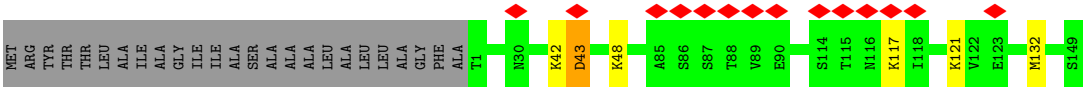
Chain Dm:





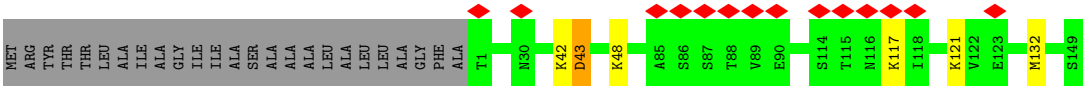
• Molecule 1: CanX

Chain Do:



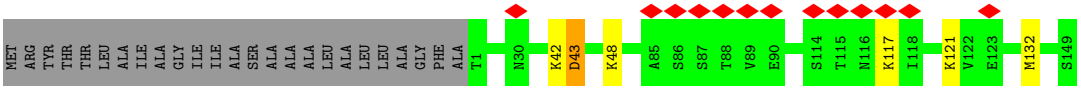
• Molecule 1: CanX

Chain Dq:



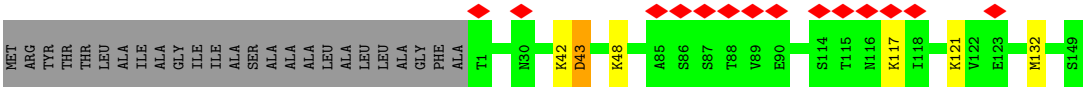
• Molecule 1: CanX

Chain Ds:



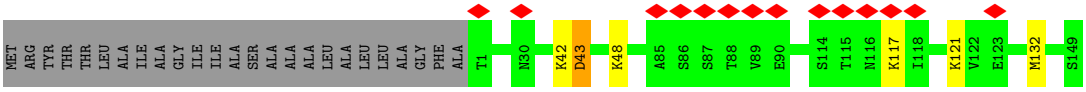
• Molecule 1: CanX

Chain Du:



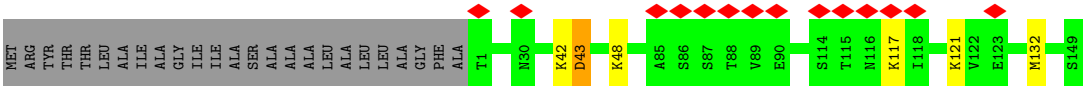
• Molecule 1: CanX

Chain Dw:



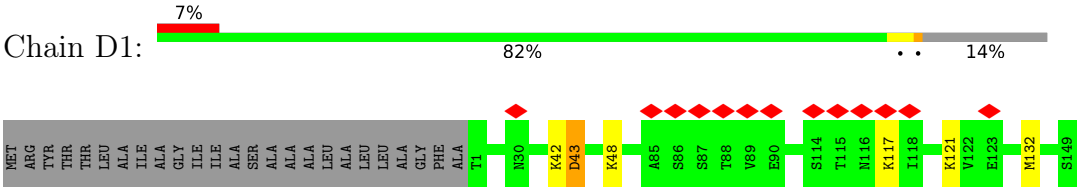
• Molecule 1: CanX

Chain Dy:



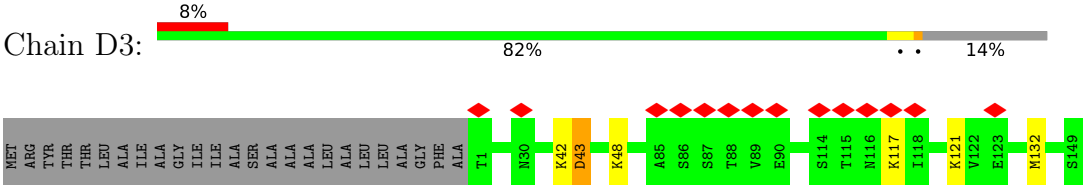
• Molecule 1: CanX

Chain D1:



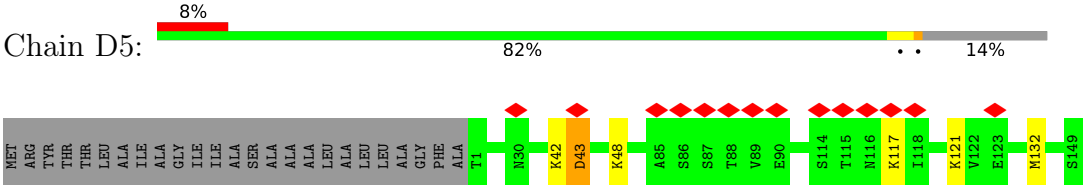
• Molecule 1: CanX

Chain D3:



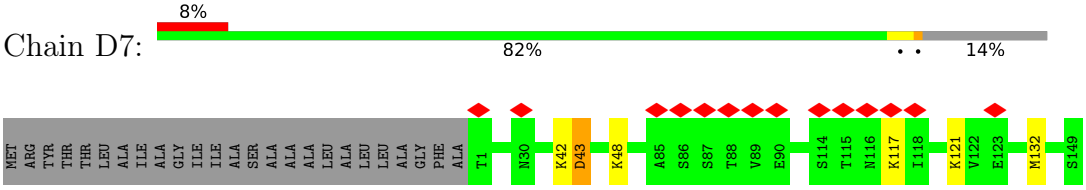
• Molecule 1: CanX

Chain D5:



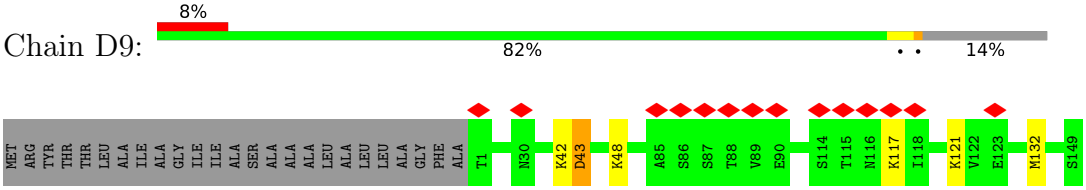
• Molecule 1: CanX

Chain D7:



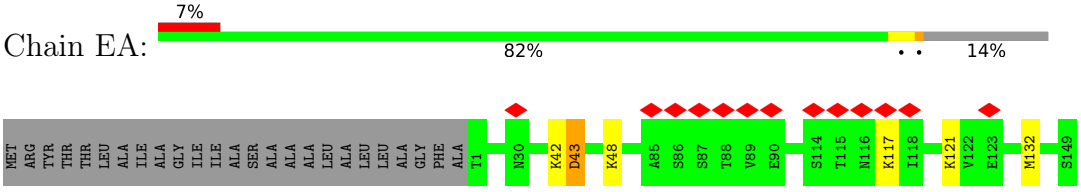
• Molecule 1: CanX

Chain D9:



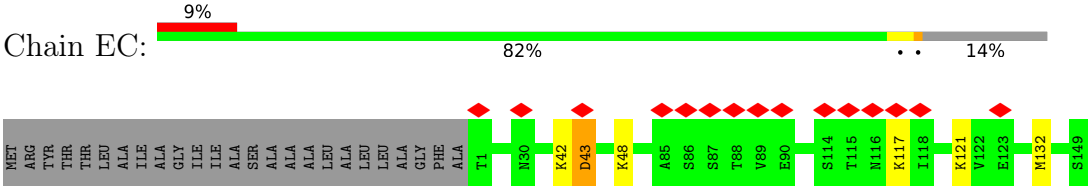
• Molecule 1: CanX

Chain EA:



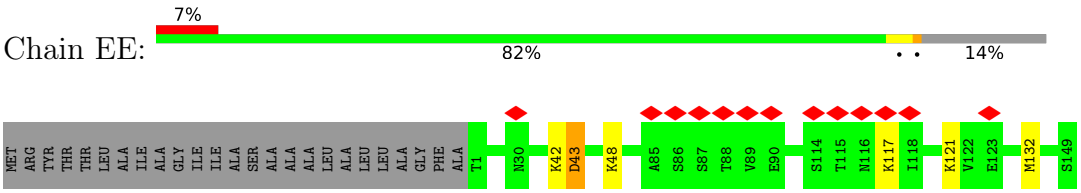
• Molecule 1: CanX

Chain EC:



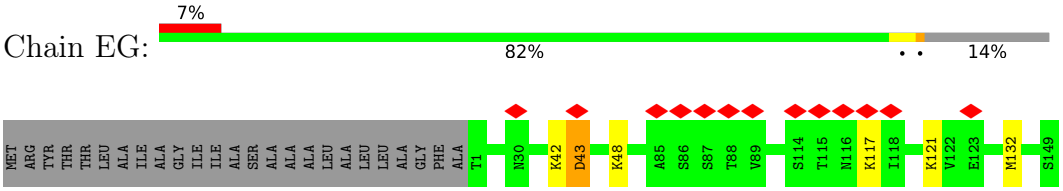
• Molecule 1: CanX

Chain EE:



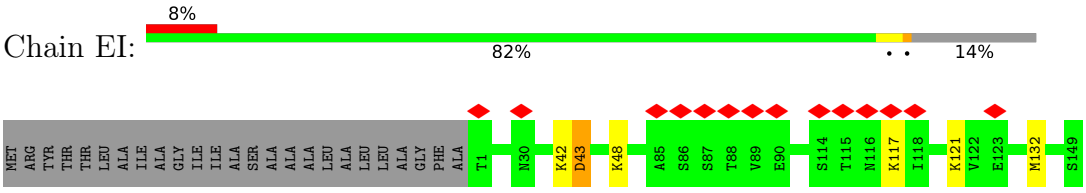
• Molecule 1: CanX

Chain EG:



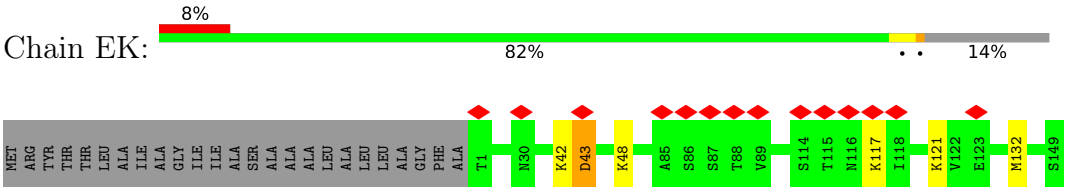
• Molecule 1: CanX

Chain EI:



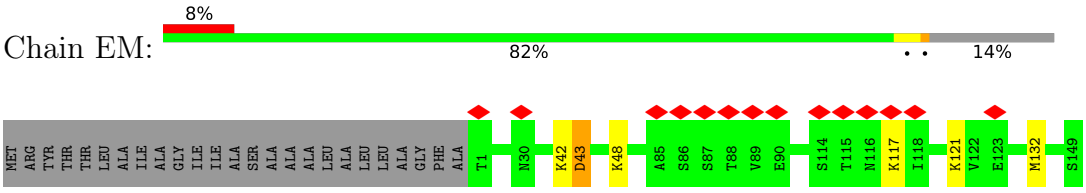
• Molecule 1: CanX

Chain EK:



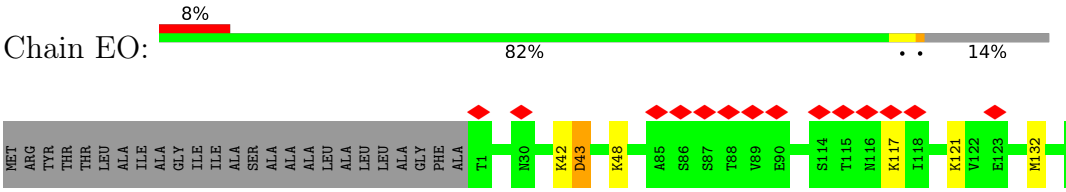
• Molecule 1: CanX

Chain EM:



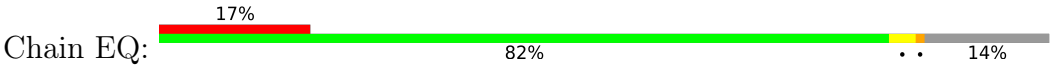
• Molecule 1: CanX

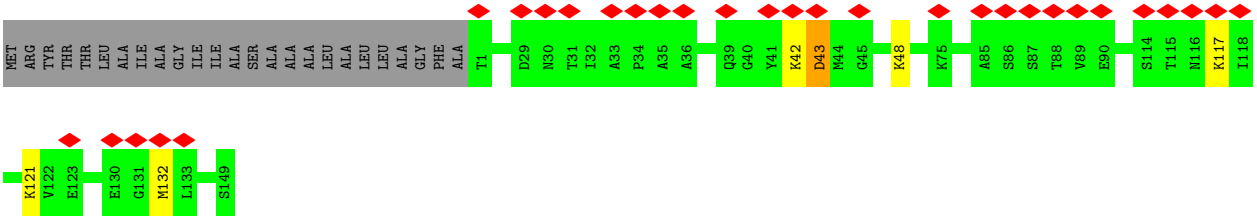
Chain EO:



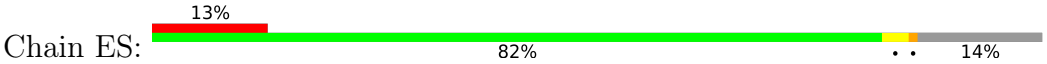
• Molecule 1: CanX

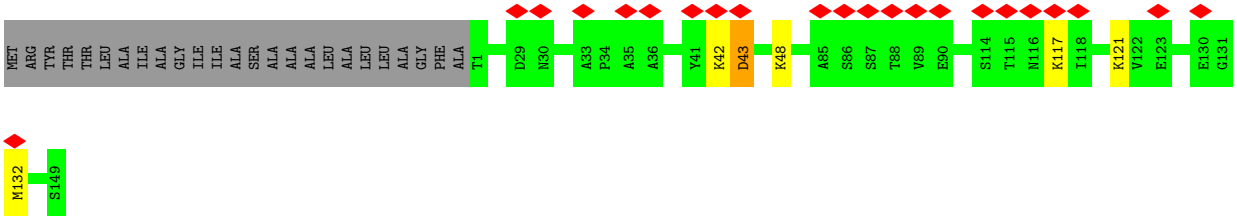
Chain EQ:



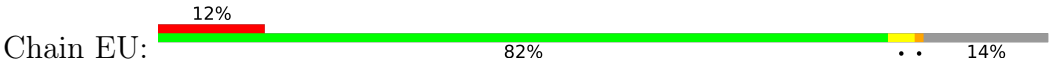


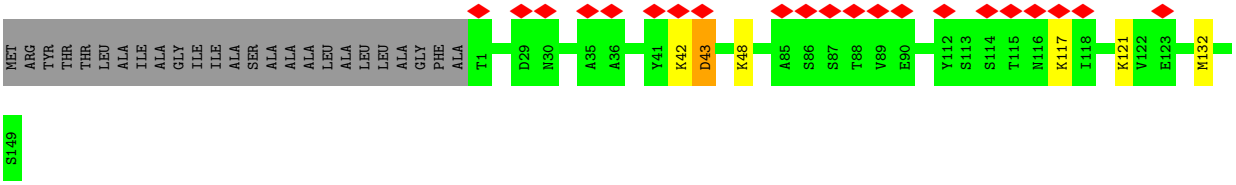
• Molecule 1: CanX



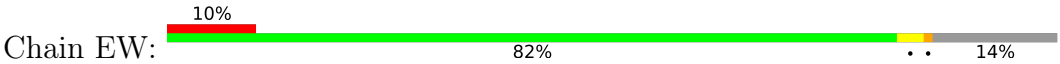


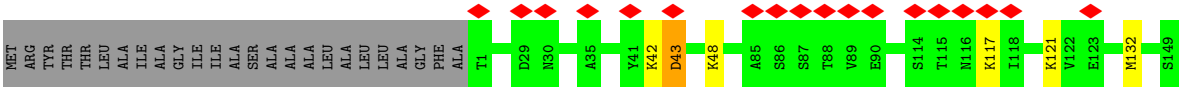
• Molecule 1: CanX



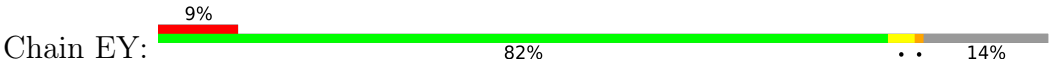


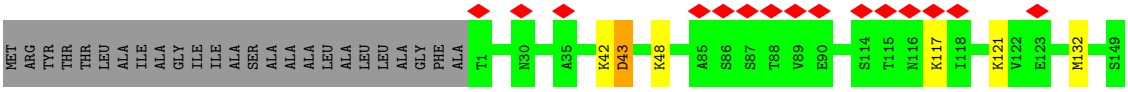
• Molecule 1: CanX



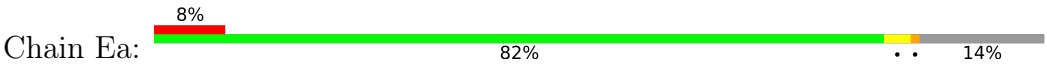


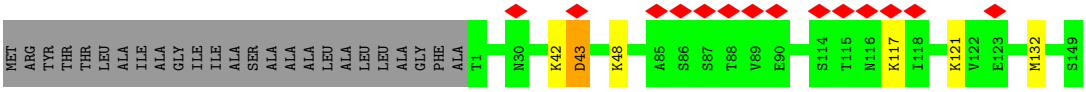
• Molecule 1: CanX





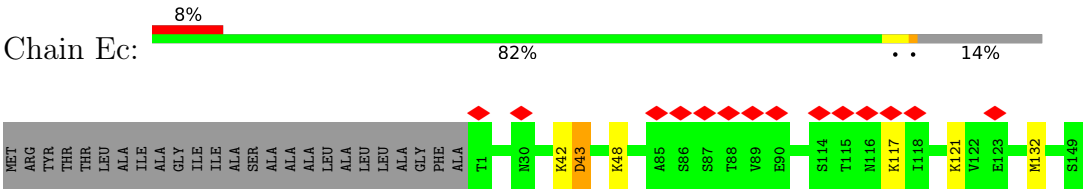
• Molecule 1: CanX





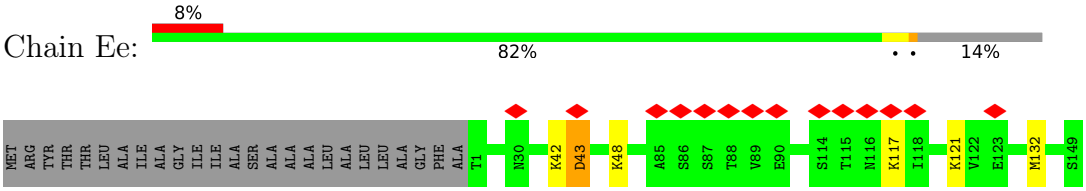
• Molecule 1: CanX

Chain Ec:



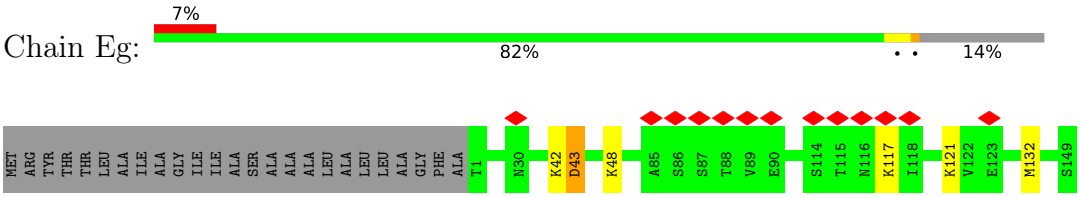
• Molecule 1: CanX

Chain Ee:



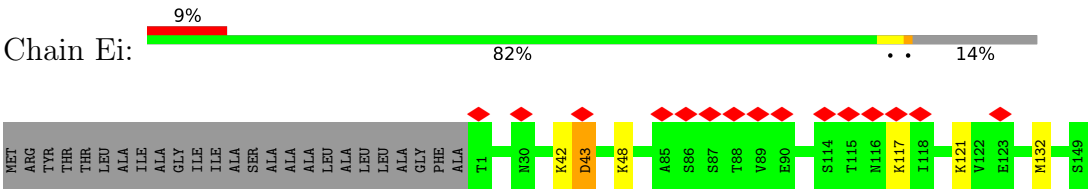
• Molecule 1: CanX

Chain Eg:



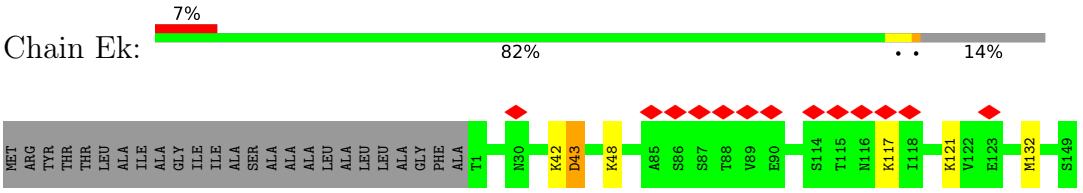
• Molecule 1: CanX

Chain Ei:



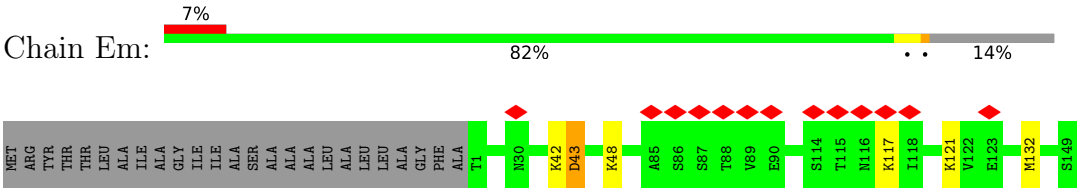
• Molecule 1: CanX

Chain Ek:



