



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 24, 2024 – 01:51 PM EDT

PDB ID : 6YF7  
Title : Virus-like particle of bacteriophage AC  
Authors : Rumnieks, J.; Kalnins, G.; Sisovs, M.; Lieknina, I.; Tars, K.  
Deposited on : 2020-03-26  
Resolution : 3.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

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>.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

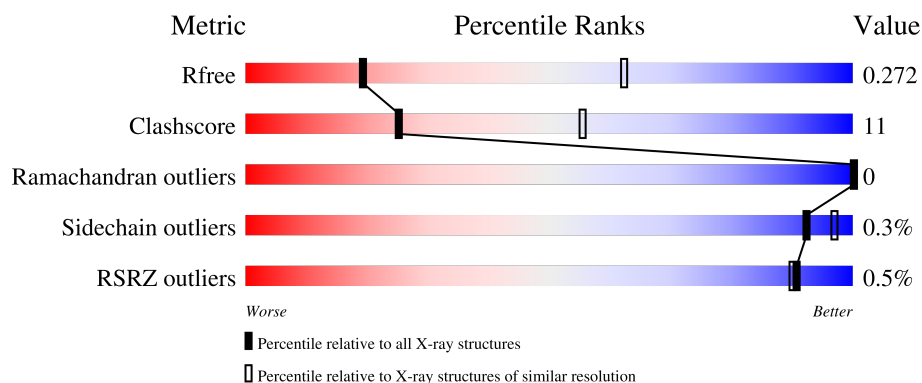
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 Å.

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
















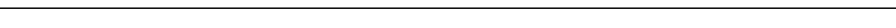











Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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

Mol	Chain	Length	Quality of chain
1	AA	115	
1	AB	115	
1	AC	115	
1	AD	115	
1	AE	115	


























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Mol	Chain	Length	Quality of chain
1	AF	115	 74% 25% .
1	AG	115	 74% 25% .
1	AH	115	 81% 18% .
1	AI	115	 76% 23% .
1	AJ	115	 77% 23% .
1	AK	115	 77% 22% .
1	AL	115	 77% 23% .
1	AM	115	 72% 27% .
1	AN	115	 76% 23% .
1	AO	115	 76% 23% .
1	AP	115	 76% 23% .
1	AQ	115	 76% 23% .
1	AR	115	 77% 23% .
1	AS	115	 69% 30% .
1	AT	115	 81% 18% .
1	AU	115	 67% 32% .
1	AV	115	 78% 21% .
1	AW	115	 80% 19% .
1	AX	115	 75% 24% .
1	AY	115	 75% 24% .
1	AZ	115	 80% 19% .
1	BA	115	 75% 24% .
1	BB	115	 77% 22% .
1	BC	115	 73% 26% .
1	BD	115	 73% 26% .












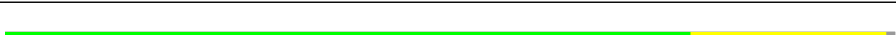

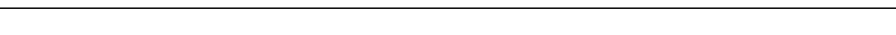
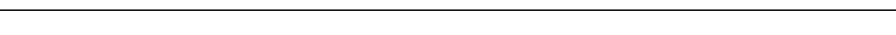
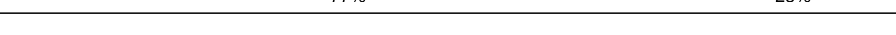