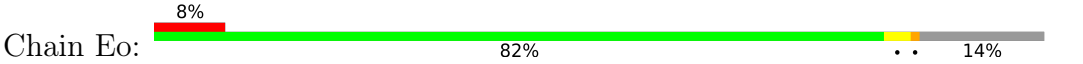
• Molecule 1: CanX

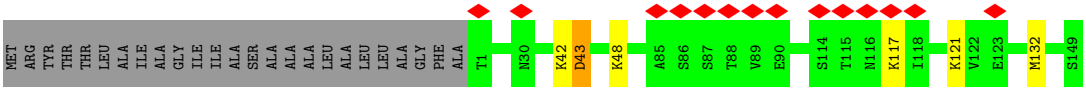
Chain Em:



• Molecule 1: CanX

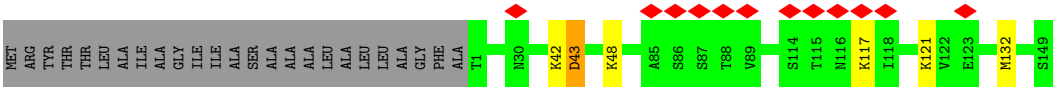
Chain Eo:





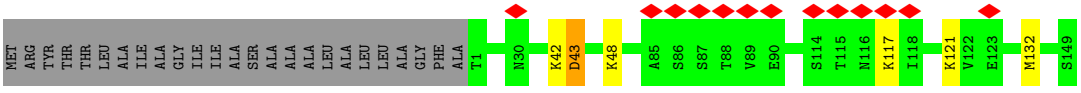
• Molecule 1: CanX

Chain Eq:



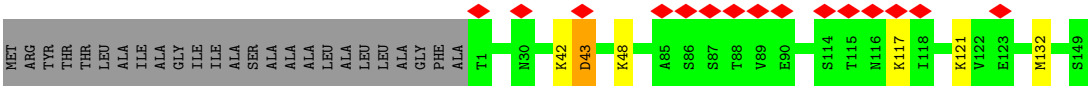
• Molecule 1: CanX

Chain Es:



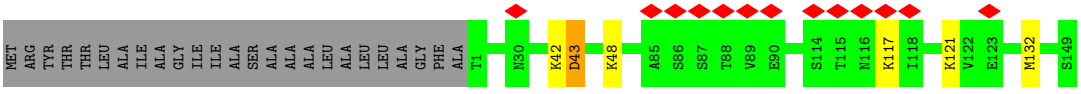
• Molecule 1: CanX

Chain Eu:



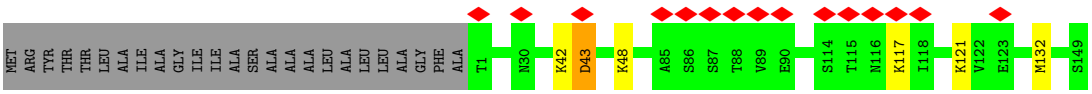
• Molecule 1: CanX

Chain Ew:



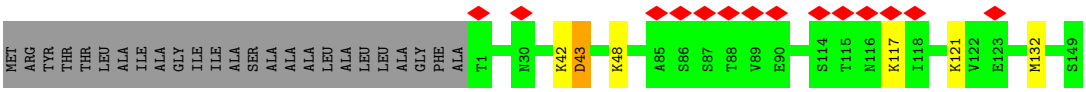
• Molecule 1: CanX

Chain Ey:



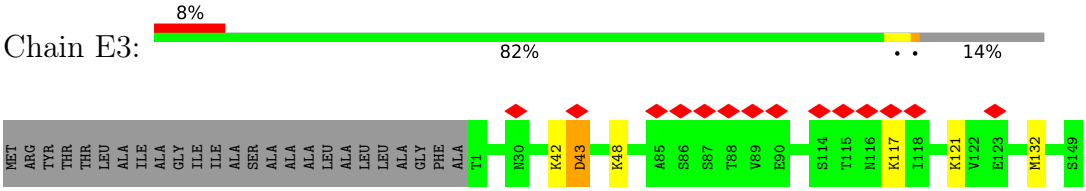
• Molecule 1: CanX

Chain E1:



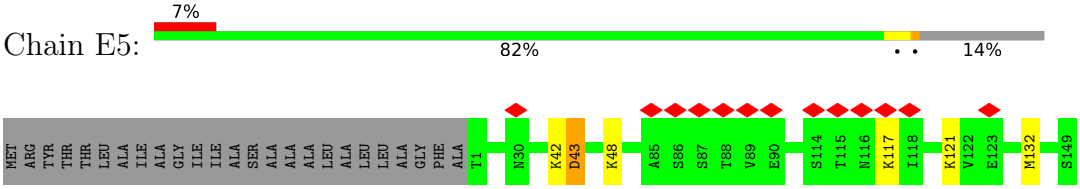
• Molecule 1: CanX

Chain E3:



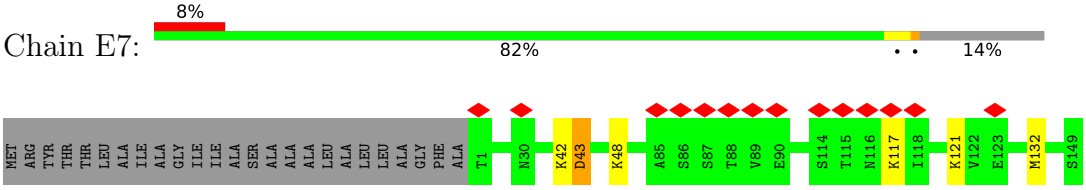
• Molecule 1: CanX

Chain E5:



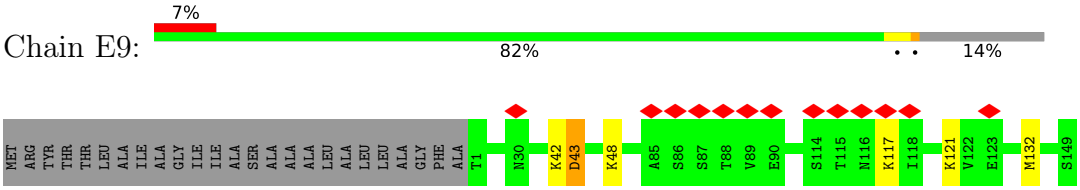
• Molecule 1: CanX

Chain E7:



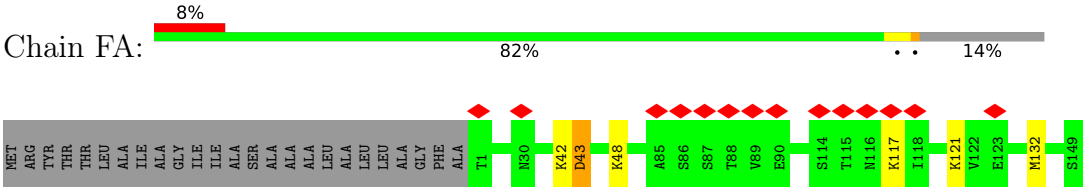
• Molecule 1: CanX

Chain E9:



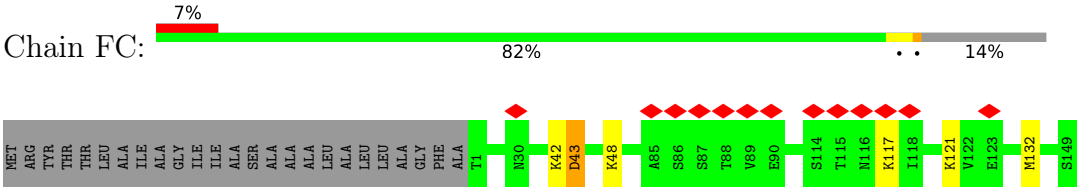
• Molecule 1: CanX

Chain FA:



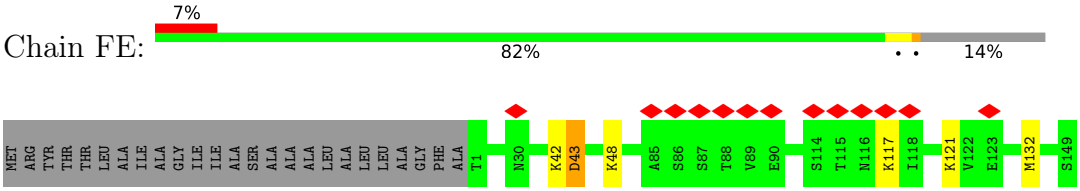
• Molecule 1: CanX

Chain FC:



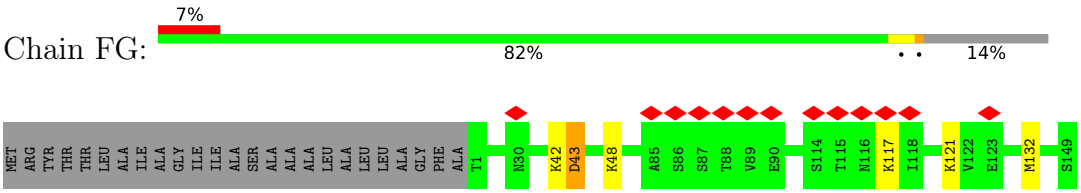
• Molecule 1: CanX

Chain FE:



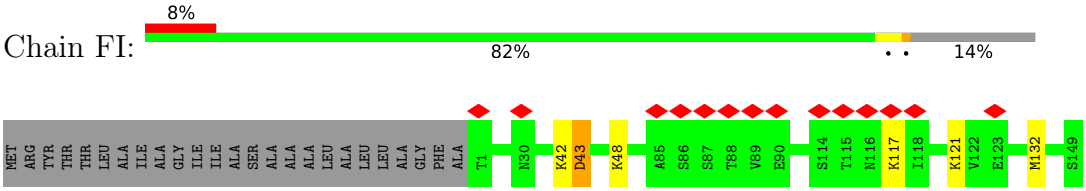
• Molecule 1: CanX

Chain FG:



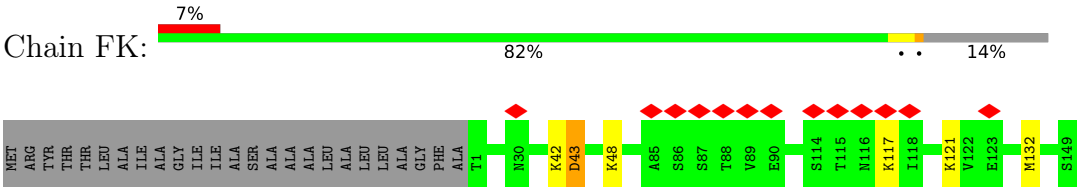
• Molecule 1: CanX

Chain FI:



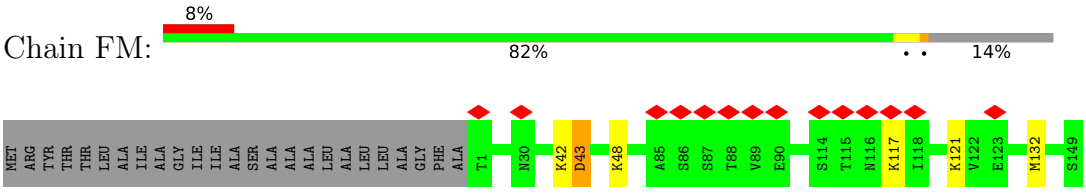
• Molecule 1: CanX

Chain FK:



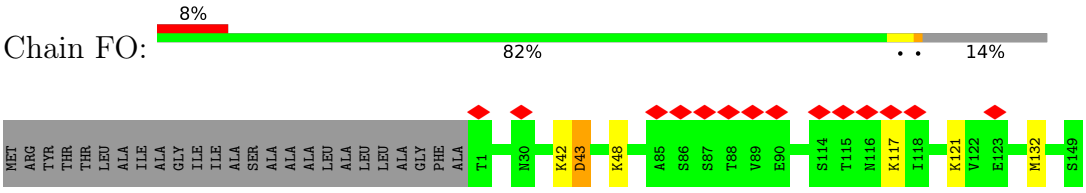
• Molecule 1: CanX

Chain FM:



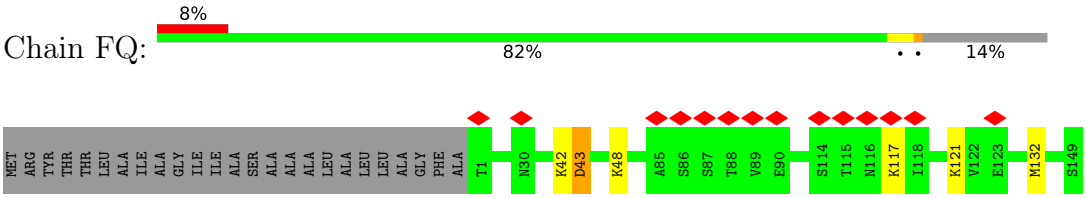
• Molecule 1: CanX

Chain FO:



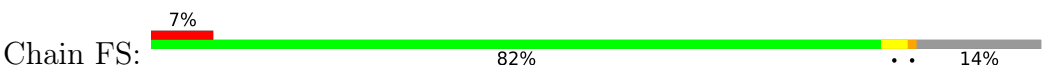
• Molecule 1: CanX

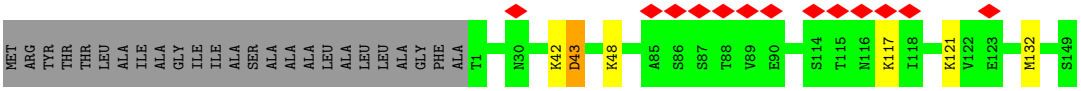
Chain FQ:



• Molecule 1: CanX

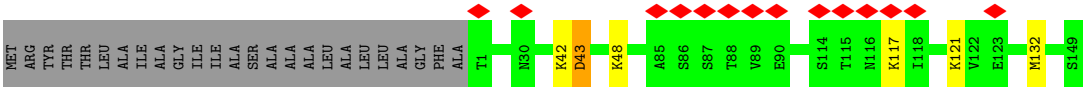
Chain FS:





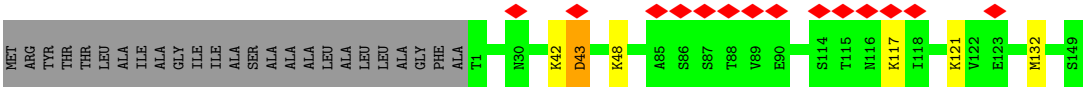
• Molecule 1: CanX

Chain FU:



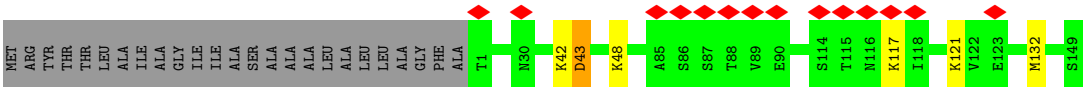
• Molecule 1: CanX

Chain FW:



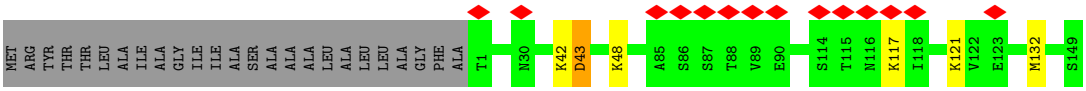
• Molecule 1: CanX

Chain FY:



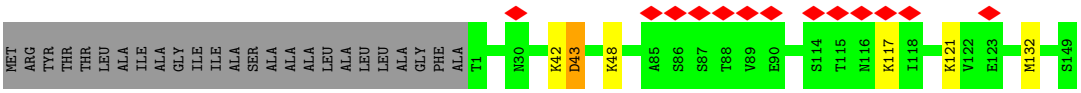
• Molecule 1: CanX

Chain Fa:



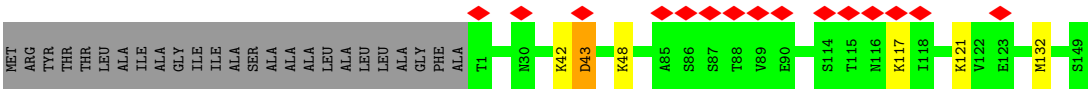
• Molecule 1: CanX

Chain Fc:



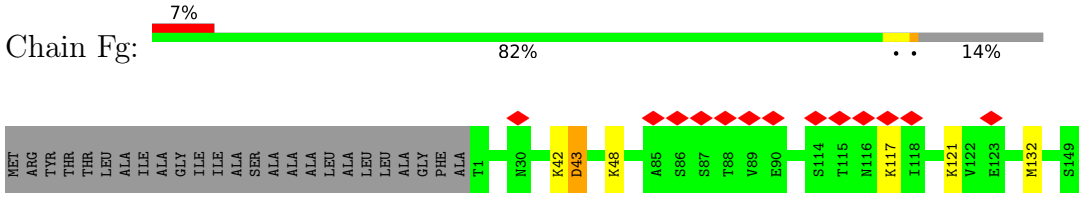
• Molecule 1: CanX

Chain Fe:



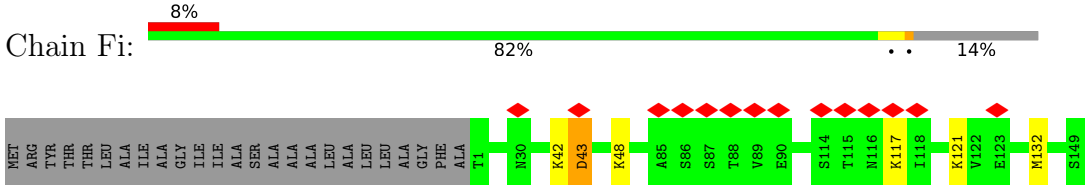
• Molecule 1: CanX

Chain Fg:



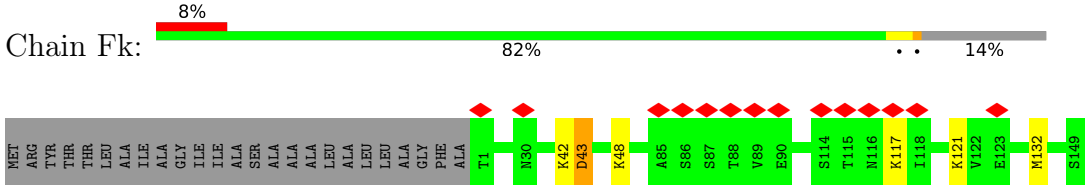
• Molecule 1: CanX

Chain Fi:



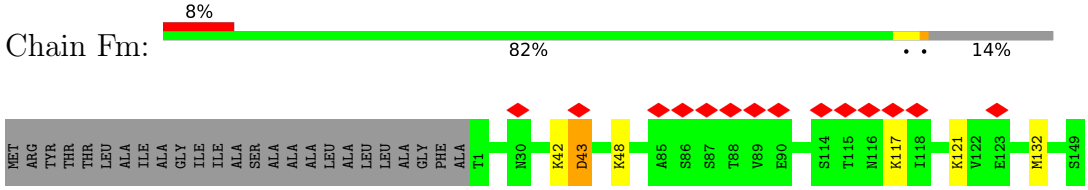
• Molecule 1: CanX

Chain Fk:



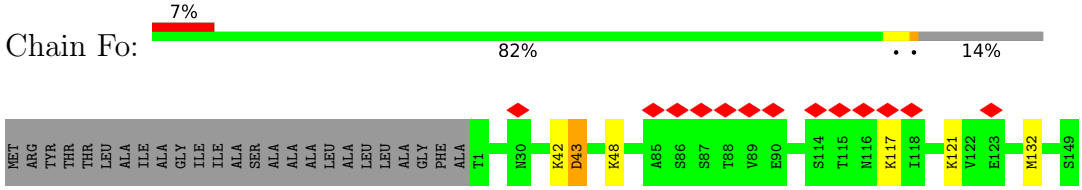
• Molecule 1: CanX

Chain Fm:



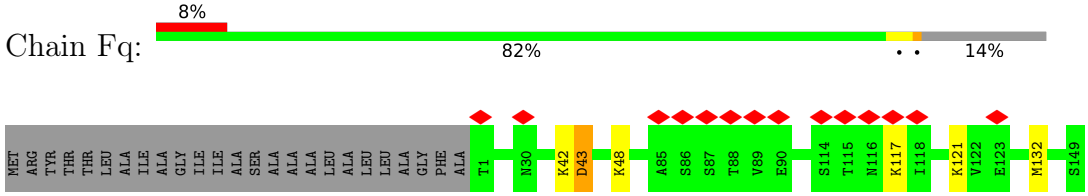
• Molecule 1: CanX

Chain Fo:



• Molecule 1: CanX

Chain Fq:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=12.094°, rise=3.178 Å, axial sym=C2	Depositor
Number of segments used	310172	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.330	Depositor
Minimum map value	-0.133	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.0691	Depositor
Map size (Å)	426.0, 426.0, 426.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.71, 0.71, 0.71	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, NAG

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	A0	0.26	0/1167	0.52	1/1590 (0.1%)
1	A1	0.26	0/1167	0.52	1/1590 (0.1%)
1	A2	0.26	0/1167	0.52	1/1590 (0.1%)
1	A3	0.26	0/1167	0.52	1/1590 (0.1%)
1	A4	0.26	0/1167	0.53	1/1590 (0.1%)
1	A5	0.26	0/1167	0.52	1/1590 (0.1%)
1	A6	0.26	0/1167	0.52	1/1590 (0.1%)
1	A7	0.26	0/1167	0.53	1/1590 (0.1%)
1	A8	0.26	0/1167	0.53	1/1590 (0.1%)
1	A9	0.26	0/1167	0.52	1/1590 (0.1%)
1	Au	0.26	0/1167	0.53	1/1590 (0.1%)
1	Av	0.26	0/1167	0.53	1/1590 (0.1%)
1	Aw	0.26	0/1167	0.53	1/1590 (0.1%)
1	Ax	0.26	0/1167	0.52	1/1590 (0.1%)
1	Ay	0.26	0/1167	0.52	1/1590 (0.1%)
1	Az	0.26	0/1167	0.53	1/1590 (0.1%)
1	B1	0.26	0/1167	0.53	1/1590 (0.1%)
1	BA	0.26	0/1167	0.52	1/1590 (0.1%)
1	BB	0.26	0/1167	0.53	1/1590 (0.1%)
1	BC	0.26	0/1167	0.53	1/1590 (0.1%)
1	BD	0.26	0/1167	0.52	1/1590 (0.1%)
1	BE	0.26	0/1167	0.52	1/1590 (0.1%)
1	BF	0.26	0/1167	0.53	1/1590 (0.1%)
1	BG	0.26	0/1167	0.53	1/1590 (0.1%)
1	BH	0.26	0/1167	0.53	1/1590 (0.1%)
1	BI	0.26	0/1167	0.53	1/1590 (0.1%)
1	BJ	0.26	0/1167	0.53	1/1590 (0.1%)
1	BK	0.26	0/1167	0.53	1/1590 (0.1%)
1	BL	0.26	0/1167	0.52	1/1590 (0.1%)
1	BM	0.26	0/1167	0.52	1/1590 (0.1%)
1	BN	0.26	0/1167	0.52	1/1590 (0.1%)
1	BO	0.26	0/1167	0.52	1/1590 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	BP	0.26	0/1167	0.52	1/1590 (0.1%)
1	BQ	0.26	0/1167	0.52	1/1590 (0.1%)
1	BR	0.26	0/1167	0.53	1/1590 (0.1%)
1	BS	0.26	0/1167	0.53	1/1590 (0.1%)
1	BT	0.26	0/1167	0.52	1/1590 (0.1%)
1	BU	0.26	0/1167	0.52	1/1590 (0.1%)
1	BV	0.26	0/1167	0.52	1/1590 (0.1%)
1	BW	0.26	0/1167	0.52	1/1590 (0.1%)
1	BX	0.26	0/1167	0.52	1/1590 (0.1%)
1	BY	0.26	0/1167	0.53	1/1590 (0.1%)
1	BZ	0.26	0/1167	0.53	1/1590 (0.1%)
1	Ba	0.26	0/1167	0.52	1/1590 (0.1%)
1	Bb	0.26	0/1167	0.53	1/1590 (0.1%)
1	Bc	0.26	0/1167	0.52	1/1590 (0.1%)
1	Bd	0.26	0/1167	0.52	1/1590 (0.1%)
1	Be	0.26	0/1167	0.53	1/1590 (0.1%)
1	Bf	0.26	0/1167	0.53	1/1590 (0.1%)
1	Bg	0.26	0/1167	0.52	1/1590 (0.1%)
1	Bh	0.26	0/1167	0.52	1/1590 (0.1%)
1	Bi	0.26	0/1167	0.52	1/1590 (0.1%)
1	Bj	0.26	0/1167	0.53	1/1590 (0.1%)
1	Bk	0.26	0/1167	0.53	1/1590 (0.1%)
1	Bl	0.26	0/1167	0.53	1/1590 (0.1%)
1	Bm	0.26	0/1167	0.52	1/1590 (0.1%)
1	Bn	0.26	0/1167	0.52	1/1590 (0.1%)
1	Bo	0.26	0/1167	0.53	1/1590 (0.1%)
1	Bp	0.26	0/1167	0.52	1/1590 (0.1%)
1	Bq	0.26	0/1167	0.52	1/1590 (0.1%)
1	Br	0.26	0/1167	0.52	1/1590 (0.1%)
1	Bs	0.26	0/1167	0.53	1/1590 (0.1%)
1	Bt	0.26	0/1167	0.53	1/1590 (0.1%)
1	Bu	0.26	0/1167	0.52	1/1590 (0.1%)
1	Bv	0.26	0/1167	0.52	1/1590 (0.1%)
1	Bw	0.26	0/1167	0.53	1/1590 (0.1%)
1	Bx	0.26	0/1167	0.52	1/1590 (0.1%)
1	By	0.26	0/1167	0.52	1/1590 (0.1%)
1	Bz	0.26	0/1167	0.53	1/1590 (0.1%)
1	C9	0.26	0/1167	0.52	1/1590 (0.1%)
1	D1	0.26	0/1167	0.53	1/1590 (0.1%)
1	D3	0.26	0/1167	0.53	1/1590 (0.1%)
1	D5	0.26	0/1167	0.52	1/1590 (0.1%)
1	D7	0.26	0/1167	0.52	1/1590 (0.1%)
1	D9	0.26	0/1167	0.53	1/1590 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	DA	0.26	0/1167	0.52	1/1590 (0.1%)
1	DC	0.26	0/1167	0.52	1/1590 (0.1%)
1	DE	0.26	0/1167	0.52	1/1590 (0.1%)
1	DG	0.26	0/1167	0.53	1/1590 (0.1%)
1	DI	0.26	0/1167	0.53	1/1590 (0.1%)
1	DK	0.26	0/1167	0.53	1/1590 (0.1%)
1	DM	0.26	0/1167	0.52	1/1590 (0.1%)
1	DO	0.26	0/1167	0.53	1/1590 (0.1%)
1	DQ	0.26	0/1167	0.52	1/1590 (0.1%)
1	DS	0.26	0/1167	0.52	1/1590 (0.1%)
1	DU	0.26	0/1167	0.53	1/1590 (0.1%)
1	DW	0.26	0/1167	0.53	1/1590 (0.1%)
1	DY	0.26	0/1167	0.52	1/1590 (0.1%)
1	Da	0.26	0/1167	0.53	1/1590 (0.1%)
1	Dc	0.26	0/1167	0.53	1/1590 (0.1%)
1	De	0.26	0/1167	0.52	1/1590 (0.1%)
1	Dg	0.26	0/1167	0.52	1/1590 (0.1%)
1	Di	0.26	0/1167	0.52	1/1590 (0.1%)
1	Dk	0.26	0/1167	0.52	1/1590 (0.1%)
1	Dm	0.26	0/1167	0.52	1/1590 (0.1%)
1	Do	0.26	0/1167	0.52	1/1590 (0.1%)
1	Dq	0.26	0/1167	0.53	1/1590 (0.1%)
1	Ds	0.26	0/1167	0.53	1/1590 (0.1%)
1	Du	0.26	0/1167	0.53	1/1590 (0.1%)
1	Dw	0.26	0/1167	0.52	1/1590 (0.1%)
1	Dy	0.26	0/1167	0.52	1/1590 (0.1%)
1	E1	0.26	0/1167	0.52	1/1590 (0.1%)
1	E3	0.26	0/1167	0.52	1/1590 (0.1%)
1	E5	0.26	0/1167	0.52	1/1590 (0.1%)
1	E7	0.26	0/1167	0.52	1/1590 (0.1%)
1	E9	0.26	0/1167	0.52	1/1590 (0.1%)
1	EA	0.26	0/1167	0.52	1/1590 (0.1%)
1	EC	0.26	0/1167	0.52	1/1590 (0.1%)
1	EE	0.26	0/1167	0.52	1/1590 (0.1%)
1	EG	0.26	0/1167	0.52	1/1590 (0.1%)
1	EI	0.26	0/1167	0.53	1/1590 (0.1%)
1	EK	0.26	0/1167	0.52	1/1590 (0.1%)
1	EM	0.26	0/1167	0.52	1/1590 (0.1%)
1	EO	0.26	0/1167	0.52	1/1590 (0.1%)
1	EQ	0.26	0/1167	0.52	1/1590 (0.1%)
1	ES	0.26	0/1167	0.53	1/1590 (0.1%)
1	EU	0.26	0/1167	0.52	1/1590 (0.1%)
1	EW	0.26	0/1167	0.53	1/1590 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	EY	0.26	0/1167	0.52	1/1590 (0.1%)
1	Ea	0.26	0/1167	0.52	1/1590 (0.1%)
1	Ec	0.26	0/1167	0.53	1/1590 (0.1%)
1	Ee	0.26	0/1167	0.52	1/1590 (0.1%)
1	Eg	0.26	0/1167	0.52	1/1590 (0.1%)
1	Ei	0.26	0/1167	0.52	1/1590 (0.1%)
1	Ek	0.26	0/1167	0.52	1/1590 (0.1%)
1	Em	0.26	0/1167	0.53	1/1590 (0.1%)
1	Eo	0.26	0/1167	0.52	1/1590 (0.1%)
1	Eq	0.26	0/1167	0.52	1/1590 (0.1%)
1	Es	0.26	0/1167	0.53	1/1590 (0.1%)
1	Eu	0.26	0/1167	0.52	1/1590 (0.1%)
1	Ew	0.26	0/1167	0.53	1/1590 (0.1%)
1	Ey	0.26	0/1167	0.53	1/1590 (0.1%)
1	FA	0.26	0/1167	0.53	1/1590 (0.1%)
1	FC	0.26	0/1167	0.52	1/1590 (0.1%)
1	FE	0.26	0/1167	0.52	1/1590 (0.1%)
1	FG	0.26	0/1167	0.53	1/1590 (0.1%)
1	FI	0.26	0/1167	0.52	1/1590 (0.1%)
1	FK	0.26	0/1167	0.52	1/1590 (0.1%)
1	FM	0.26	0/1167	0.53	1/1590 (0.1%)
1	FO	0.26	0/1167	0.52	1/1590 (0.1%)
1	FQ	0.26	0/1167	0.53	1/1590 (0.1%)
1	FS	0.26	0/1167	0.52	1/1590 (0.1%)
1	FU	0.26	0/1167	0.53	1/1590 (0.1%)
1	FW	0.26	0/1167	0.52	1/1590 (0.1%)
1	FY	0.26	0/1167	0.53	1/1590 (0.1%)
1	Fa	0.26	0/1167	0.53	1/1590 (0.1%)
1	Fc	0.26	0/1167	0.52	1/1590 (0.1%)
1	Fe	0.26	0/1167	0.53	1/1590 (0.1%)
1	Fg	0.26	0/1167	0.52	1/1590 (0.1%)
1	Fi	0.26	0/1167	0.53	1/1590 (0.1%)
1	Fk	0.26	0/1167	0.52	1/1590 (0.1%)
1	Fm	0.26	0/1167	0.52	1/1590 (0.1%)
1	Fo	0.26	0/1167	0.53	1/1590 (0.1%)
1	Fq	0.26	0/1167	0.53	1/1590 (0.1%)
All	All	0.26	0/179718	0.52	154/244860 (0.1%)

There are no bond length outliers.

All (154) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	DY	43	ASP	CB-CG-OD2	5.75	123.48	118.30
1	Ew	43	ASP	CB-CG-OD2	5.75	123.48	118.30
1	FA	43	ASP	CB-CG-OD2	5.75	123.48	118.30
1	Aw	43	ASP	CB-CG-OD2	5.75	123.47	118.30
1	Bw	43	ASP	CB-CG-OD2	5.74	123.47	118.30
1	A3	43	ASP	CB-CG-OD2	5.73	123.46	118.30
1	BH	43	ASP	CB-CG-OD2	5.73	123.46	118.30
1	Fe	43	ASP	CB-CG-OD2	5.73	123.45	118.30
1	A4	43	ASP	CB-CG-OD2	5.72	123.45	118.30
1	Bm	43	ASP	CB-CG-OD2	5.72	123.45	118.30
1	Bp	43	ASP	CB-CG-OD2	5.72	123.45	118.30
1	Fk	43	ASP	CB-CG-OD2	5.72	123.45	118.30
1	Av	43	ASP	CB-CG-OD2	5.72	123.45	118.30
1	A7	43	ASP	CB-CG-OD2	5.72	123.45	118.30
1	Bn	43	ASP	CB-CG-OD2	5.72	123.45	118.30
1	Dq	43	ASP	CB-CG-OD2	5.72	123.45	118.30
1	D9	43	ASP	CB-CG-OD2	5.72	123.45	118.30
1	FY	43	ASP	CB-CG-OD2	5.72	123.45	118.30
1	EO	43	ASP	CB-CG-OD2	5.72	123.44	118.30
1	E7	43	ASP	CB-CG-OD2	5.72	123.44	118.30
1	Fq	43	ASP	CB-CG-OD2	5.72	123.44	118.30
1	DK	43	ASP	CB-CG-OD2	5.71	123.44	118.30
1	EE	43	ASP	CB-CG-OD2	5.71	123.44	118.30
1	EW	43	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A5	43	ASP	CB-CG-OD2	5.71	123.44	118.30
1	Bg	43	ASP	CB-CG-OD2	5.71	123.44	118.30
1	BS	43	ASP	CB-CG-OD2	5.71	123.44	118.30
1	DI	43	ASP	CB-CG-OD2	5.71	123.44	118.30
1	BY	43	ASP	CB-CG-OD2	5.71	123.44	118.30
1	Bt	43	ASP	CB-CG-OD2	5.71	123.44	118.30
1	Fi	43	ASP	CB-CG-OD2	5.71	123.44	118.30
1	BA	43	ASP	CB-CG-OD2	5.71	123.44	118.30
1	Bx	43	ASP	CB-CG-OD2	5.71	123.44	118.30
1	DQ	43	ASP	CB-CG-OD2	5.71	123.44	118.30
1	ES	43	ASP	CB-CG-OD2	5.71	123.44	118.30
1	Em	43	ASP	CB-CG-OD2	5.71	123.43	118.30
1	Fo	43	ASP	CB-CG-OD2	5.71	123.43	118.30
1	Bj	43	ASP	CB-CG-OD2	5.70	123.43	118.30
1	Ek	43	ASP	CB-CG-OD2	5.70	123.43	118.30
1	BO	43	ASP	CB-CG-OD2	5.70	123.43	118.30
1	DO	43	ASP	CB-CG-OD2	5.70	123.43	118.30
1	FQ	43	ASP	CB-CG-OD2	5.70	123.43	118.30
1	Bs	43	ASP	CB-CG-OD2	5.70	123.43	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	DW	43	ASP	CB-CG-OD2	5.70	123.43	118.30
1	Ey	43	ASP	CB-CG-OD2	5.70	123.43	118.30
1	BB	43	ASP	CB-CG-OD2	5.70	123.43	118.30
1	BJ	43	ASP	CB-CG-OD2	5.70	123.43	118.30
1	Bl	43	ASP	CB-CG-OD2	5.70	123.43	118.30
1	EI	43	ASP	CB-CG-OD2	5.70	123.43	118.30
1	Bv	43	ASP	CB-CG-OD2	5.69	123.42	118.30
1	BK	43	ASP	CB-CG-OD2	5.69	123.42	118.30
1	Bb	43	ASP	CB-CG-OD2	5.69	123.42	118.30
1	DU	43	ASP	CB-CG-OD2	5.69	123.42	118.30
1	Dy	43	ASP	CB-CG-OD2	5.69	123.42	118.30
1	FE	43	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A1	43	ASP	CB-CG-OD2	5.69	123.42	118.30
1	BM	43	ASP	CB-CG-OD2	5.69	123.42	118.30
1	BW	43	ASP	CB-CG-OD2	5.69	123.42	118.30
1	FG	43	ASP	CB-CG-OD2	5.69	123.42	118.30
1	Bd	43	ASP	CB-CG-OD2	5.69	123.42	118.30
1	DS	43	ASP	CB-CG-OD2	5.69	123.42	118.30
1	Eu	43	ASP	CB-CG-OD2	5.69	123.42	118.30
1	FC	43	ASP	CB-CG-OD2	5.69	123.42	118.30
1	Bh	43	ASP	CB-CG-OD2	5.69	123.42	118.30
1	FM	43	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A8	43	ASP	CB-CG-OD2	5.68	123.42	118.30
1	BI	43	ASP	CB-CG-OD2	5.68	123.42	118.30
1	Ba	43	ASP	CB-CG-OD2	5.68	123.42	118.30
1	Bk	43	ASP	CB-CG-OD2	5.68	123.42	118.30
1	Bz	43	ASP	CB-CG-OD2	5.68	123.42	118.30
1	B1	43	ASP	CB-CG-OD2	5.68	123.42	118.30
1	C9	43	ASP	CB-CG-OD2	5.68	123.42	118.30
1	DA	43	ASP	CB-CG-OD2	5.68	123.42	118.30
1	EY	43	ASP	CB-CG-OD2	5.68	123.42	118.30
1	Es	43	ASP	CB-CG-OD2	5.68	123.42	118.30
1	Au	43	ASP	CB-CG-OD2	5.68	123.41	118.30
1	A0	43	ASP	CB-CG-OD2	5.68	123.41	118.30
1	BG	43	ASP	CB-CG-OD2	5.68	123.42	118.30
1	BQ	43	ASP	CB-CG-OD2	5.68	123.41	118.30
1	Bf	43	ASP	CB-CG-OD2	5.68	123.41	118.30
1	Bu	43	ASP	CB-CG-OD2	5.68	123.41	118.30
1	Ds	43	ASP	CB-CG-OD2	5.68	123.41	118.30
1	EA	43	ASP	CB-CG-OD2	5.68	123.41	118.30
1	Do	43	ASP	CB-CG-OD2	5.68	123.41	118.30
1	Da	43	ASP	CB-CG-OD2	5.68	123.41	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Dk	43	ASP	CB-CG-OD2	5.68	123.41	118.30
1	D1	43	ASP	CB-CG-OD2	5.68	123.41	118.30
1	BE	43	ASP	CB-CG-OD2	5.68	123.41	118.30
1	Bc	43	ASP	CB-CG-OD2	5.68	123.41	118.30
1	Dc	43	ASP	CB-CG-OD2	5.68	123.41	118.30
1	EC	43	ASP	CB-CG-OD2	5.67	123.41	118.30
1	EK	43	ASP	CB-CG-OD2	5.67	123.41	118.30
1	FU	43	ASP	CB-CG-OD2	5.67	123.41	118.30
1	Fc	43	ASP	CB-CG-OD2	5.67	123.41	118.30
1	Fm	43	ASP	CB-CG-OD2	5.67	123.41	118.30
1	FK	43	ASP	CB-CG-OD2	5.67	123.41	118.30
1	BL	43	ASP	CB-CG-OD2	5.67	123.41	118.30
1	Du	43	ASP	CB-CG-OD2	5.67	123.41	118.30
1	Ec	43	ASP	CB-CG-OD2	5.67	123.41	118.30
1	E3	43	ASP	CB-CG-OD2	5.67	123.40	118.30
1	Bo	43	ASP	CB-CG-OD2	5.67	123.40	118.30
1	Be	43	ASP	CB-CG-OD2	5.67	123.40	118.30
1	Di	43	ASP	CB-CG-OD2	5.67	123.40	118.30
1	Ax	43	ASP	CB-CG-OD2	5.67	123.40	118.30
1	BT	43	ASP	CB-CG-OD2	5.67	123.40	118.30
1	De	43	ASP	CB-CG-OD2	5.66	123.40	118.30
1	Ee	43	ASP	CB-CG-OD2	5.66	123.40	118.30
1	DM	43	ASP	CB-CG-OD2	5.66	123.40	118.30
1	D7	43	ASP	CB-CG-OD2	5.66	123.40	118.30
1	Ay	43	ASP	CB-CG-OD2	5.66	123.39	118.30
1	BU	43	ASP	CB-CG-OD2	5.66	123.39	118.30
1	Br	43	ASP	CB-CG-OD2	5.66	123.39	118.30
1	DG	43	ASP	CB-CG-OD2	5.66	123.39	118.30
1	FS	43	ASP	CB-CG-OD2	5.66	123.39	118.30
1	BP	43	ASP	CB-CG-OD2	5.66	123.39	118.30
1	D5	43	ASP	CB-CG-OD2	5.66	123.39	118.30
1	EU	43	ASP	CB-CG-OD2	5.66	123.39	118.30
1	FW	43	ASP	CB-CG-OD2	5.66	123.39	118.30
1	BC	43	ASP	CB-CG-OD2	5.66	123.39	118.30
1	BZ	43	ASP	CB-CG-OD2	5.66	123.39	118.30
1	Bi	43	ASP	CB-CG-OD2	5.66	123.39	118.30
1	A6	43	ASP	CB-CG-OD2	5.66	123.39	118.30
1	DE	43	ASP	CB-CG-OD2	5.66	123.39	118.30
1	FI	43	ASP	CB-CG-OD2	5.66	123.39	118.30
1	Fa	43	ASP	CB-CG-OD2	5.66	123.39	118.30
1	Az	43	ASP	CB-CG-OD2	5.65	123.39	118.30
1	DC	43	ASP	CB-CG-OD2	5.65	123.39	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	BF	43	ASP	CB-CG-OD2	5.65	123.39	118.30
1	Eo	43	ASP	CB-CG-OD2	5.65	123.39	118.30
1	Dw	43	ASP	CB-CG-OD2	5.65	123.39	118.30
1	Ei	43	ASP	CB-CG-OD2	5.65	123.39	118.30
1	FO	43	ASP	CB-CG-OD2	5.65	123.39	118.30
1	Ea	43	ASP	CB-CG-OD2	5.65	123.38	118.30
1	E9	43	ASP	CB-CG-OD2	5.65	123.38	118.30
1	A2	43	ASP	CB-CG-OD2	5.65	123.38	118.30
1	EM	43	ASP	CB-CG-OD2	5.65	123.38	118.30
1	Eg	43	ASP	CB-CG-OD2	5.65	123.38	118.30
1	Bq	43	ASP	CB-CG-OD2	5.65	123.38	118.30
1	Eq	43	ASP	CB-CG-OD2	5.64	123.38	118.30
1	BD	43	ASP	CB-CG-OD2	5.64	123.38	118.30
1	By	43	ASP	CB-CG-OD2	5.64	123.38	118.30
1	Dg	43	ASP	CB-CG-OD2	5.64	123.38	118.30
1	EQ	43	ASP	CB-CG-OD2	5.64	123.38	118.30
1	Fg	43	ASP	CB-CG-OD2	5.64	123.38	118.30
1	BX	43	ASP	CB-CG-OD2	5.64	123.37	118.30
1	BR	43	ASP	CB-CG-OD2	5.63	123.37	118.30
1	A9	43	ASP	CB-CG-OD2	5.63	123.37	118.30
1	Dm	43	ASP	CB-CG-OD2	5.63	123.37	118.30
1	EG	43	ASP	CB-CG-OD2	5.63	123.37	118.30
1	E1	43	ASP	CB-CG-OD2	5.63	123.37	118.30
1	D3	43	ASP	CB-CG-OD2	5.63	123.36	118.30
1	BV	43	ASP	CB-CG-OD2	5.62	123.36	118.30
1	BN	43	ASP	CB-CG-OD2	5.61	123.35	118.30
1	E5	43	ASP	CB-CG-OD2	5.60	123.34	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A0	147/174 (84%)	139 (95%)	8 (5%)	0	100	100
1	A1	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	A2	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	A3	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	A4	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	A5	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	A6	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	A7	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	A8	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	A9	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	Au	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	Av	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	Aw	147/174 (84%)	139 (95%)	8 (5%)	0	100	100
1	Ax	147/174 (84%)	139 (95%)	8 (5%)	0	100	100
1	Ay	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	Az	147/174 (84%)	139 (95%)	8 (5%)	0	100	100
1	B1	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	BA	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	BB	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	BC	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	BD	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	BE	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	BF	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	BG	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	BH	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	BI	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	BJ	147/174 (84%)	139 (95%)	8 (5%)	0	100	100
1	BK	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	BL	147/174 (84%)	140 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BM	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	BN	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	BO	147/174 (84%)	139 (95%)	8 (5%)	0	100	100
1	BP	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	BQ	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	BR	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	BS	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	BT	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	BU	147/174 (84%)	139 (95%)	8 (5%)	0	100	100
1	BV	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	BW	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	BX	147/174 (84%)	139 (95%)	8 (5%)	0	100	100
1	BY	147/174 (84%)	139 (95%)	8 (5%)	0	100	100
1	BZ	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	Ba	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	Bb	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	Bc	147/174 (84%)	139 (95%)	8 (5%)	0	100	100
1	Bd	147/174 (84%)	139 (95%)	8 (5%)	0	100	100
1	Be	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	Bf	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	Bg	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	Bh	147/174 (84%)	139 (95%)	8 (5%)	0	100	100
1	Bi	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	Bj	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	Bk	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	Bl	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	Bm	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	Bn	147/174 (84%)	139 (95%)	8 (5%)	0	100	100
1	Bo	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	Bp	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	Bq	147/174 (84%)	140 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Br	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	Bs	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	Bt	147/174 (84%)	139 (95%)	8 (5%)	0	100	100
1	Bu	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	Bv	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	Bw	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	Bx	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	By	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	Bz	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	C9	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	D1	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	D3	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	D5	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	D7	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	D9	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	DA	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	DC	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	DE	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	DG	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	DI	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	DK	147/174 (84%)	139 (95%)	8 (5%)	0	100	100
1	DM	147/174 (84%)	139 (95%)	8 (5%)	0	100	100
1	DO	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	DQ	147/174 (84%)	139 (95%)	8 (5%)	0	100	100
1	DS	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	DU	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	DW	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	DY	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	Da	147/174 (84%)	139 (95%)	8 (5%)	0	100	100
1	Dc	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	De	147/174 (84%)	140 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Dg	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	Di	147/174 (84%)	139 (95%)	8 (5%)	0	100	100
1	Dk	147/174 (84%)	139 (95%)	8 (5%)	0	100	100
1	Dm	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	Do	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	Dq	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	Ds	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	Du	147/174 (84%)	139 (95%)	8 (5%)	0	100	100
1	Dw	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	Dy	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	E1	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	E3	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	E5	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	E7	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	E9	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	EA	147/174 (84%)	139 (95%)	8 (5%)	0	100	100
1	EC	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	EE	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	EG	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	EI	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	EK	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	EM	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	EO	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	EQ	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	ES	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	EU	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	EW	147/174 (84%)	139 (95%)	8 (5%)	0	100	100
1	EY	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	Ea	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	Ec	147/174 (84%)	139 (95%)	8 (5%)	0	100	100
1	Ee	147/174 (84%)	140 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Eg	147/174 (84%)	139 (95%)	8 (5%)	0	100	100
1	Ei	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	Ek	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	Em	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	Eo	147/174 (84%)	139 (95%)	8 (5%)	0	100	100
1	Eq	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	Es	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	Eu	147/174 (84%)	139 (95%)	8 (5%)	0	100	100
1	Ew	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	Ey	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	FA	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	FC	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	FE	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	FG	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	FI	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	FK	147/174 (84%)	139 (95%)	8 (5%)	0	100	100
1	FM	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	FO	147/174 (84%)	139 (95%)	8 (5%)	0	100	100
1	FQ	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	FS	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	FU	147/174 (84%)	139 (95%)	8 (5%)	0	100	100
1	FW	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	FY	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	Fa	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	Fc	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	Fe	147/174 (84%)	139 (95%)	8 (5%)	0	100	100
1	Fg	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	Fi	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	Fk	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	Fm	147/174 (84%)	140 (95%)	7 (5%)	0	100	100
1	Fo	147/174 (84%)	140 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Fq	147/174 (84%)	139 (95%)	8 (5%)	0	100	100
All	All	22638/26796 (84%)	21528 (95%)	1110 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A0	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	A1	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	A2	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	A3	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	A4	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	A5	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	A6	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	A7	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	A8	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	A9	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Au	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Av	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Aw	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Ax	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Ay	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Az	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	B1	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	BA	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	BB	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	BC	129/143 (90%)	123 (95%)	6 (5%)	22	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BD	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	BE	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	BF	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	BG	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	BH	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	BI	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	BJ	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	BK	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	BL	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	BM	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	BN	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	BO	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	BP	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	BQ	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	BR	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	BS	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	BT	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	BU	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	BV	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	BW	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	BX	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	BY	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	BZ	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Ba	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Bb	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Bc	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Bd	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Be	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Bf	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Bg	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Bh	129/143 (90%)	123 (95%)	6 (5%)	22	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Bi	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Bj	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Bk	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Bl	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Bm	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Bn	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Bo	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Bp	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Bq	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Br	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Bs	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Bt	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Bu	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Bv	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Bw	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Bx	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	By	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Bz	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	C9	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	D1	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	D3	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	D5	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	D7	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	D9	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	DA	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	DC	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	DE	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	DG	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	DI	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	DK	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	DM	129/143 (90%)	123 (95%)	6 (5%)	22	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	DO	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	DQ	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	DS	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	DU	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	DW	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	DY	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Da	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Dc	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	De	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Dg	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Di	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Dk	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Dm	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Do	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Dq	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Ds	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Du	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Dw	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Dy	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	E1	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	E3	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	E5	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	E7	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	E9	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	EA	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	EC	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	EE	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	EG	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	EI	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	EK	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	EM	129/143 (90%)	123 (95%)	6 (5%)	22	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	EO	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	EQ	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	ES	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	EU	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	EW	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	EY	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Ea	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Ec	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Ee	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Eg	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Ei	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Ek	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Em	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Eo	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Eq	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Es	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Eu	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Ew	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Ey	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	FA	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	FC	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	FE	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	FG	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	FI	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	FK	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	FM	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	FO	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	FQ	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	FS	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	FU	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	FW	129/143 (90%)	123 (95%)	6 (5%)	22	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	FY	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Fa	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Fc	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Fe	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Fg	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Fi	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Fk	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Fm	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Fo	129/143 (90%)	123 (95%)	6 (5%)	22	32
1	Fq	129/143 (90%)	123 (95%)	6 (5%)	22	32
All	All	19866/22022 (90%)	18942 (95%)	924 (5%)	24	32