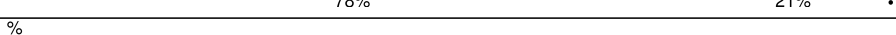







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Mol	Chain	Length	Quality of chain
1	BE	115	 78% 21% .
1	BF	115	 74% 25% .
1	BG	115	 75% 24% .
1	BH	115	 77% 22% .
1	BI	115	 80% 19% .
1	BJ	115	 76% 23% .
1	BK	115	 80% 19% .
1	BL	115	 79% 20% .
1	BM	115	 77% 22% .
1	BN	115	 79% 20% .
1	BO	115	 80% 19% .
1	BP	115	 74% 25% .
1	BQ	115	 78% 21% .
1	BR	115	 78% 21% .
1	BS	115	 77% 22% .
1	BT	115	 77% 23% .
1	BU	115	 77% 22% .
1	BV	115	 77% 23% .
1	BW	115	 76% 23% .
1	BX	115	 79% 20% .
1	BY	115	 76% 23% .
1	BZ	115	 70% 29% .
1	CA	115	 71% 28% .
1	CB	115	 76% 23% .
1	CC	115	 71% 28% .



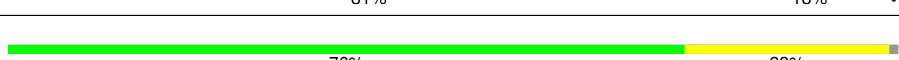
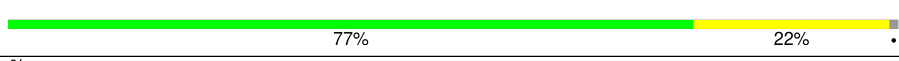
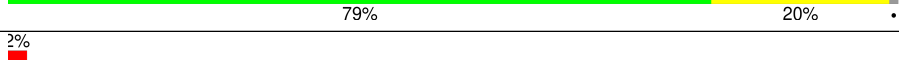
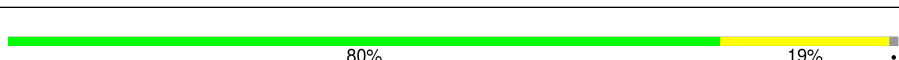
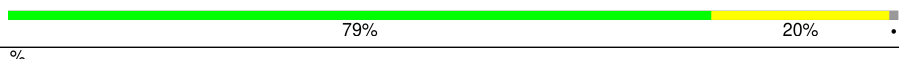
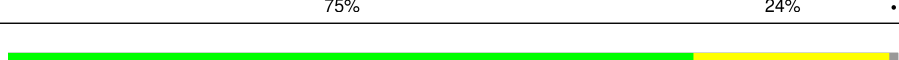

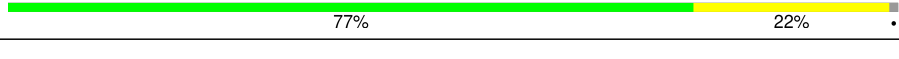

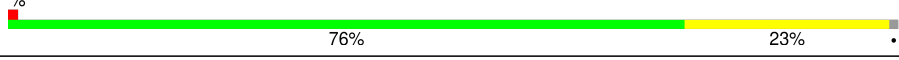
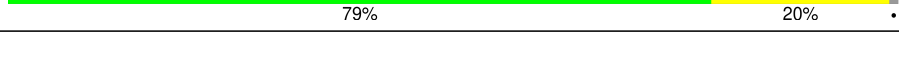

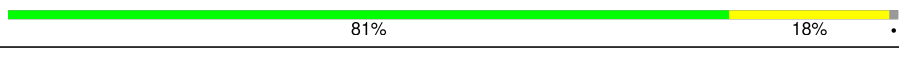
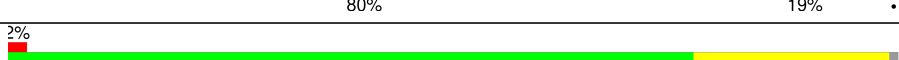





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Mol	Chain	Length	Quality of chain
1	CD	115	 78% 21% .
1	CE	115	 77% 22% .
1	CF	115	 77% 22% .
1	CG	115	 72% 27% .
1	CH	115	 68% 31% .
1	CI	115	 77% 23% .
1	CJ	115	 75% 24% .
1	CK	115	 77% 22% .
1	CL	115	 73% 26% .
1	CM	115	 77% 22% .
1	CN	115	 72% 27% .
1	CO	115	 77% 22% .
1	CP	115	 80% 19% .
1	CQ	115	 76% 23% .
1	CR	115	 77% 23% .
1	CS	115	 81% 18% .
1	CT	115	 78% 21% .
1	CU	115	 78% 21% .
1	CV	115	 80% 19% .
1	CW	115	 78% 21% .
1	CX	115	 79% 20% .
1	CY	115	 77% 23% .
1	CZ	115	 74% 25% .
1	DA	115	 80% 19% .
1	DB	115	 81% 18% .