All (924) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Au	42	LYS
1	Au	43	ASP
1	Au	48	LYS
1	Au	117	LYS
1	Au	121	LYS
1	Au	132	MET
1	Av	42	LYS
1	Av	43	ASP
1	Av	48	LYS
1	Av	117	LYS
1	Av	121	LYS
1	Av	132	MET
1	Aw	42	LYS
1	Aw	43	ASP
1	Aw	48	LYS
1	Aw	117	LYS
1	Aw	121	LYS
1	Aw	132	MET
1	Ax	42	LYS
1	Ax	43	ASP
1	Ax	48	LYS
1	Ax	117	LYS
1	Ax	121	LYS

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Mol	Chain	Res	Type
1	Ax	132	MET
1	Ay	42	LYS
1	Ay	43	ASP
1	Ay	48	LYS
1	Ay	117	LYS
1	Ay	121	LYS
1	Ay	132	MET
1	Az	42	LYS
1	Az	43	ASP
1	Az	48	LYS
1	Az	117	LYS
1	Az	121	LYS
1	Az	132	MET
1	A1	42	LYS
1	A1	43	ASP
1	A1	48	LYS
1	A1	117	LYS
1	A1	121	LYS
1	A1	132	MET
1	A2	42	LYS
1	A2	43	ASP
1	A2	48	LYS
1	A2	117	LYS
1	A2	121	LYS
1	A2	132	MET
1	A3	42	LYS
1	A3	43	ASP
1	A3	48	LYS
1	A3	117	LYS
1	A3	121	LYS
1	A3	132	MET
1	A4	42	LYS
1	A4	43	ASP
1	A4	48	LYS
1	A4	117	LYS
1	A4	121	LYS
1	A4	132	MET
1	A5	42	LYS
1	A5	43	ASP
1	A5	48	LYS
1	A5	117	LYS
1	A5	121	LYS

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Mol	Chain	Res	Type
1	A5	132	MET
1	A6	42	LYS
1	A6	43	ASP
1	A6	48	LYS
1	A6	117	LYS
1	A6	121	LYS
1	A6	132	MET
1	A7	42	LYS
1	A7	43	ASP
1	A7	48	LYS
1	A7	117	LYS
1	A7	121	LYS
1	A7	132	MET
1	A8	42	LYS
1	A8	43	ASP
1	A8	48	LYS
1	A8	117	LYS
1	A8	121	LYS
1	A8	132	MET
1	A9	42	LYS
1	A9	43	ASP
1	A9	48	LYS
1	A9	117	LYS
1	A9	121	LYS
1	A9	132	MET
1	A0	42	LYS
1	A0	43	ASP
1	A0	48	LYS
1	A0	117	LYS
1	A0	121	LYS
1	A0	132	MET
1	BA	42	LYS
1	BA	43	ASP
1	BA	48	LYS
1	BA	117	LYS
1	BA	121	LYS
1	BA	132	MET
1	BB	42	LYS
1	BB	43	ASP
1	BB	48	LYS
1	BB	117	LYS
1	BB	121	LYS

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Mol	Chain	Res	Type
1	BB	132	MET
1	BC	42	LYS
1	BC	43	ASP
1	BC	48	LYS
1	BC	117	LYS
1	BC	121	LYS
1	BC	132	MET
1	BD	42	LYS
1	BD	43	ASP
1	BD	48	LYS
1	BD	117	LYS
1	BD	121	LYS
1	BD	132	MET
1	BE	42	LYS
1	BE	43	ASP
1	BE	48	LYS
1	BE	117	LYS
1	BE	121	LYS
1	BE	132	MET
1	BF	42	LYS
1	BF	43	ASP
1	BF	48	LYS
1	BF	117	LYS
1	BF	121	LYS
1	BF	132	MET
1	BG	42	LYS
1	BG	43	ASP
1	BG	48	LYS
1	BG	117	LYS
1	BG	121	LYS
1	BG	132	MET
1	BH	42	LYS
1	BH	43	ASP
1	BH	48	LYS
1	BH	117	LYS
1	BH	121	LYS
1	BH	132	MET
1	BI	42	LYS
1	BI	43	ASP
1	BI	48	LYS
1	BI	117	LYS
1	BI	121	LYS

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Mol	Chain	Res	Type
1	BI	132	MET
1	BJ	42	LYS
1	BJ	43	ASP
1	BJ	48	LYS
1	BJ	117	LYS
1	BJ	121	LYS
1	BJ	132	MET
1	BK	42	LYS
1	BK	43	ASP
1	BK	48	LYS
1	BK	117	LYS
1	BK	121	LYS
1	BK	132	MET
1	BL	42	LYS
1	BL	43	ASP
1	BL	48	LYS
1	BL	117	LYS
1	BL	121	LYS
1	BL	132	MET
1	BM	42	LYS
1	BM	43	ASP
1	BM	48	LYS
1	BM	117	LYS
1	BM	121	LYS
1	BM	132	MET
1	BN	42	LYS
1	BN	43	ASP
1	BN	48	LYS
1	BN	117	LYS
1	BN	121	LYS
1	BN	132	MET
1	BO	42	LYS
1	BO	43	ASP
1	BO	48	LYS
1	BO	117	LYS
1	BO	121	LYS
1	BO	132	MET
1	BP	42	LYS
1	BP	43	ASP
1	BP	48	LYS
1	BP	117	LYS
1	BP	121	LYS

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Mol	Chain	Res	Type
1	BP	132	MET
1	BQ	42	LYS
1	BQ	43	ASP
1	BQ	48	LYS
1	BQ	117	LYS
1	BQ	121	LYS
1	BQ	132	MET
1	BR	42	LYS
1	BR	43	ASP
1	BR	48	LYS
1	BR	117	LYS
1	BR	121	LYS
1	BR	132	MET
1	BS	42	LYS
1	BS	43	ASP
1	BS	48	LYS
1	BS	117	LYS
1	BS	121	LYS
1	BS	132	MET
1	BT	42	LYS
1	BT	43	ASP
1	BT	48	LYS
1	BT	117	LYS
1	BT	121	LYS
1	BT	132	MET
1	BU	42	LYS
1	BU	43	ASP
1	BU	48	LYS
1	BU	117	LYS
1	BU	121	LYS
1	BU	132	MET
1	BV	42	LYS
1	BV	43	ASP
1	BV	48	LYS
1	BV	117	LYS
1	BV	121	LYS
1	BV	132	MET
1	BW	42	LYS
1	BW	43	ASP
1	BW	48	LYS
1	BW	117	LYS
1	BW	121	LYS

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Mol	Chain	Res	Type
1	BW	132	MET
1	BX	42	LYS
1	BX	43	ASP
1	BX	48	LYS
1	BX	117	LYS
1	BX	121	LYS
1	BX	132	MET
1	BY	42	LYS
1	BY	43	ASP
1	BY	48	LYS
1	BY	117	LYS
1	BY	121	LYS
1	BY	132	MET
1	BZ	42	LYS
1	BZ	43	ASP
1	BZ	48	LYS
1	BZ	117	LYS
1	BZ	121	LYS
1	BZ	132	MET
1	Ba	42	LYS
1	Ba	43	ASP
1	Ba	48	LYS
1	Ba	117	LYS
1	Ba	121	LYS
1	Ba	132	MET
1	Bb	42	LYS
1	Bb	43	ASP
1	Bb	48	LYS
1	Bb	117	LYS
1	Bb	121	LYS
1	Bb	132	MET
1	Bc	42	LYS
1	Bc	43	ASP
1	Bc	48	LYS
1	Bc	117	LYS
1	Bc	121	LYS
1	Bc	132	MET
1	Bd	42	LYS
1	Bd	43	ASP
1	Bd	48	LYS
1	Bd	117	LYS
1	Bd	121	LYS

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Mol	Chain	Res	Type
1	Bd	132	MET
1	Be	42	LYS
1	Be	43	ASP
1	Be	48	LYS
1	Be	117	LYS
1	Be	121	LYS
1	Be	132	MET
1	Bf	42	LYS
1	Bf	43	ASP
1	Bf	48	LYS
1	Bf	117	LYS
1	Bf	121	LYS
1	Bf	132	MET
1	Bg	42	LYS
1	Bg	43	ASP
1	Bg	48	LYS
1	Bg	117	LYS
1	Bg	121	LYS
1	Bg	132	MET
1	Bh	42	LYS
1	Bh	43	ASP
1	Bh	48	LYS
1	Bh	117	LYS
1	Bh	121	LYS
1	Bh	132	MET
1	Bi	42	LYS
1	Bi	43	ASP
1	Bi	48	LYS
1	Bi	117	LYS
1	Bi	121	LYS
1	Bi	132	MET
1	Bj	42	LYS
1	Bj	43	ASP
1	Bj	48	LYS
1	Bj	117	LYS
1	Bj	121	LYS
1	Bj	132	MET
1	Bk	42	LYS
1	Bk	43	ASP
1	Bk	48	LYS
1	Bk	117	LYS
1	Bk	121	LYS

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Mol	Chain	Res	Type
1	Bk	132	MET
1	Bl	42	LYS
1	Bl	43	ASP
1	Bl	48	LYS
1	Bl	117	LYS
1	Bl	121	LYS
1	Bl	132	MET
1	Bm	42	LYS
1	Bm	43	ASP
1	Bm	48	LYS
1	Bm	117	LYS
1	Bm	121	LYS
1	Bm	132	MET
1	Bn	42	LYS
1	Bn	43	ASP
1	Bn	48	LYS
1	Bn	117	LYS
1	Bn	121	LYS
1	Bn	132	MET
1	Bo	42	LYS
1	Bo	43	ASP
1	Bo	48	LYS
1	Bo	117	LYS
1	Bo	121	LYS
1	Bo	132	MET
1	Bp	42	LYS
1	Bp	43	ASP
1	Bp	48	LYS
1	Bp	117	LYS
1	Bp	121	LYS
1	Bp	132	MET
1	Bq	42	LYS
1	Bq	43	ASP
1	Bq	48	LYS
1	Bq	117	LYS
1	Bq	121	LYS
1	Bq	132	MET
1	Br	42	LYS
1	Br	43	ASP
1	Br	48	LYS
1	Br	117	LYS
1	Br	121	LYS

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Mol	Chain	Res	Type
1	Br	132	MET
1	Bs	42	LYS
1	Bs	43	ASP
1	Bs	48	LYS
1	Bs	117	LYS
1	Bs	121	LYS
1	Bs	132	MET
1	Bt	42	LYS
1	Bt	43	ASP
1	Bt	48	LYS
1	Bt	117	LYS
1	Bt	121	LYS
1	Bt	132	MET
1	Bu	42	LYS
1	Bu	43	ASP
1	Bu	48	LYS
1	Bu	117	LYS
1	Bu	121	LYS
1	Bu	132	MET
1	Bv	42	LYS
1	Bv	43	ASP
1	Bv	48	LYS
1	Bv	117	LYS
1	Bv	121	LYS
1	Bv	132	MET
1	Bw	42	LYS
1	Bw	43	ASP
1	Bw	48	LYS
1	Bw	117	LYS
1	Bw	121	LYS
1	Bw	132	MET
1	Bx	42	LYS
1	Bx	43	ASP
1	Bx	48	LYS
1	Bx	117	LYS
1	Bx	121	LYS
1	Bx	132	MET
1	By	42	LYS
1	By	43	ASP
1	By	48	LYS
1	By	117	LYS
1	By	121	LYS

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Mol	Chain	Res	Type
1	By	132	MET
1	Bz	42	LYS
1	Bz	43	ASP
1	Bz	48	LYS
1	Bz	117	LYS
1	Bz	121	LYS
1	Bz	132	MET
1	B1	42	LYS
1	B1	43	ASP
1	B1	48	LYS
1	B1	117	LYS
1	B1	121	LYS
1	B1	132	MET
1	C9	42	LYS
1	C9	43	ASP
1	C9	48	LYS
1	C9	117	LYS
1	C9	121	LYS
1	C9	132	MET
1	DA	42	LYS
1	DA	43	ASP
1	DA	48	LYS
1	DA	117	LYS
1	DA	121	LYS
1	DA	132	MET
1	DC	42	LYS
1	DC	43	ASP
1	DC	48	LYS
1	DC	117	LYS
1	DC	121	LYS
1	DC	132	MET
1	DE	42	LYS
1	DE	43	ASP
1	DE	48	LYS
1	DE	117	LYS
1	DE	121	LYS
1	DE	132	MET
1	DG	42	LYS
1	DG	43	ASP
1	DG	48	LYS
1	DG	117	LYS
1	DG	121	LYS

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Mol	Chain	Res	Type
1	DG	132	MET
1	DI	42	LYS
1	DI	43	ASP
1	DI	48	LYS
1	DI	117	LYS
1	DI	121	LYS
1	DI	132	MET
1	DK	42	LYS
1	DK	43	ASP
1	DK	48	LYS
1	DK	117	LYS
1	DK	121	LYS
1	DK	132	MET
1	DM	42	LYS
1	DM	43	ASP
1	DM	48	LYS
1	DM	117	LYS
1	DM	121	LYS
1	DM	132	MET
1	DO	42	LYS
1	DO	43	ASP
1	DO	48	LYS
1	DO	117	LYS
1	DO	121	LYS
1	DO	132	MET
1	DQ	42	LYS
1	DQ	43	ASP
1	DQ	48	LYS
1	DQ	117	LYS
1	DQ	121	LYS
1	DQ	132	MET
1	DS	42	LYS
1	DS	43	ASP
1	DS	48	LYS
1	DS	117	LYS
1	DS	121	LYS
1	DS	132	MET
1	DU	42	LYS
1	DU	43	ASP
1	DU	48	LYS
1	DU	117	LYS
1	DU	121	LYS

Continued on next page...

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Mol	Chain	Res	Type
1	DU	132	MET
1	DW	42	LYS
1	DW	43	ASP
1	DW	48	LYS
1	DW	117	LYS
1	DW	121	LYS
1	DW	132	MET
1	DY	42	LYS
1	DY	43	ASP
1	DY	48	LYS
1	DY	117	LYS
1	DY	121	LYS
1	DY	132	MET
1	Da	42	LYS
1	Da	43	ASP
1	Da	48	LYS
1	Da	117	LYS
1	Da	121	LYS
1	Da	132	MET
1	Dc	42	LYS
1	Dc	43	ASP
1	Dc	48	LYS
1	Dc	117	LYS
1	Dc	121	LYS
1	Dc	132	MET
1	De	42	LYS
1	De	43	ASP
1	De	48	LYS
1	De	117	LYS
1	De	121	LYS
1	De	132	MET
1	Dg	42	LYS
1	Dg	43	ASP
1	Dg	48	LYS
1	Dg	117	LYS
1	Dg	121	LYS
1	Dg	132	MET
1	Di	42	LYS
1	Di	43	ASP
1	Di	48	LYS
1	Di	117	LYS
1	Di	121	LYS

Continued on next page...