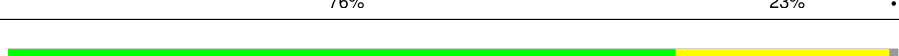

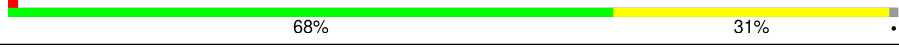
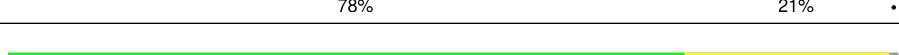

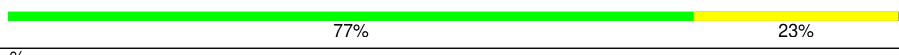
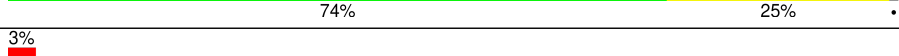
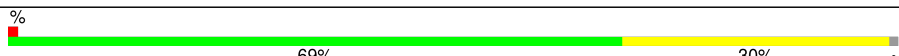

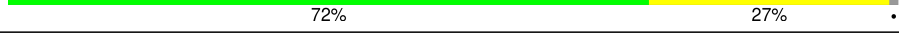
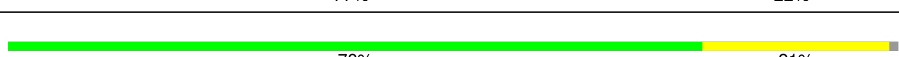





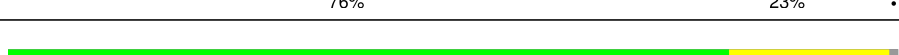



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Mol	Chain	Length	Quality of chain
1	DC	115	
1	DD	115	
1	DE	115	
1	DF	115	
1	DG	115	
1	DH	115	
1	DI	115	
1	DJ	115	
1	DK	115	
1	DL	115	
1	DM	115	
1	DN	115	
1	DO	115	
1	DP	115	
1	DQ	115	
1	DR	115	
1	DS	115	
1	DT	115	
1	DU	115	
1	DV	115	
1	DW	115	
1	DX	115	
1	DY	115	
1	DZ	115	
1	EA	115	






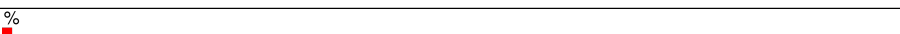


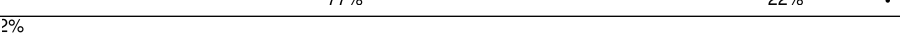

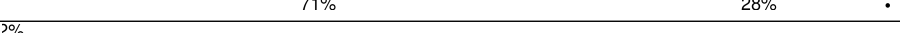














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Mol	Chain	Length	Quality of chain
1	EB	115	
1	EC	115	
1	ED	115	
1	EE	115	
1	EF	115	
1	EG	115	
1	EH	115	
1	EI	115	
1	EJ	115	
1	EK	115	
1	EL	115	
1	EM	115	
1	EN	115	
1	EO	115	
1	EP	115	
1	EQ	115	
1	ER	115	
1	ES	115	
1	ET	115	
1	EU	115	
1	EV	115	
1	EW	115	
1	EX	115	
1	EY	115	
1	EZ	115	