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Mol	Chain	Res	Type
1	Di	132	MET
1	Dk	42	LYS
1	Dk	43	ASP
1	Dk	48	LYS
1	Dk	117	LYS
1	Dk	121	LYS
1	Dk	132	MET
1	Dm	42	LYS
1	Dm	43	ASP
1	Dm	48	LYS
1	Dm	117	LYS
1	Dm	121	LYS
1	Dm	132	MET
1	Do	42	LYS
1	Do	43	ASP
1	Do	48	LYS
1	Do	117	LYS
1	Do	121	LYS
1	Do	132	MET
1	Dq	42	LYS
1	Dq	43	ASP
1	Dq	48	LYS
1	Dq	117	LYS
1	Dq	121	LYS
1	Dq	132	MET
1	Ds	42	LYS
1	Ds	43	ASP
1	Ds	48	LYS
1	Ds	117	LYS
1	Ds	121	LYS
1	Ds	132	MET
1	Du	42	LYS
1	Du	43	ASP
1	Du	48	LYS
1	Du	117	LYS
1	Du	121	LYS
1	Du	132	MET
1	Dw	42	LYS
1	Dw	43	ASP
1	Dw	48	LYS
1	Dw	117	LYS
1	Dw	121	LYS

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Mol	Chain	Res	Type
1	Dw	132	MET
1	Dy	42	LYS
1	Dy	43	ASP
1	Dy	48	LYS
1	Dy	117	LYS
1	Dy	121	LYS
1	Dy	132	MET
1	D1	42	LYS
1	D1	43	ASP
1	D1	48	LYS
1	D1	117	LYS
1	D1	121	LYS
1	D1	132	MET
1	D3	42	LYS
1	D3	43	ASP
1	D3	48	LYS
1	D3	117	LYS
1	D3	121	LYS
1	D3	132	MET
1	D5	42	LYS
1	D5	43	ASP
1	D5	48	LYS
1	D5	117	LYS
1	D5	121	LYS
1	D5	132	MET
1	D7	42	LYS
1	D7	43	ASP
1	D7	48	LYS
1	D7	117	LYS
1	D7	121	LYS
1	D7	132	MET
1	D9	42	LYS
1	D9	43	ASP
1	D9	48	LYS
1	D9	117	LYS
1	D9	121	LYS
1	D9	132	MET
1	EA	42	LYS
1	EA	43	ASP
1	EA	48	LYS
1	EA	117	LYS
1	EA	121	LYS

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Mol	Chain	Res	Type
1	EA	132	MET
1	EC	42	LYS
1	EC	43	ASP
1	EC	48	LYS
1	EC	117	LYS
1	EC	121	LYS
1	EC	132	MET
1	EE	42	LYS
1	EE	43	ASP
1	EE	48	LYS
1	EE	117	LYS
1	EE	121	LYS
1	EE	132	MET
1	EG	42	LYS
1	EG	43	ASP
1	EG	48	LYS
1	EG	117	LYS
1	EG	121	LYS
1	EG	132	MET
1	EI	42	LYS
1	EI	43	ASP
1	EI	48	LYS
1	EI	117	LYS
1	EI	121	LYS
1	EI	132	MET
1	EK	42	LYS
1	EK	43	ASP
1	EK	48	LYS
1	EK	117	LYS
1	EK	121	LYS
1	EK	132	MET
1	EM	42	LYS
1	EM	43	ASP
1	EM	48	LYS
1	EM	117	LYS
1	EM	121	LYS
1	EM	132	MET
1	EO	42	LYS
1	EO	43	ASP
1	EO	48	LYS
1	EO	117	LYS
1	EO	121	LYS

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Mol	Chain	Res	Type
1	EO	132	MET
1	EQ	42	LYS
1	EQ	43	ASP
1	EQ	48	LYS
1	EQ	117	LYS
1	EQ	121	LYS
1	EQ	132	MET
1	ES	42	LYS
1	ES	43	ASP
1	ES	48	LYS
1	ES	117	LYS
1	ES	121	LYS
1	ES	132	MET
1	EU	42	LYS
1	EU	43	ASP
1	EU	48	LYS
1	EU	117	LYS
1	EU	121	LYS
1	EU	132	MET
1	EW	42	LYS
1	EW	43	ASP
1	EW	48	LYS
1	EW	117	LYS
1	EW	121	LYS
1	EW	132	MET
1	EY	42	LYS
1	EY	43	ASP
1	EY	48	LYS
1	EY	117	LYS
1	EY	121	LYS
1	EY	132	MET
1	Ea	42	LYS
1	Ea	43	ASP
1	Ea	48	LYS
1	Ea	117	LYS
1	Ea	121	LYS
1	Ea	132	MET
1	Ec	42	LYS
1	Ec	43	ASP
1	Ec	48	LYS
1	Ec	117	LYS
1	Ec	121	LYS

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Mol	Chain	Res	Type
1	Ec	132	MET
1	Ee	42	LYS
1	Ee	43	ASP
1	Ee	48	LYS
1	Ee	117	LYS
1	Ee	121	LYS
1	Ee	132	MET
1	Eg	42	LYS
1	Eg	43	ASP
1	Eg	48	LYS
1	Eg	117	LYS
1	Eg	121	LYS
1	Eg	132	MET
1	Ei	42	LYS
1	Ei	43	ASP
1	Ei	48	LYS
1	Ei	117	LYS
1	Ei	121	LYS
1	Ei	132	MET
1	Ek	42	LYS
1	Ek	43	ASP
1	Ek	48	LYS
1	Ek	117	LYS
1	Ek	121	LYS
1	Ek	132	MET
1	Em	42	LYS
1	Em	43	ASP
1	Em	48	LYS
1	Em	117	LYS
1	Em	121	LYS
1	Em	132	MET
1	Eo	42	LYS
1	Eo	43	ASP
1	Eo	48	LYS
1	Eo	117	LYS
1	Eo	121	LYS
1	Eo	132	MET
1	Eq	42	LYS
1	Eq	43	ASP
1	Eq	48	LYS
1	Eq	117	LYS
1	Eq	121	LYS

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Mol	Chain	Res	Type
1	Eq	132	MET
1	Es	42	LYS
1	Es	43	ASP
1	Es	48	LYS
1	Es	117	LYS
1	Es	121	LYS
1	Es	132	MET
1	Eu	42	LYS
1	Eu	43	ASP
1	Eu	48	LYS
1	Eu	117	LYS
1	Eu	121	LYS
1	Eu	132	MET
1	Ew	42	LYS
1	Ew	43	ASP
1	Ew	48	LYS
1	Ew	117	LYS
1	Ew	121	LYS
1	Ew	132	MET
1	Ey	42	LYS
1	Ey	43	ASP
1	Ey	48	LYS
1	Ey	117	LYS
1	Ey	121	LYS
1	Ey	132	MET
1	E1	42	LYS
1	E1	43	ASP
1	E1	48	LYS
1	E1	117	LYS
1	E1	121	LYS
1	E1	132	MET
1	E3	42	LYS
1	E3	43	ASP
1	E3	48	LYS
1	E3	117	LYS
1	E3	121	LYS
1	E3	132	MET
1	E5	42	LYS
1	E5	43	ASP
1	E5	48	LYS
1	E5	117	LYS
1	E5	121	LYS

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Mol	Chain	Res	Type
1	E5	132	MET
1	E7	42	LYS
1	E7	43	ASP
1	E7	48	LYS
1	E7	117	LYS
1	E7	121	LYS
1	E7	132	MET
1	E9	42	LYS
1	E9	43	ASP
1	E9	48	LYS
1	E9	117	LYS
1	E9	121	LYS
1	E9	132	MET
1	FA	42	LYS
1	FA	43	ASP
1	FA	48	LYS
1	FA	117	LYS
1	FA	121	LYS
1	FA	132	MET
1	FC	42	LYS
1	FC	43	ASP
1	FC	48	LYS
1	FC	117	LYS
1	FC	121	LYS
1	FC	132	MET
1	FE	42	LYS
1	FE	43	ASP
1	FE	48	LYS
1	FE	117	LYS
1	FE	121	LYS
1	FE	132	MET
1	FG	42	LYS
1	FG	43	ASP
1	FG	48	LYS
1	FG	117	LYS
1	FG	121	LYS
1	FG	132	MET
1	FI	42	LYS
1	FI	43	ASP
1	FI	48	LYS
1	FI	117	LYS
1	FI	121	LYS

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Mol	Chain	Res	Type
1	FI	132	MET
1	FK	42	LYS
1	FK	43	ASP
1	FK	48	LYS
1	FK	117	LYS
1	FK	121	LYS
1	FK	132	MET
1	FM	42	LYS
1	FM	43	ASP
1	FM	48	LYS
1	FM	117	LYS
1	FM	121	LYS
1	FM	132	MET
1	FO	42	LYS
1	FO	43	ASP
1	FO	48	LYS
1	FO	117	LYS
1	FO	121	LYS
1	FO	132	MET
1	FQ	42	LYS
1	FQ	43	ASP
1	FQ	48	LYS
1	FQ	117	LYS
1	FQ	121	LYS
1	FQ	132	MET
1	FS	42	LYS
1	FS	43	ASP
1	FS	48	LYS
1	FS	117	LYS
1	FS	121	LYS
1	FS	132	MET
1	FU	42	LYS
1	FU	43	ASP
1	FU	48	LYS
1	FU	117	LYS
1	FU	121	LYS
1	FU	132	MET
1	FW	42	LYS
1	FW	43	ASP
1	FW	48	LYS
1	FW	117	LYS
1	FW	121	LYS

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Mol	Chain	Res	Type
1	FW	132	MET
1	FY	42	LYS
1	FY	43	ASP
1	FY	48	LYS
1	FY	117	LYS
1	FY	121	LYS
1	FY	132	MET
1	Fa	42	LYS
1	Fa	43	ASP
1	Fa	48	LYS
1	Fa	117	LYS
1	Fa	121	LYS
1	Fa	132	MET
1	Fc	42	LYS
1	Fc	43	ASP
1	Fc	48	LYS
1	Fc	117	LYS
1	Fc	121	LYS
1	Fc	132	MET
1	Fe	42	LYS
1	Fe	43	ASP
1	Fe	48	LYS
1	Fe	117	LYS
1	Fe	121	LYS
1	Fe	132	MET
1	Fg	42	LYS
1	Fg	43	ASP
1	Fg	48	LYS
1	Fg	117	LYS
1	Fg	121	LYS
1	Fg	132	MET
1	Fi	42	LYS
1	Fi	43	ASP
1	Fi	48	LYS
1	Fi	117	LYS
1	Fi	121	LYS
1	Fi	132	MET
1	Fk	42	LYS
1	Fk	43	ASP
1	Fk	48	LYS
1	Fk	117	LYS
1	Fk	121	LYS

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Mol	Chain	Res	Type
1	Fk	132	MET
1	Fm	42	LYS
1	Fm	43	ASP
1	Fm	48	LYS
1	Fm	117	LYS
1	Fm	121	LYS
1	Fm	132	MET
1	Fo	42	LYS
1	Fo	43	ASP
1	Fo	48	LYS
1	Fo	117	LYS
1	Fo	121	LYS
1	Fo	132	MET
1	Fq	42	LYS
1	Fq	43	ASP
1	Fq	48	LYS
1	Fq	117	LYS
1	Fq	121	LYS
1	Fq	132	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (426) such sidechains are listed below:

Mol	Chain	Res	Type
1	Au	3	GLN
1	Au	144	GLN
1	Av	3	GLN
1	Av	144	GLN
1	Aw	3	GLN
1	Aw	84	ASN
1	Aw	144	GLN
1	Ax	3	GLN
1	Ax	144	GLN
1	Ay	3	GLN
1	Ay	144	GLN
1	Az	3	GLN
1	Az	84	ASN
1	Az	144	GLN
1	A1	3	GLN
1	A1	84	ASN
1	A1	144	GLN
1	A2	3	GLN
1	A2	84	ASN

Continued on next page...

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Mol	Chain	Res	Type
1	A2	144	GLN
1	A3	3	GLN
1	A3	84	ASN
1	A3	144	GLN
1	A4	3	GLN
1	A4	84	ASN
1	A4	144	GLN
1	A5	3	GLN
1	A5	84	ASN
1	A5	144	GLN
1	A6	3	GLN
1	A6	144	GLN
1	A7	3	GLN
1	A7	84	ASN
1	A7	144	GLN
1	A8	3	GLN
1	A8	144	GLN
1	A9	3	GLN
1	A9	144	GLN
1	A0	3	GLN
1	A0	84	ASN
1	A0	144	GLN
1	BA	3	GLN
1	BA	84	ASN
1	BA	144	GLN
1	BB	3	GLN
1	BB	84	ASN
1	BB	144	GLN
1	BC	3	GLN
1	BC	84	ASN
1	BC	144	GLN
1	BD	3	GLN
1	BD	84	ASN
1	BD	144	GLN
1	BE	3	GLN
1	BE	84	ASN
1	BE	144	GLN
1	BF	3	GLN
1	BF	84	ASN
1	BF	144	GLN
1	BG	3	GLN
1	BG	84	ASN

Continued on next page...

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Mol	Chain	Res	Type
1	BG	144	GLN
1	BH	3	GLN
1	BH	84	ASN
1	BH	144	GLN
1	BI	3	GLN
1	BI	144	GLN
1	BJ	3	GLN
1	BJ	84	ASN
1	BJ	144	GLN
1	BK	3	GLN
1	BK	84	ASN
1	BK	144	GLN
1	BL	3	GLN
1	BL	84	ASN
1	BL	144	GLN
1	BM	3	GLN
1	BM	84	ASN
1	BM	144	GLN
1	BN	3	GLN
1	BN	84	ASN
1	BN	144	GLN
1	BO	3	GLN
1	BO	144	GLN
1	BP	3	GLN
1	BP	144	GLN
1	BQ	3	GLN
1	BQ	84	ASN
1	BQ	144	GLN
1	BR	3	GLN
1	BR	84	ASN
1	BR	144	GLN
1	BS	3	GLN
1	BS	84	ASN
1	BS	144	GLN
1	BT	3	GLN
1	BT	84	ASN
1	BT	144	GLN
1	BU	3	GLN
1	BU	84	ASN
1	BU	144	GLN
1	BV	3	GLN
1	BV	84	ASN

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Mol	Chain	Res	Type
1	BV	144	GLN
1	BW	3	GLN
1	BW	84	ASN
1	BW	144	GLN
1	BX	3	GLN
1	BX	84	ASN
1	BX	144	GLN
1	BY	3	GLN
1	BY	84	ASN
1	BY	144	GLN
1	BZ	3	GLN
1	BZ	144	GLN
1	Ba	3	GLN
1	Ba	84	ASN
1	Ba	144	GLN
1	Bb	3	GLN
1	Bb	84	ASN
1	Bb	144	GLN
1	Bc	3	GLN
1	Bc	84	ASN
1	Bc	144	GLN
1	Bd	3	GLN
1	Bd	84	ASN
1	Bd	144	GLN
1	Be	3	GLN
1	Be	84	ASN
1	Be	144	GLN
1	Bf	3	GLN
1	Bf	144	GLN
1	Bg	3	GLN
1	Bg	144	GLN
1	Bh	3	GLN
1	Bh	84	ASN
1	Bh	144	GLN
1	Bi	3	GLN
1	Bi	84	ASN
1	Bi	144	GLN
1	Bj	3	GLN
1	Bj	84	ASN
1	Bj	144	GLN
1	Bk	3	GLN
1	Bk	84	ASN

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Mol	Chain	Res	Type
1	Bk	144	GLN
1	Bl	3	GLN
1	Bl	84	ASN
1	Bl	144	GLN
1	Bm	3	GLN
1	Bm	84	ASN
1	Bm	144	GLN
1	Bn	3	GLN
1	Bn	84	ASN
1	Bn	144	GLN
1	Bo	3	GLN
1	Bo	84	ASN
1	Bo	144	GLN
1	Bp	3	GLN
1	Bp	84	ASN
1	Bp	144	GLN
1	Bq	3	GLN
1	Bq	144	GLN
1	Br	3	GLN
1	Br	144	GLN
1	Bs	3	GLN
1	Bs	84	ASN
1	Bs	144	GLN
1	Bt	3	GLN
1	Bt	144	GLN
1	Bu	3	GLN
1	Bu	144	GLN
1	Bv	3	GLN
1	Bv	84	ASN
1	Bv	144	GLN
1	Bw	3	GLN
1	Bw	84	ASN
1	Bw	144	GLN
1	Bx	3	GLN
1	Bx	84	ASN
1	Bx	144	GLN
1	By	3	GLN
1	By	84	ASN
1	By	144	GLN
1	Bz	3	GLN
1	Bz	84	ASN
1	Bz	144	GLN

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Mol	Chain	Res	Type
1	B1	3	GLN
1	B1	84	ASN
1	B1	144	GLN
1	C9	3	GLN
1	C9	84	ASN
1	C9	144	GLN
1	DA	3	GLN
1	DA	84	ASN
1	DA	144	GLN
1	DC	3	GLN
1	DC	84	ASN
1	DC	144	GLN
1	DE	3	GLN
1	DE	84	ASN
1	DE	144	GLN
1	DG	3	GLN
1	DG	84	ASN
1	DG	144	GLN
1	DI	3	GLN
1	DI	84	ASN
1	DI	144	GLN
1	DK	3	GLN
1	DK	84	ASN
1	DK	144	GLN
1	DM	3	GLN
1	DM	84	ASN
1	DM	144	GLN
1	DO	3	GLN
1	DO	144	GLN
1	DQ	3	GLN
1	DQ	84	ASN
1	DQ	144	GLN
1	DS	3	GLN
1	DS	144	GLN
1	DU	3	GLN
1	DU	84	ASN
1	DU	144	GLN
1	DW	3	GLN
1	DW	84	ASN
1	DW	144	GLN
1	DY	3	GLN
1	DY	144	GLN

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Mol	Chain	Res	Type
1	Da	3	GLN
1	Da	84	ASN
1	Da	144	GLN
1	Dc	3	GLN
1	Dc	84	ASN
1	Dc	144	GLN
1	De	3	GLN
1	De	84	ASN
1	De	144	GLN
1	Dg	3	GLN
1	Dg	144	GLN
1	Di	3	GLN
1	Di	84	ASN
1	Di	144	GLN
1	Dk	3	GLN
1	Dk	144	GLN
1	Dm	3	GLN
1	Dm	84	ASN
1	Dm	144	GLN
1	Do	3	GLN
1	Do	84	ASN
1	Do	144	GLN
1	Dq	3	GLN
1	Dq	84	ASN
1	Dq	144	GLN
1	Ds	3	GLN
1	Ds	84	ASN
1	Ds	144	GLN
1	Du	3	GLN
1	Du	144	GLN
1	Dw	3	GLN
1	Dw	84	ASN
1	Dw	144	GLN
1	Dy	3	GLN
1	Dy	84	ASN
1	Dy	144	GLN
1	D1	3	GLN
1	D1	84	ASN
1	D1	144	GLN
1	D3	3	GLN
1	D3	84	ASN
1	D3	144	GLN

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Mol	Chain	Res	Type
1	D5	3	GLN
1	D5	84	ASN
1	D5	144	GLN
1	D7	3	GLN
1	D7	84	ASN
1	D7	144	GLN
1	D9	3	GLN
1	D9	84	ASN
1	D9	144	GLN
1	EA	3	GLN
1	EA	84	ASN
1	EA	144	GLN
1	EC	3	GLN
1	EC	84	ASN
1	EC	144	GLN
1	EE	3	GLN
1	EE	84	ASN
1	EE	144	GLN
1	EG	3	GLN
1	EG	144	GLN
1	EI	3	GLN
1	EI	144	GLN
1	EK	3	GLN
1	EK	84	ASN
1	EK	144	GLN
1	EM	3	GLN
1	EM	144	GLN
1	EO	3	GLN
1	EO	84	ASN
1	EO	144	GLN
1	EQ	3	GLN
1	EQ	144	GLN
1	ES	3	GLN
1	ES	84	ASN
1	ES	144	GLN
1	EU	3	GLN
1	EU	84	ASN
1	EU	144	GLN
1	EW	3	GLN
1	EW	144	GLN
1	EY	3	GLN
1	EY	84	ASN

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Mol	Chain	Res	Type
1	EY	144	GLN
1	Ea	3	GLN
1	Ea	84	ASN
1	Ea	144	GLN
1	Ec	3	GLN
1	Ec	84	ASN
1	Ec	144	GLN
1	Ee	3	GLN
1	Ee	84	ASN
1	Ee	144	GLN
1	Eg	3	GLN
1	Eg	84	ASN
1	Eg	144	GLN
1	Ei	3	GLN
1	Ei	144	GLN
1	Ek	3	GLN
1	Ek	84	ASN
1	Ek	144	GLN
1	Em	3	GLN
1	Em	84	ASN
1	Em	144	GLN
1	Eo	3	GLN
1	Eo	84	ASN
1	Eo	144	GLN
1	Eq	3	GLN
1	Eq	84	ASN
1	Eq	144	GLN
1	Es	3	GLN
1	Es	84	ASN
1	Es	144	GLN
1	Eu	3	GLN
1	Eu	84	ASN
1	Eu	144	GLN
1	Ew	3	GLN
1	Ew	84	ASN
1	Ew	144	GLN
1	Ey	3	GLN
1	Ey	84	ASN
1	Ey	144	GLN
1	E1	3	GLN
1	E1	84	ASN
1	E1	144	GLN

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Mol	Chain	Res	Type
1	E3	3	GLN
1	E3	84	ASN
1	E3	144	GLN
1	E5	3	GLN
1	E5	84	ASN
1	E5	144	GLN
1	E7	3	GLN
1	E7	84	ASN
1	E7	144	GLN
1	E9	3	GLN
1	E9	84	ASN
1	E9	144	GLN
1	FA	3	GLN
1	FA	84	ASN
1	FA	144	GLN
1	FC	3	GLN
1	FC	84	ASN
1	FC	144	GLN
1	FE	3	GLN
1	FE	84	ASN
1	FE	144	GLN
1	FG	3	GLN
1	FG	84	ASN
1	FG	144	GLN
1	FI	3	GLN
1	FI	84	ASN
1	FI	144	GLN
1	FK	3	GLN
1	FK	144	GLN
1	FM	3	GLN
1	FM	84	ASN
1	FM	144	GLN
1	FO	3	GLN
1	FO	144	GLN
1	FQ	3	GLN
1	FQ	84	ASN
1	FQ	144	GLN
1	FS	3	GLN
1	FS	84	ASN
1	FS	144	GLN
1	FU	3	GLN
1	FU	84	ASN

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Mol	Chain	Res	Type
1	FU	144	GLN
1	FW	3	GLN
1	FW	144	GLN
1	FY	3	GLN
1	FY	84	ASN
1	FY	144	GLN
1	Fa	3	GLN
1	Fa	84	ASN
1	Fa	144	GLN
1	Fc	3	GLN
1	Fc	144	GLN
1	Fe	3	GLN
1	Fe	84	ASN
1	Fe	144	GLN
1	Fg	3	GLN
1	Fg	144	GLN
1	Fi	3	GLN
1	Fi	84	ASN
1	Fi	144	GLN
1	Fk	3	GLN
1	Fk	84	ASN
1	Fk	144	GLN
1	Fm	3	GLN
1	Fm	84	ASN
1	Fm	144	GLN
1	Fo	3	GLN
1	Fo	144	GLN
1	Fq	3	GLN
1	Fq	144	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 616 ligands modelled in this entry, 462 are monoatomic - leaving 154 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	A8	201	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	Bj	203	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	DC	203	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	Ds	201	1	14,14,15	0.77	0	17,19,21	0.93	0
3	NAG	Aw	202	1	14,14,15	0.77	0	17,19,21	0.93	0
3	NAG	Dw	203	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	BH	201	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	DQ	201	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	DW	203	1	14,14,15	0.77	0	17,19,21	0.94	0
3	NAG	BZ	202	1	14,14,15	0.77	0	17,19,21	0.93	0
3	NAG	Eq	201	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	Bs	202	1	14,14,15	0.77	0	17,19,21	0.93	0
3	NAG	Bo	201	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	Be	201	1	14,14,15	0.77	0	17,19,21	0.93	0
3	NAG	BG	203	1	14,14,15	0.77	0	17,19,21	0.94	0
3	NAG	BN	201	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	Bb	202	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	Ey	201	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	Bf	201	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	FM	202	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	BX	202	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	Ei	201	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	BE	202	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	EQ	202	1	14,14,15	0.76	0	17,19,21	0.94	0
3	NAG	BR	202	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	DS	201	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	EC	201	1	14,14,15	0.77	0	17,19,21	0.93	0
3	NAG	D9	201	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	BS	202	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	DU	202	1	14,14,15	0.77	0	17,19,21	0.93	0
3	NAG	Fg	202	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	Fo	201	1	14,14,15	0.76	0	17,19,21	0.93	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	E7	201	1	14,14,15	0.77	0	17,19,21	0.93	0
3	NAG	A3	201	1	14,14,15	0.76	0	17,19,21	0.94	0
3	NAG	Bg	202	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	BA	202	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	Ay	203	1	14,14,15	0.77	0	17,19,21	0.93	0
3	NAG	Bd	201	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	BU	201	1	14,14,15	0.77	0	17,19,21	0.93	0
3	NAG	Dm	203	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	Do	201	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	EM	202	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	Dk	201	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	Fc	202	1	14,14,15	0.77	0	17,19,21	0.94	0
3	NAG	A0	203	1	14,14,15	0.76	0	17,19,21	0.94	0
3	NAG	De	201	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	EK	201	1	14,14,15	0.76	0	17,19,21	0.94	0
3	NAG	Es	201	1	14,14,15	0.77	0	17,19,21	0.93	0
3	NAG	FK	202	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	A7	203	1	14,14,15	0.76	0	17,19,21	0.94	0
3	NAG	Bx	202	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	D5	202	1	14,14,15	0.76	0	17,19,21	0.94	0
3	NAG	Fe	202	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	BD	202	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	FW	202	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	Ew	202	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	EO	201	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	EW	202	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	By	202	1	14,14,15	0.77	0	17,19,21	0.93	0
3	NAG	EE	201	1	14,14,15	0.77	0	17,19,21	0.93	0
3	NAG	FU	201	1	14,14,15	0.76	0	17,19,21	0.94	0
3	NAG	BV	201	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	FY	202	1	14,14,15	0.77	0	17,19,21	0.93	0
3	NAG	Eg	202	1	14,14,15	0.77	0	17,19,21	0.94	0
3	NAG	A6	202	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	Bp	202	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	EY	201	1	14,14,15	0.77	0	17,19,21	0.94	0
3	NAG	Eo	201	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	D7	201	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	BT	201	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	Bk	202	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	Ax	201	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	Br	203	1	14,14,15	0.77	0	17,19,21	0.93	0
3	NAG	E3	202	1	14,14,15	0.77	0	17,19,21	0.93	0
3	NAG	Fi	201	1	14,14,15	0.76	0	17,19,21	0.93	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	BP	201	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	Di	202	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	Bn	201	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	FG	201	1	14,14,15	0.77	0	17,19,21	0.93	0
3	NAG	ES	201	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	FO	202	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	DG	202	1	14,14,15	0.77	0	17,19,21	0.93	0
3	NAG	E5	202	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	BL	201	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	Fa	201	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	EU	201	1	14,14,15	0.77	0	17,19,21	0.93	0
3	NAG	Em	201	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	DK	203	1	14,14,15	0.77	0	17,19,21	0.93	0
3	NAG	Ek	202	1	14,14,15	0.76	0	17,19,21	0.94	0
3	NAG	D3	201	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	Az	203	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	BK	201	1	14,14,15	0.77	0	17,19,21	0.93	0
3	NAG	Bq	203	1	14,14,15	0.77	0	17,19,21	0.93	0
3	NAG	Ec	201	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	BY	201	1	14,14,15	0.77	0	17,19,21	0.93	0
3	NAG	BJ	202	1	14,14,15	0.77	0	17,19,21	0.93	0
3	NAG	FS	201	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	BI	201	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	BC	201	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	BO	203	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	DI	201	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	Du	202	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	EA	201	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	EI	202	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	DM	201	1	14,14,15	0.77	0	17,19,21	0.93	0
3	NAG	Eu	202	1	14,14,15	0.77	0	17,19,21	0.94	0
3	NAG	EG	201	1	14,14,15	0.77	0	17,19,21	0.93	0
3	NAG	E1	201	1	14,14,15	0.77	0	17,19,21	0.93	0
3	NAG	Da	202	1	14,14,15	0.76	0	17,19,21	0.94	0
3	NAG	Fq	201	1	14,14,15	0.77	0	17,19,21	0.93	0
3	NAG	A2	202	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	FE	201	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	DA	201	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	FC	201	1	14,14,15	0.77	0	17,19,21	0.93	0
3	NAG	FA	201	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	A9	202	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	Bh	202	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	E9	201	1	14,14,15	0.76	0	17,19,21	0.93	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	Bz	202	1	14,14,15	0.77	0	17,19,21	0.93	0
3	NAG	BW	201	1	14,14,15	0.77	0	17,19,21	0.93	0
3	NAG	Bl	202	1	14,14,15	0.77	0	17,19,21	0.93	0
3	NAG	Bu	203	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	BQ	201	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	Ba	201	1	14,14,15	0.77	0	17,19,21	0.93	0
3	NAG	Dy	202	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	DY	203	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	BF	201	1	14,14,15	0.76	0	17,19,21	0.94	0
3	NAG	Av	202	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	BB	201	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	Dq	203	1	14,14,15	0.76	0	17,19,21	0.94	0
3	NAG	Dc	201	1	14,14,15	0.77	0	17,19,21	0.93	0
3	NAG	Fm	201	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	D1	202	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	Bm	201	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	Bc	201	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	Fk	202	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	A1	203	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	FI	201	1	14,14,15	0.77	0	17,19,21	0.93	0
3	NAG	Bi	201	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	DO	201	1	14,14,15	0.77	0	17,19,21	0.93	0
3	NAG	Dg	201	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	FQ	201	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	C9	203	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	Bt	201	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	B1	202	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	A5	202	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	DE	201	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	A4	202	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	Bw	202	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	Ee	202	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	BM	201	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	Au	202	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	Bv	201	1	14,14,15	0.76	0	17,19,21	0.93	0
3	NAG	Ea	201	1	14,14,15	0.77	0	17,19,21	0.93	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A8	201	1	-	0/6/23/26	0/1/1/1
3	NAG	Bj	203	1	-	0/6/23/26	0/1/1/1
3	NAG	DC	203	1	-	0/6/23/26	0/1/1/1
3	NAG	Ds	201	1	-	0/6/23/26	0/1/1/1
3	NAG	Aw	202	1	-	0/6/23/26	0/1/1/1
3	NAG	Dw	203	1	-	0/6/23/26	0/1/1/1
3	NAG	BH	201	1	-	0/6/23/26	0/1/1/1
3	NAG	DQ	201	1	-	0/6/23/26	0/1/1/1
3	NAG	DW	203	1	-	0/6/23/26	0/1/1/1
3	NAG	BZ	202	1	-	0/6/23/26	0/1/1/1
3	NAG	Eq	201	1	-	0/6/23/26	0/1/1/1
3	NAG	Bs	202	1	-	0/6/23/26	0/1/1/1
3	NAG	Bo	201	1	-	0/6/23/26	0/1/1/1
3	NAG	Be	201	1	-	0/6/23/26	0/1/1/1
3	NAG	BG	203	1	-	0/6/23/26	0/1/1/1
3	NAG	BN	201	1	-	0/6/23/26	0/1/1/1
3	NAG	Bb	202	1	-	0/6/23/26	0/1/1/1
3	NAG	Ey	201	1	-	0/6/23/26	0/1/1/1
3	NAG	Bf	201	1	-	0/6/23/26	0/1/1/1
3	NAG	FM	202	1	-	0/6/23/26	0/1/1/1
3	NAG	BX	202	1	-	0/6/23/26	0/1/1/1
3	NAG	Ei	201	1	-	0/6/23/26	0/1/1/1
3	NAG	BE	202	1	-	0/6/23/26	0/1/1/1
3	NAG	EQ	202	1	-	0/6/23/26	0/1/1/1
3	NAG	BR	202	1	-	0/6/23/26	0/1/1/1
3	NAG	DS	201	1	-	0/6/23/26	0/1/1/1
3	NAG	EC	201	1	-	0/6/23/26	0/1/1/1
3	NAG	D9	201	1	-	0/6/23/26	0/1/1/1
3	NAG	BS	202	1	-	0/6/23/26	0/1/1/1
3	NAG	DU	202	1	-	0/6/23/26	0/1/1/1
3	NAG	Fg	202	1	-	0/6/23/26	0/1/1/1
3	NAG	Fo	201	1	-	0/6/23/26	0/1/1/1
3	NAG	E7	201	1	-	0/6/23/26	0/1/1/1
3	NAG	A3	201	1	-	0/6/23/26	0/1/1/1
3	NAG	Bg	202	1	-	0/6/23/26	0/1/1/1
3	NAG	BA	202	1	-	0/6/23/26	0/1/1/1
3	NAG	Ay	203	1	-	0/6/23/26	0/1/1/1
3	NAG	Bd	201	1	-	0/6/23/26	0/1/1/1
3	NAG	BU	201	1	-	0/6/23/26	0/1/1/1
3	NAG	Dm	203	1	-	0/6/23/26	0/1/1/1
3	NAG	Do	201	1	-	0/6/23/26	0/1/1/1
3	NAG	EM	202	1	-	0/6/23/26	0/1/1/1
3	NAG	Dk	201	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	Fc	202	1	-	0/6/23/26	0/1/1/1
3	NAG	A0	203	1	-	0/6/23/26	0/1/1/1
3	NAG	De	201	1	-	0/6/23/26	0/1/1/1
3	NAG	EK	201	1	-	0/6/23/26	0/1/1/1
3	NAG	Es	201	1	-	0/6/23/26	0/1/1/1
3	NAG	FK	202	1	-	0/6/23/26	0/1/1/1
3	NAG	A7	203	1	-	0/6/23/26	0/1/1/1
3	NAG	Bx	202	1	-	0/6/23/26	0/1/1/1
3	NAG	D5	202	1	-	0/6/23/26	0/1/1/1
3	NAG	Fe	202	1	-	0/6/23/26	0/1/1/1
3	NAG	BD	202	1	-	0/6/23/26	0/1/1/1
3	NAG	FW	202	1	-	0/6/23/26	0/1/1/1
3	NAG	Ew	202	1	-	0/6/23/26	0/1/1/1
3	NAG	EO	201	1	-	0/6/23/26	0/1/1/1
3	NAG	EW	202	1	-	0/6/23/26	0/1/1/1
3	NAG	By	202	1	-	0/6/23/26	0/1/1/1
3	NAG	EE	201	1	-	0/6/23/26	0/1/1/1
3	NAG	FU	201	1	-	0/6/23/26	0/1/1/1
3	NAG	BV	201	1	-	0/6/23/26	0/1/1/1
3	NAG	FY	202	1	-	0/6/23/26	0/1/1/1
3	NAG	Eg	202	1	-	0/6/23/26	0/1/1/1
3	NAG	A6	202	1	-	0/6/23/26	0/1/1/1
3	NAG	Bp	202	1	-	0/6/23/26	0/1/1/1
3	NAG	EY	201	1	-	0/6/23/26	0/1/1/1
3	NAG	Eo	201	1	-	0/6/23/26	0/1/1/1
3	NAG	D7	201	1	-	0/6/23/26	0/1/1/1
3	NAG	BT	201	1	-	0/6/23/26	0/1/1/1
3	NAG	Bk	202	1	-	0/6/23/26	0/1/1/1
3	NAG	Ax	201	1	-	0/6/23/26	0/1/1/1
3	NAG	Br	203	1	-	0/6/23/26	0/1/1/1
3	NAG	E3	202	1	-	0/6/23/26	0/1/1/1
3	NAG	Fi	201	1	-	0/6/23/26	0/1/1/1
3	NAG	BP	201	1	-	0/6/23/26	0/1/1/1
3	NAG	Di	202	1	-	0/6/23/26	0/1/1/1
3	NAG	Bn	201	1	-	0/6/23/26	0/1/1/1
3	NAG	FG	201	1	-	0/6/23/26	0/1/1/1
3	NAG	ES	201	1	-	0/6/23/26	0/1/1/1
3	NAG	FO	202	1	-	0/6/23/26	0/1/1/1
3	NAG	DG	202	1	-	0/6/23/26	0/1/1/1
3	NAG	E5	202	1	-	0/6/23/26	0/1/1/1
3	NAG	BL	201	1	-	0/6/23/26	0/1/1/1
3	NAG	Fa	201	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	EU	201	1	-	0/6/23/26	0/1/1/1
3	NAG	Em	201	1	-	0/6/23/26	0/1/1/1
3	NAG	DK	203	1	-	0/6/23/26	0/1/1/1
3	NAG	Ek	202	1	-	0/6/23/26	0/1/1/1
3	NAG	D3	201	1	-	0/6/23/26	0/1/1/1
3	NAG	Az	203	1	-	0/6/23/26	0/1/1/1
3	NAG	BK	201	1	-	0/6/23/26	0/1/1/1
3	NAG	Bq	203	1	-	0/6/23/26	0/1/1/1
3	NAG	Ec	201	1	-	0/6/23/26	0/1/1/1
3	NAG	BY	201	1	-	0/6/23/26	0/1/1/1
3	NAG	BJ	202	1	-	0/6/23/26	0/1/1/1
3	NAG	FS	201	1	-	0/6/23/26	0/1/1/1
3	NAG	BI	201	1	-	0/6/23/26	0/1/1/1
3	NAG	BC	201	1	-	0/6/23/26	0/1/1/1
3	NAG	BO	203	1	-	0/6/23/26	0/1/1/1
3	NAG	DI	201	1	-	0/6/23/26	0/1/1/1
3	NAG	Du	202	1	-	0/6/23/26	0/1/1/1
3	NAG	EA	201	1	-	0/6/23/26	0/1/1/1
3	NAG	EI	202	1	-	0/6/23/26	0/1/1/1
3	NAG	DM	201	1	-	0/6/23/26	0/1/1/1
3	NAG	Eu	202	1	-	0/6/23/26	0/1/1/1
3	NAG	EG	201	1	-	0/6/23/26	0/1/1/1
3	NAG	E1	201	1	-	0/6/23/26	0/1/1/1
3	NAG	Da	202	1	-	0/6/23/26	0/1/1/1
3	NAG	Fq	201	1	-	0/6/23/26	0/1/1/1
3	NAG	A2	202	1	-	0/6/23/26	0/1/1/1
3	NAG	FE	201	1	-	0/6/23/26	0/1/1/1
3	NAG	DA	201	1	-	0/6/23/26	0/1/1/1
3	NAG	FC	201	1	-	0/6/23/26	0/1/1/1
3	NAG	FA	201	1	-	0/6/23/26	0/1/1/1
3	NAG	A9	202	1	-	0/6/23/26	0/1/1/1
3	NAG	Bh	202	1	-	0/6/23/26	0/1/1/1
3	NAG	E9	201	1	-	0/6/23/26	0/1/1/1
3	NAG	Bz	202	1	-	0/6/23/26	0/1/1/1
3	NAG	BW	201	1	-	0/6/23/26	0/1/1/1
3	NAG	Bl	202	1	-	0/6/23/26	0/1/1/1
3	NAG	Bu	203	1	-	0/6/23/26	0/1/1/1
3	NAG	BQ	201	1	-	0/6/23/26	0/1/1/1
3	NAG	Ba	201	1	-	0/6/23/26	0/1/1/1
3	NAG	Dy	202	1	-	0/6/23/26	0/1/1/1
3	NAG	DY	203	1	-	0/6/23/26	0/1/1/1
3	NAG	BF	201	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	Av	202	1	-	0/6/23/26	0/1/1/1
3	NAG	BB	201	1	-	0/6/23/26	0/1/1/1
3	NAG	Dq	203	1	-	0/6/23/26	0/1/1/1
3	NAG	Dc	201	1	-	0/6/23/26	0/1/1/1
3	NAG	Fm	201	1	-	0/6/23/26	0/1/1/1
3	NAG	D1	202	1	-	0/6/23/26	0/1/1/1
3	NAG	Bm	201	1	-	0/6/23/26	0/1/1/1
3	NAG	Bc	201	1	-	0/6/23/26	0/1/1/1
3	NAG	Fk	202	1	-	0/6/23/26	0/1/1/1
3	NAG	A1	203	1	-	0/6/23/26	0/1/1/1
3	NAG	FI	201	1	-	0/6/23/26	0/1/1/1
3	NAG	Bi	201	1	-	0/6/23/26	0/1/1/1
3	NAG	DO	201	1	-	0/6/23/26	0/1/1/1
3	NAG	Dg	201	1	-	0/6/23/26	0/1/1/1
3	NAG	FQ	201	1	-	0/6/23/26	0/1/1/1
3	NAG	C9	203	1	-	0/6/23/26	0/1/1/1
3	NAG	Bt	201	1	-	0/6/23/26	0/1/1/1
3	NAG	B1	202	1	-	0/6/23/26	0/1/1/1
3	NAG	A5	202	1	-	0/6/23/26	0/1/1/1
3	NAG	DE	201	1	-	0/6/23/26	0/1/1/1
3	NAG	A4	202	1	-	0/6/23/26	0/1/1/1
3	NAG	Bw	202	1	-	0/6/23/26	0/1/1/1
3	NAG	Ee	202	1	-	0/6/23/26	0/1/1/1
3	NAG	BM	201	1	-	0/6/23/26	0/1/1/1
3	NAG	Au	202	1	-	0/6/23/26	0/1/1/1
3	NAG	Bv	201	1	-	0/6/23/26	0/1/1/1
3	NAG	Ea	201	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

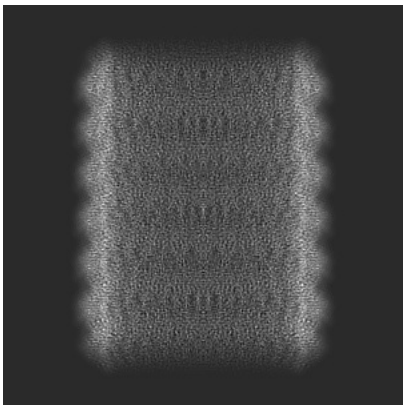
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-51935. These allow visual inspection of the internal detail of the map and identification of artifacts.

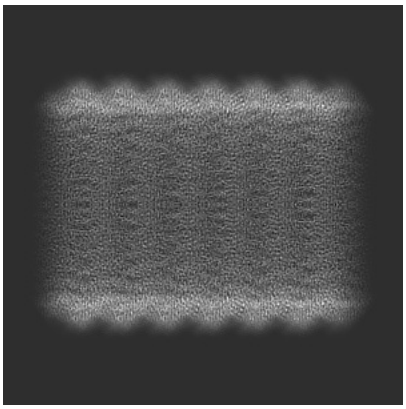
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

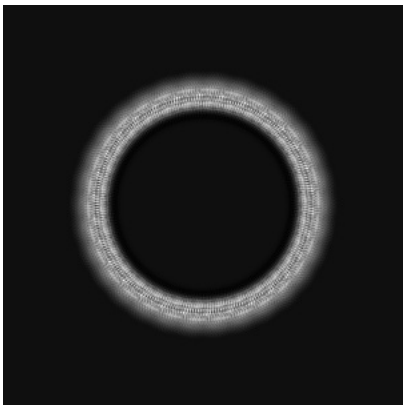
6.1.1 Primary map



X

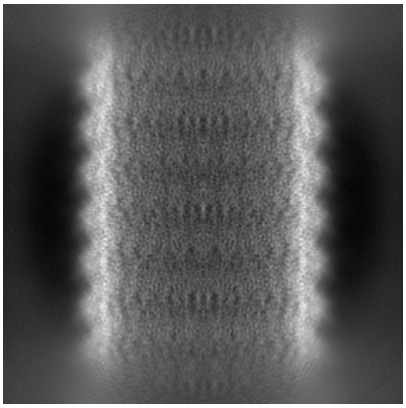


Y

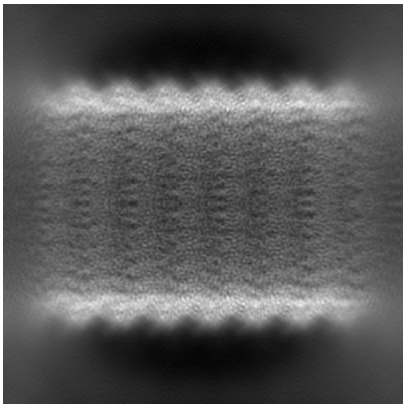


Z

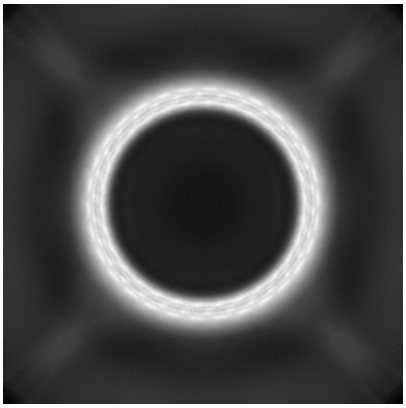
6.1.2 Raw map



X



Y

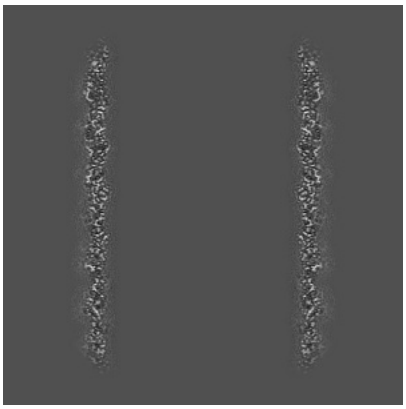


Z

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

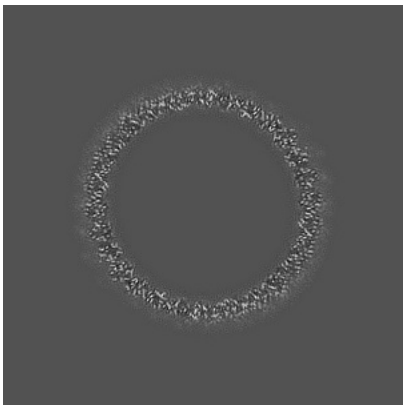
6.2 Central slices (i)

6.2.1 Primary map



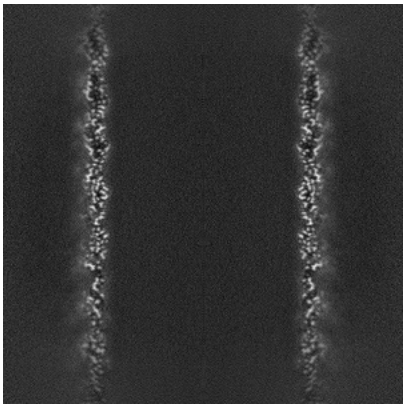
X Index: 300

Y Index: 300

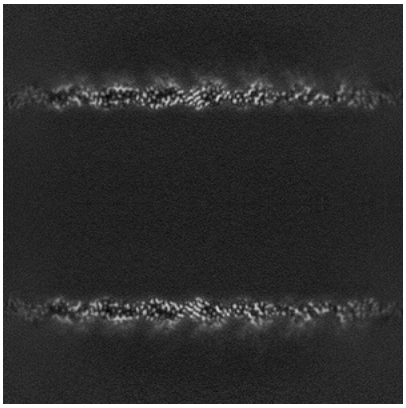


Z Index: 300

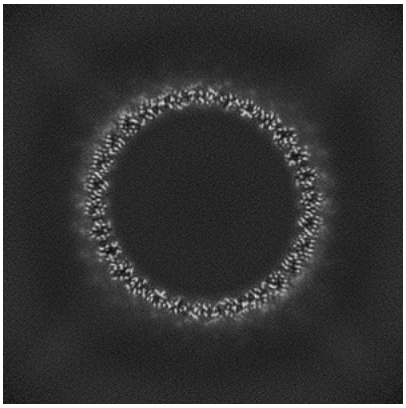
6.2.2 Raw map



X Index: 300



Y Index: 300

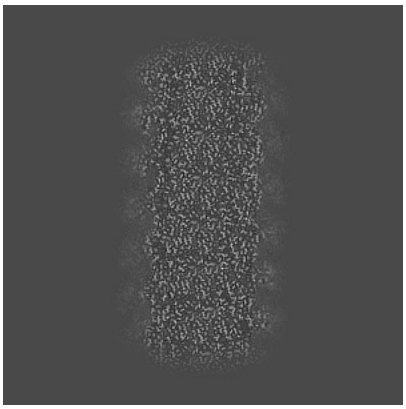


Z Index: 300

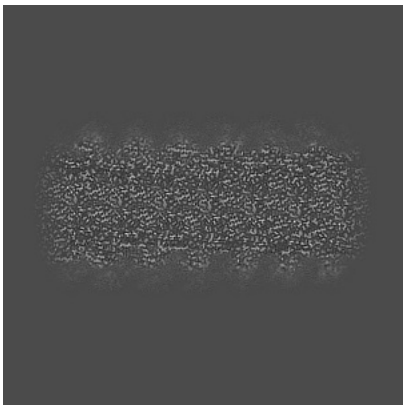
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

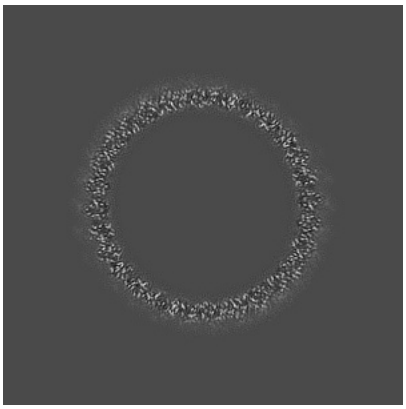
6.3.1 Primary map



X Index: 452

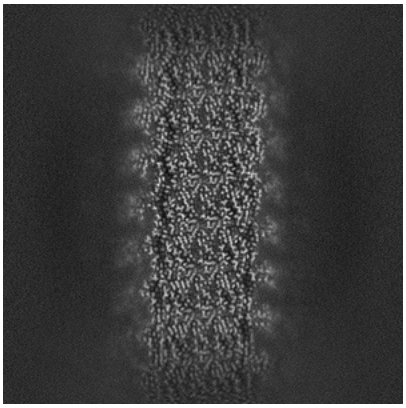


Y Index: 452

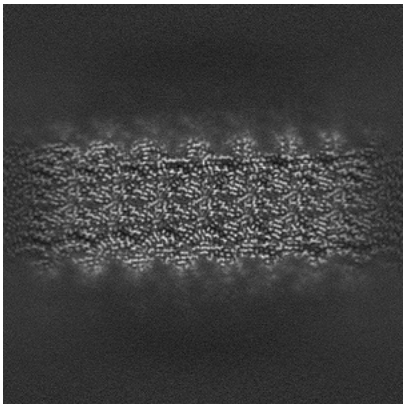


Z Index: 295

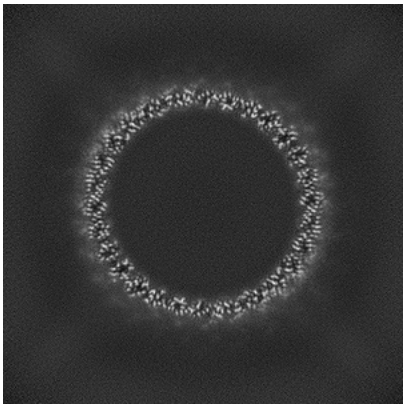
6.3.2 Raw map



X Index: 451



Y Index: 149

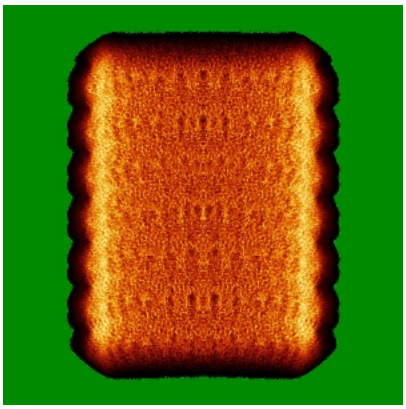


Z Index: 304

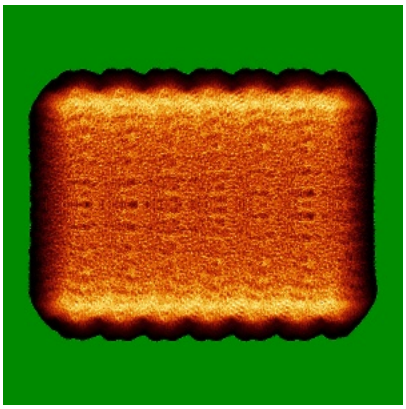
The images above show the largest variance slices of the map in three orthogonal directions.

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

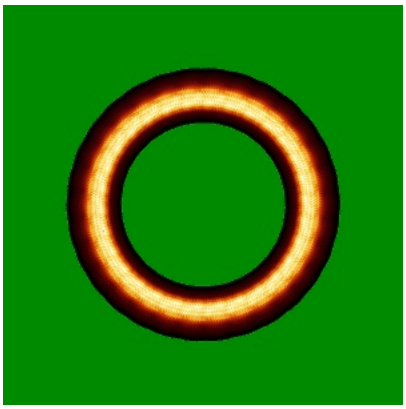
6.4.1 Primary map



X

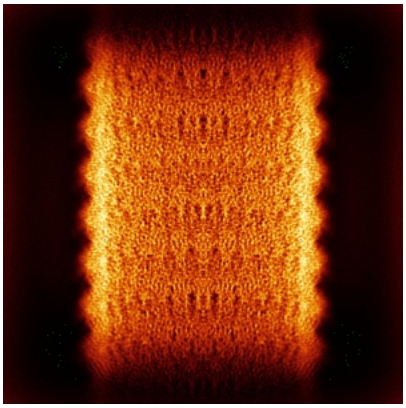


Y

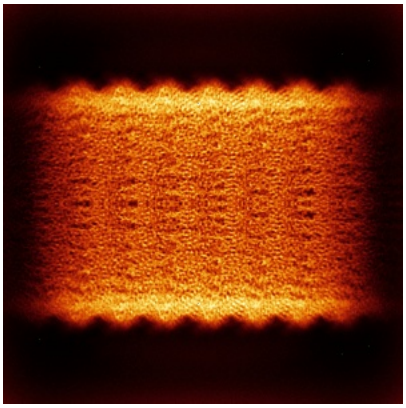


Z

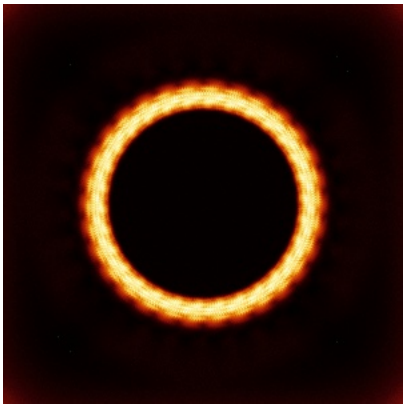
6.4.2 Raw map



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.

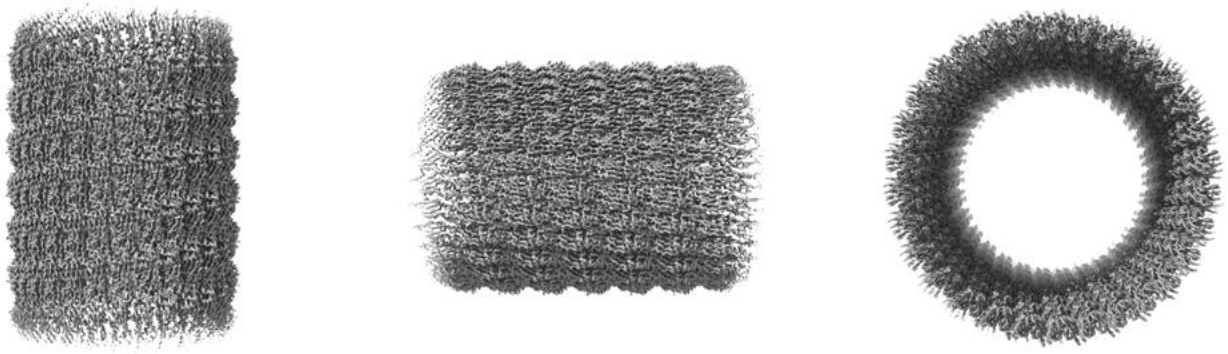
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0691. 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



X Y Z

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.

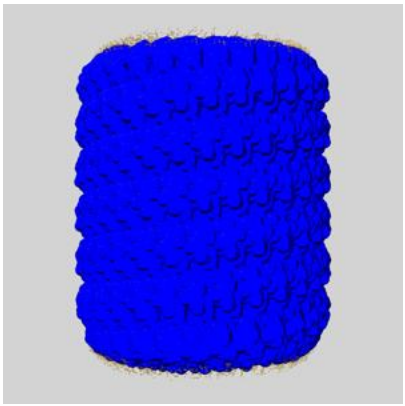
6.6 Mask visualisation

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

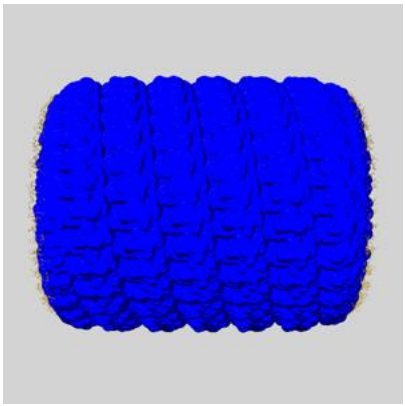
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

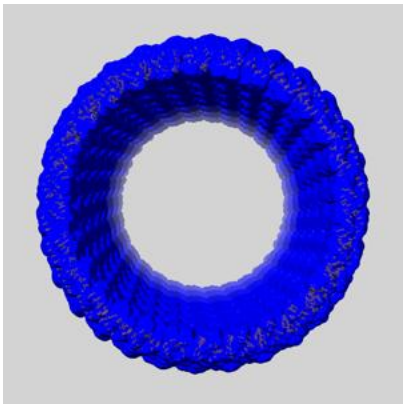
6.6.1 emd_51935_msk_1.map



X



Y

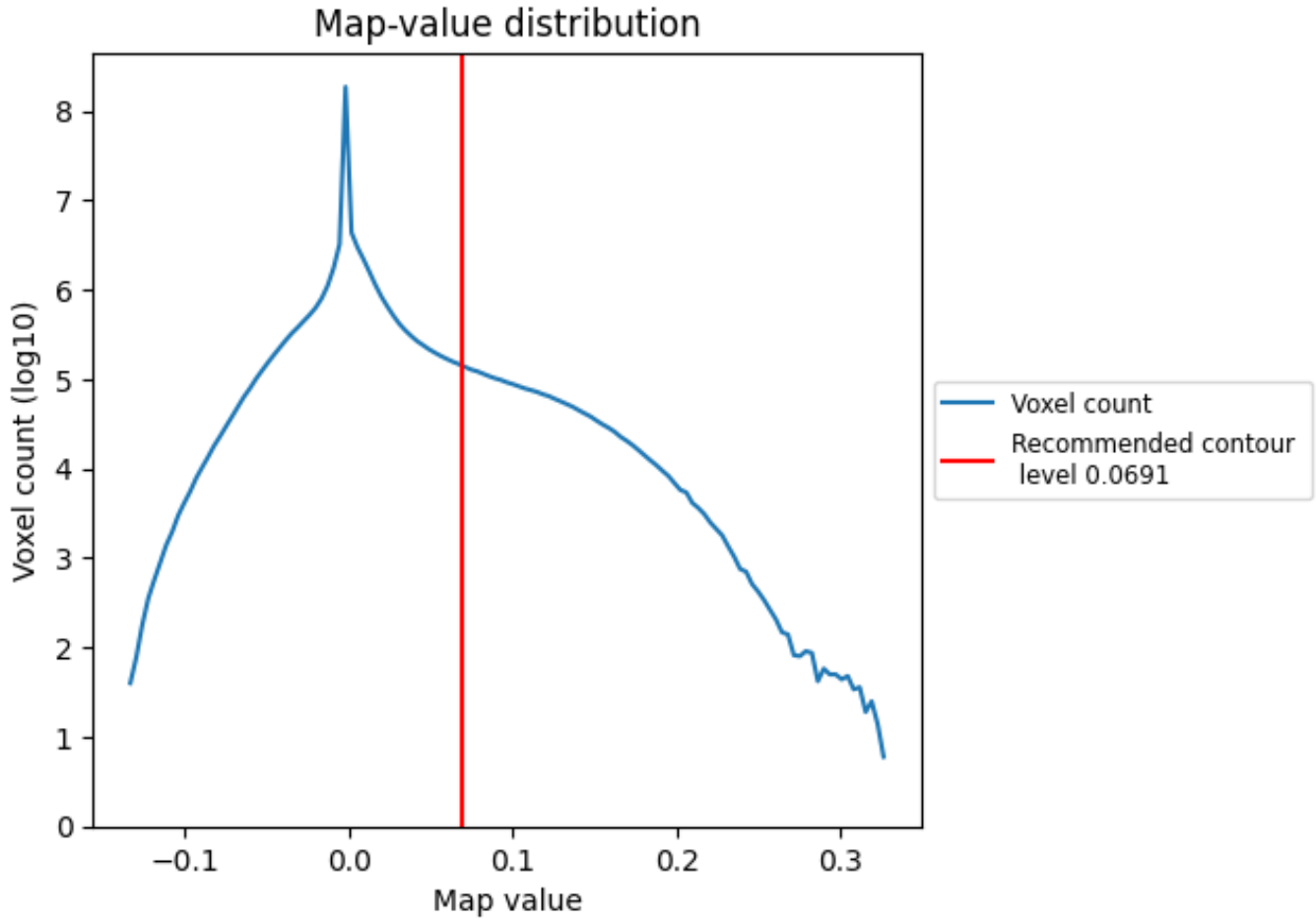


Z

7 Map analysis

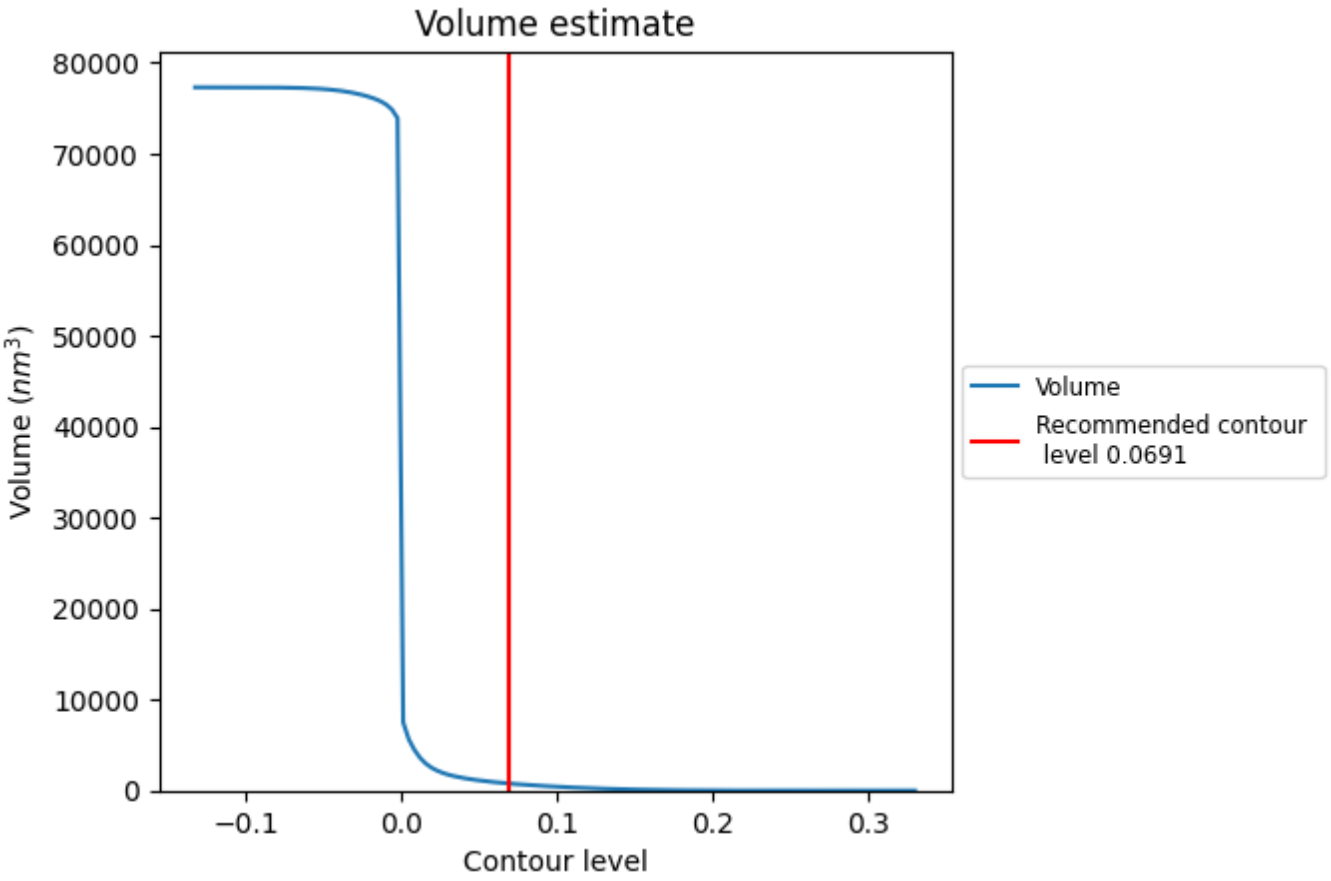
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

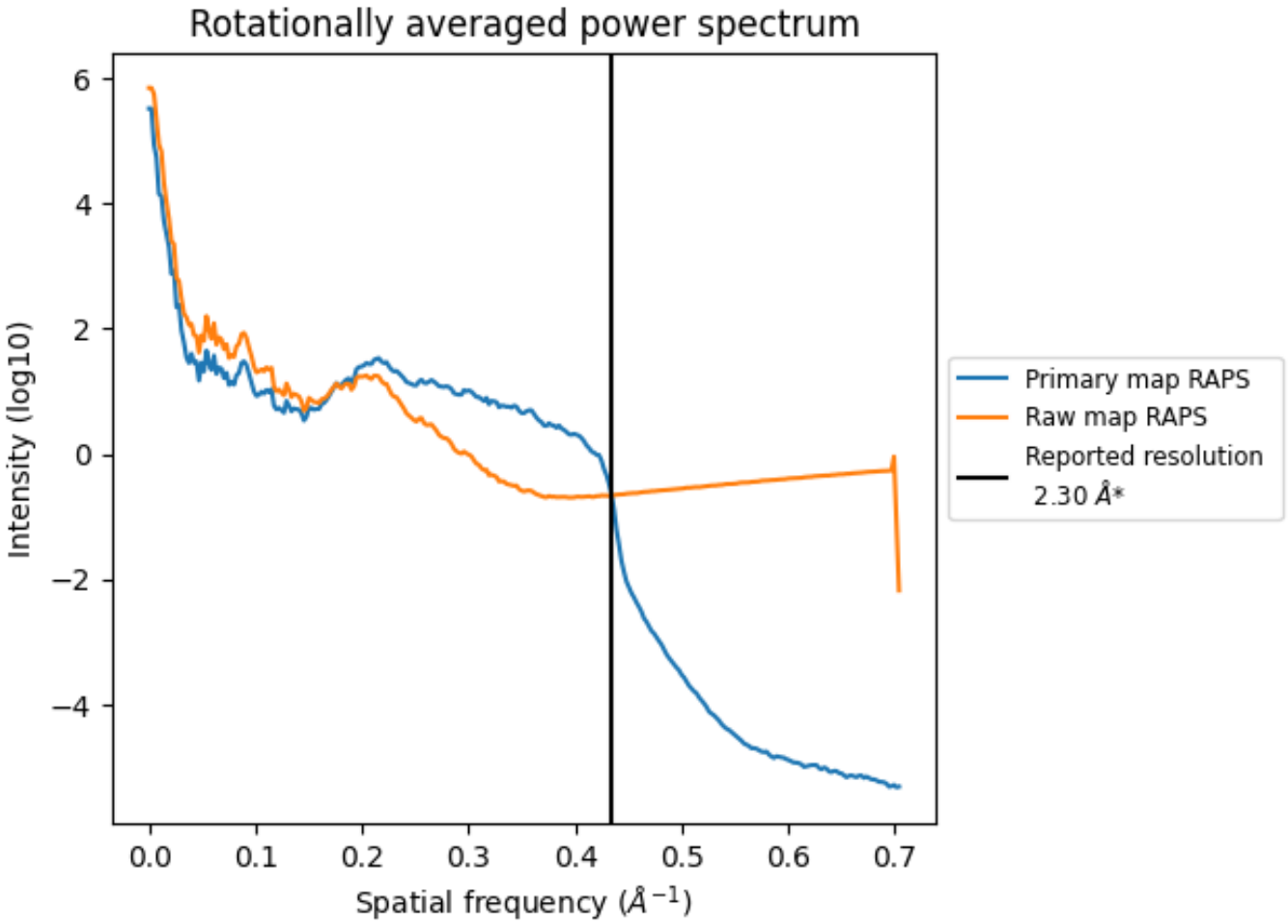
7.2 Volume estimate



The volume at the recommended contour level is 771 nm^3; this corresponds to an approximate mass of 696 kDa.

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

7.3 Rotationally averaged power spectrum (i)

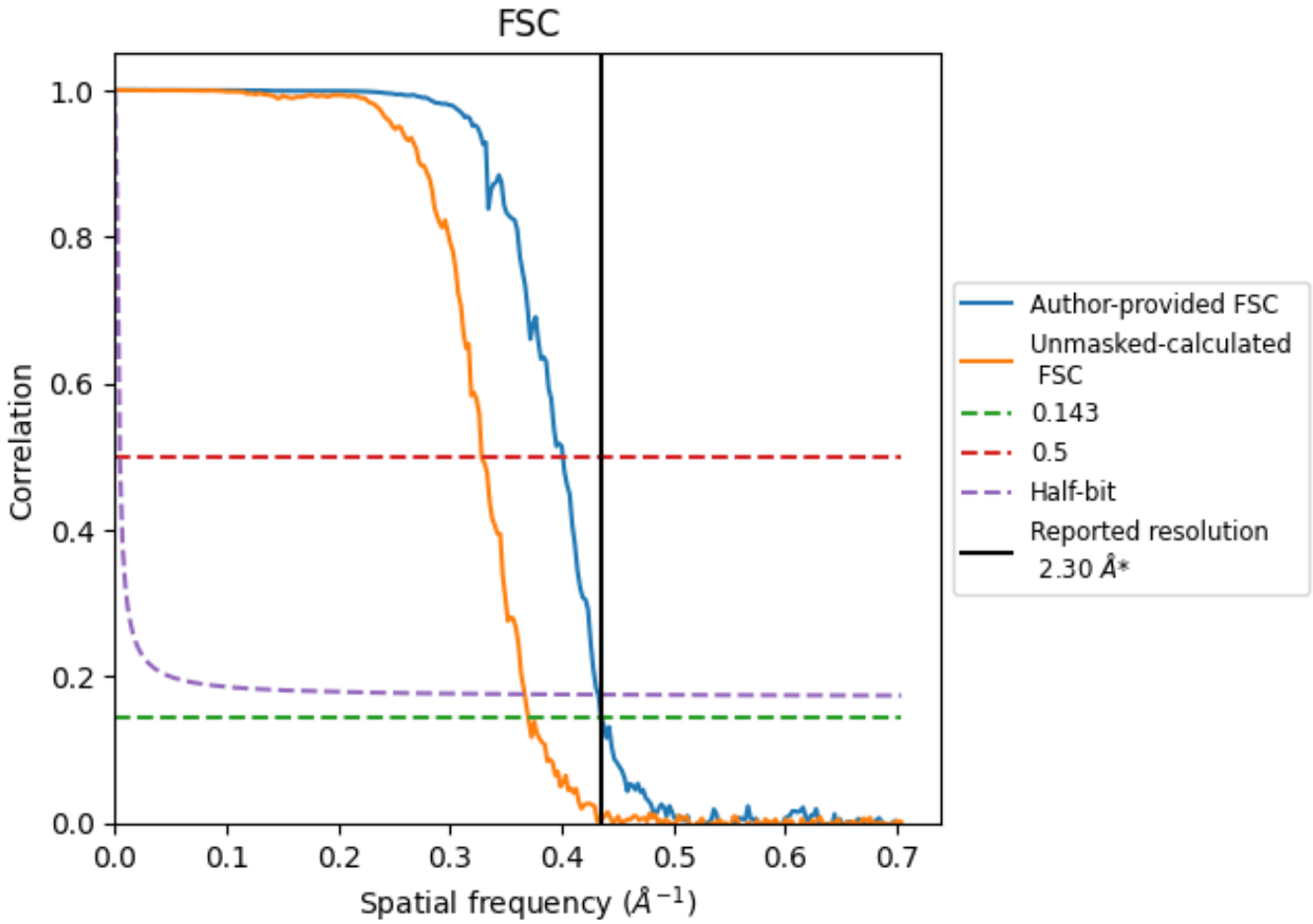


*Reported resolution corresponds to spatial frequency of 0.435 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.435 $Å^{-1}$

8.2 Resolution estimates (i)

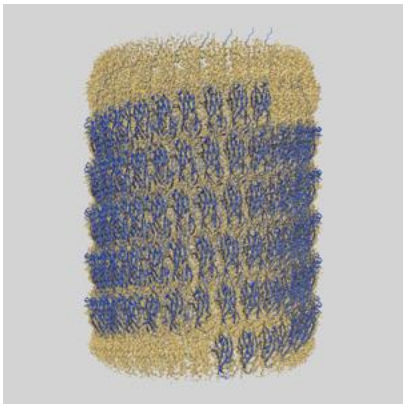
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.30	-	-
Author-provided FSC curve	2.30	2.49	2.31
Unmasked-calculated*	2.70	3.04	2.73

*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 2.70 differs from the reported value 2.3 by more than 10 %

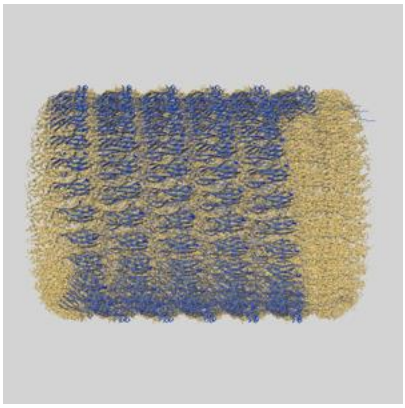
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-51935 and PDB model 9H8B. Per-residue inclusion information can be found in section 3 on page 32.

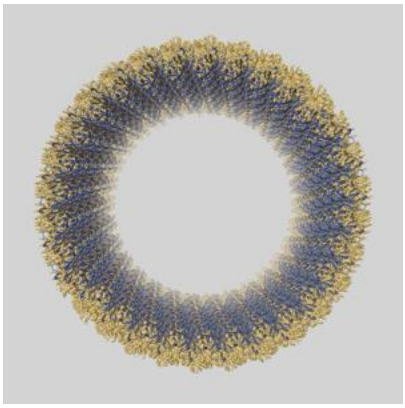
9.1 Map-model overlay



X



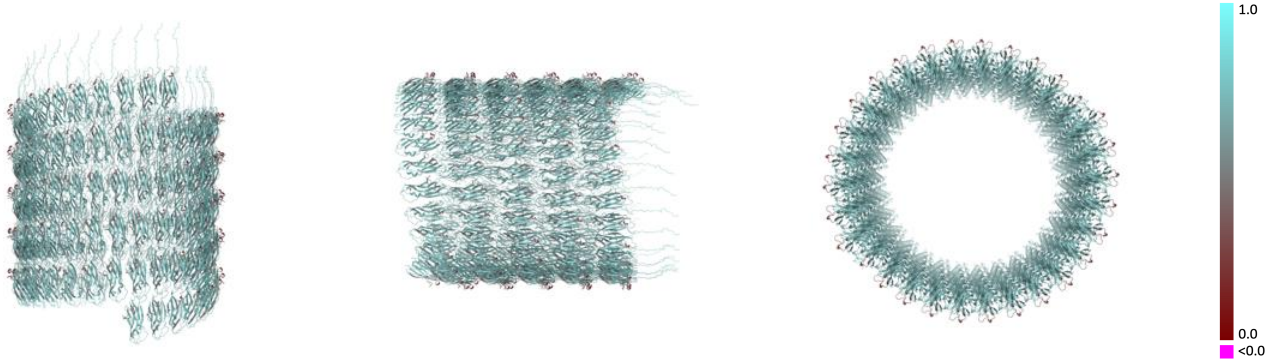
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0691 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

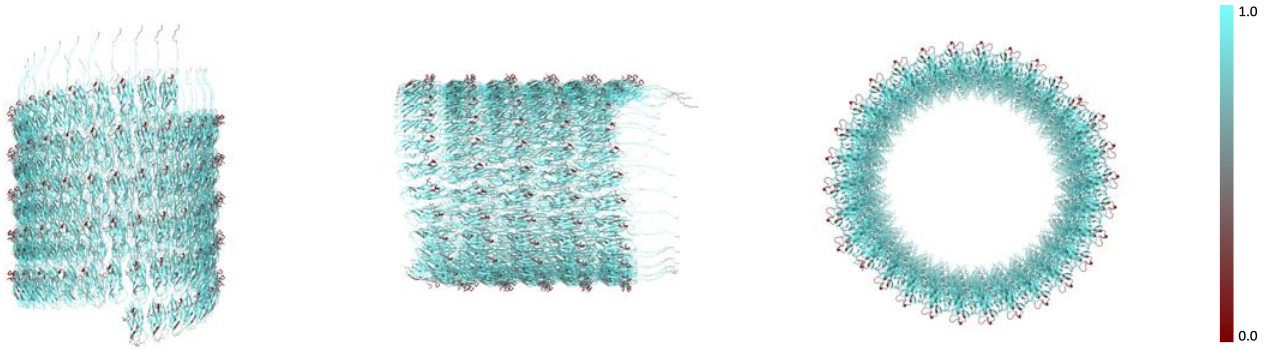
9.2 Q-score mapped to coordinate model



X Y Z

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

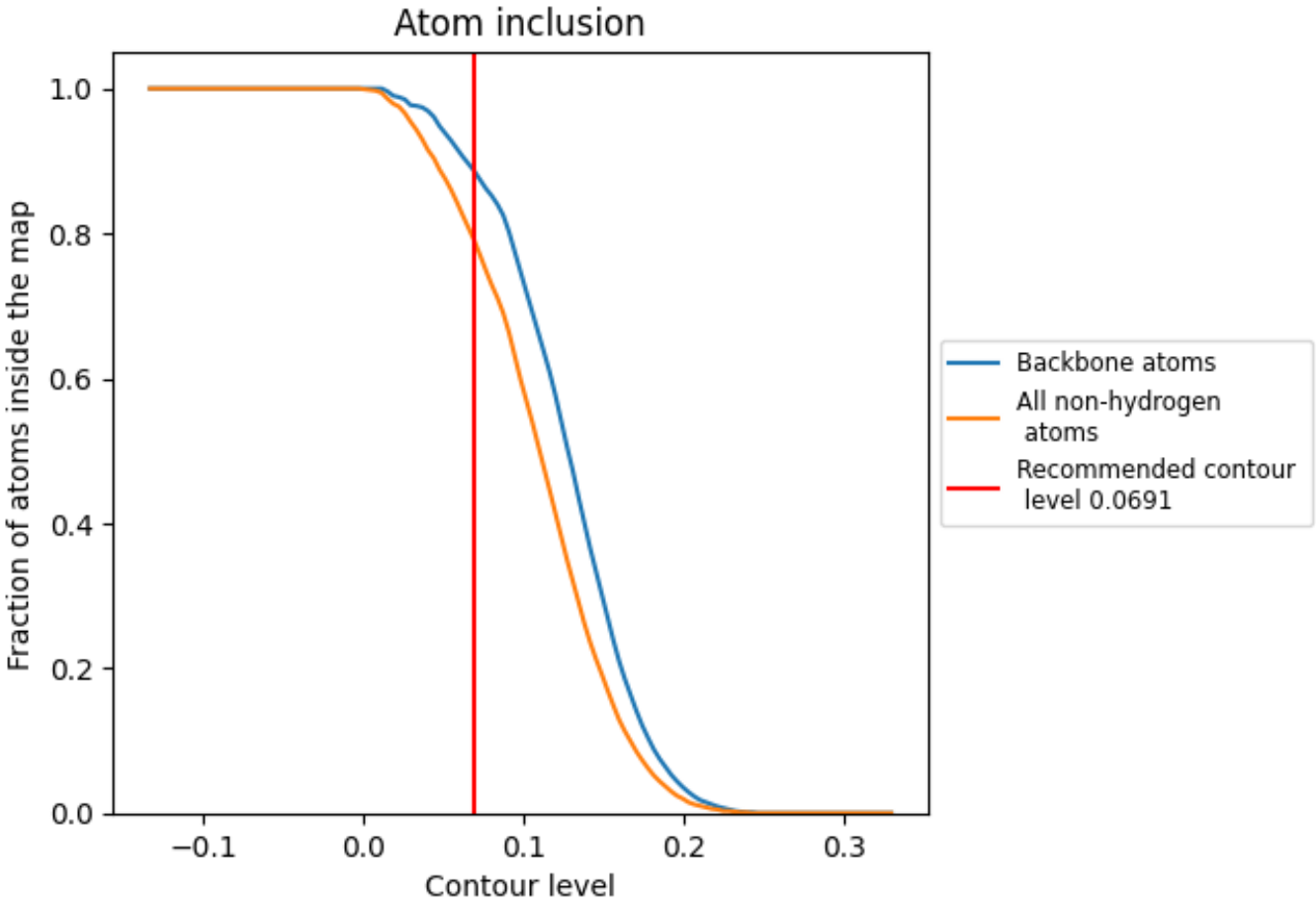
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0691).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 79% 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 (0.0691) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7920	0.6470
A0	0.7920	0.6470
A1	0.7960	0.6470
A2	0.8000	0.6450
A3	0.7950	0.6460
A4	0.7910	0.6460
A5	0.7920	0.6470
A6	0.7930	0.6480
A7	0.7960	0.6470
A8	0.7990	0.6470
A9	0.7960	0.6460
Au	0.7960	0.6460
Av	0.7960	0.6460
Aw	0.7960	0.6460
Ax	0.7950	0.6460
Ay	0.7930	0.6450
Az	0.8000	0.6470
B1	0.7900	0.6480
BA	0.7940	0.6480
BB	0.7990	0.6490
BC	0.7930	0.6490
BD	0.8020	0.6480
BE	0.8000	0.6470
BF	0.7980	0.6470
BG	0.7980	0.6480
BH	0.7950	0.6480
BI	0.7940	0.6470
BJ	0.7920	0.6460
BK	0.7990	0.6450
BL	0.7840	0.6460
BM	0.7760	0.6460
BN	0.7660	0.6460
BO	0.7530	0.6470
BP	0.7510	0.6460
BQ	0.7950	0.6470

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Chain	Atom inclusion	Q-score
BR	0.7960	0.6480
BS	0.7950	0.6490
BT	0.7950	0.6490
BU	0.7950	0.6470
BV	0.8020	0.6480
BW	0.7970	0.6470
BX	0.8010	0.6480
BY	0.7980	0.6480
BZ	0.7930	0.6470
Ba	0.7930	0.6460
Bb	0.7940	0.6460
Bc	0.7970	0.6450
Bd	0.7970	0.6450
Be	0.7980	0.6450
Bf	0.7940	0.6460
Bg	0.7930	0.6460
Bh	0.7980	0.6450
Bi	0.7930	0.6460
Bj	0.8020	0.6460
Bk	0.7990	0.6460
Bl	0.7980	0.6460
Bm	0.7960	0.6450
Bn	0.7940	0.6450
Bo	0.7950	0.6460
Bp	0.7930	0.6480
Bq	0.7990	0.6470
Br	0.7830	0.6480
Bs	0.7750	0.6470
Bt	0.7660	0.6470
Bu	0.7520	0.6470
Bv	0.7490	0.6480
Bw	0.7110	0.6470
Bx	0.7480	0.6470
By	0.7610	0.6480
Bz	0.7810	0.6490
C9	0.7940	0.6470
D1	0.7980	0.6490
D3	0.7940	0.6490
D5	0.7950	0.6480
D7	0.7950	0.6470
D9	0.7950	0.6470
DA	0.7940	0.6460

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Chain	Atom inclusion	Q-score
DC	0.7990	0.6480
DE	0.7970	0.6480
DG	0.7940	0.6470
DI	0.7980	0.6460
DK	0.7970	0.6450
DM	0.7990	0.6460
DO	0.8000	0.6460
DQ	0.7960	0.6460
DS	0.7960	0.6460
DU	0.7970	0.6460
DW	0.7980	0.6460
DY	0.7960	0.6460
Da	0.7980	0.6450
Dc	0.7960	0.6470
De	0.7910	0.6460
Dg	0.7980	0.6460
Di	0.7970	0.6450
Dk	0.7990	0.6460
Dm	0.7970	0.6470
Do	0.7970	0.6480
Dq	0.7970	0.6470
Ds	0.7970	0.6470
Du	0.7970	0.6460
Dw	0.7960	0.6460
Dy	0.7950	0.6470
E1	0.7950	0.6490
E3	0.8000	0.6470
E5	0.7940	0.6480
E7	0.7920	0.6460
E9	0.8000	0.6480
EA	0.7980	0.6480
EC	0.7940	0.6480
EE	0.8010	0.6470
EG	0.7980	0.6460
EI	0.7950	0.6460
EK	0.7970	0.6450
EM	0.7980	0.6460
EO	0.7990	0.6460
EQ	0.7120	0.6460
ES	0.7510	0.6460
EU	0.7590	0.6460
EW	0.7810	0.6460

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Chain	Atom inclusion	Q-score
EY	0.7900	0.6450
Ea	0.7940	0.6460
Ec	0.7940	0.6460
Ee	0.7990	0.6450
Eg	0.7970	0.6450
Ei	0.7930	0.6460
Ek	0.7980	0.6460
Em	0.7970	0.6470
Eo	0.7970	0.6470
Eq	0.8000	0.6470
Es	0.7950	0.6460
Eu	0.7940	0.6460
Ew	0.7960	0.6470
Ey	0.7970	0.6480
FA	0.7980	0.6480
FC	0.8000	0.6480
FE	0.7970	0.6460
FG	0.7980	0.6460
FI	0.7960	0.6460
FK	0.7980	0.6460
FM	0.7960	0.6460
FO	0.7960	0.6460
FQ	0.7930	0.6460
FS	0.7980	0.6460
FU	0.7920	0.6460
FW	0.7940	0.6450
FY	0.7940	0.6470
Fa	0.7930	0.6470
Fc	0.7990	0.6450
Fe	0.7930	0.6450
Fg	0.7970	0.6460
Fi	0.7950	0.6460
Fk	0.7940	0.6480
Fm	0.7960	0.6460
Fo	0.7980	0.6470
Fq	0.8000	0.6460