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Mol	Chain	Length	Quality of chain
1	FA	115	 80% 19%
1	FB	115	 2% 77% 23%
1	FC	115	 77% 22%
1	FD	115	 79% 20%
1	FE	115	 78% 21%
1	FF	115	 1% 76% 23%
1	FG	115	 75% 24%
1	FH	115	 77% 22%
1	FI	115	 2% 81% 18%
1	FJ	115	 1% 71% 28%
1	FK	115	 2% 73% 26%
1	FL	115	 77% 23%
1	FM	115	 77% 23%
1	FN	115	 75% 24%
1	FO	115	 73% 26%
1	FP	115	 79% 20%
1	FQ	115	 77% 22%
1	FR	115	 3% 71% 28%
1	FS	115	 76% 23%
1	FT	115	 70% 29%
1	FU	115	 72% 27%
1	FV	115	 80% 19%
1	FW	115	 4% 75% 24%
1	FX	115	 77% 22%
1	FY	115	 77% 23%

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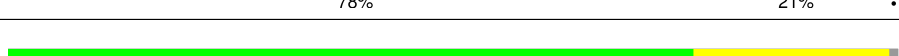

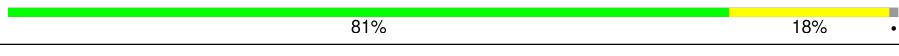
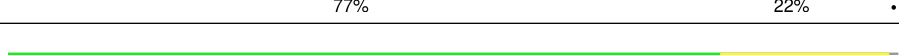

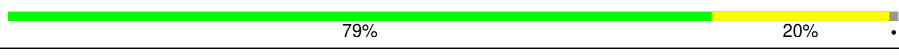
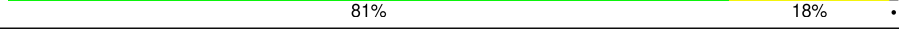
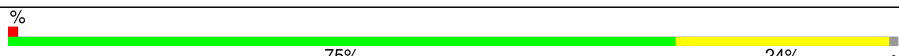

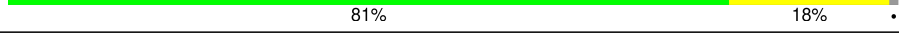
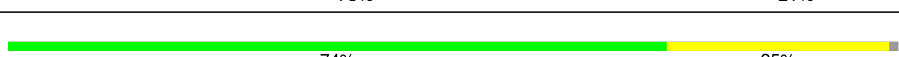





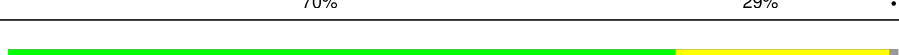





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Mol	Chain	Length	Quality of chain
1	FZ	115	 3% 77% 23%
1	GA	115	 74% 25%
1	GB	115	 73% 26%
1	GC	115	 75% 24%
1	GD	115	 80% 19%
1	GE	115	 79% 20%
1	GF	115	 2% 77% 23%
1	GG	115	 77% 22%
1	GH	115	 % 76% 23%
1	GI	115	 2% 76% 23%
1	GJ	115	 79% 20%
1	GK	115	 72% 27%
1	GL	115	 2% 75% 24%
1	GM	115	 78% 21%
1	GN	115	 80% 19%
1	GO	115	 75% 24%
1	GP	115	 77% 22%
1	GQ	115	 81% 18%
1	GR	115	 77% 23%
1	GS	115	 80% 19%
1	GT	115	 78% 21%
1	GU	115	 75% 24%
1	GV	115	 79% 20%
1	GW	115	 80% 19%
1	GX	115	 % 74% 25%


























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Mol	Chain	Length	Quality of chain
1	GY	115	
1	GZ	115	
1	HA	115	
1	HB	115	
1	HC	115	
1	HD	115	
1	HE	115	
1	HF	115	
1	HG	115	
1	HH	115	
1	HI	115	
1	HJ	115	
1	HK	115	
1	HL	115	
1	HM	115	
1	HN	115	
1	HO	115	
1	HP	115	
1	HQ	115	
1	HR	115	
1	HS	115	
1	HT	115	
1	HU	115	
1	HV	115	
1	HW	115	

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Mol	Chain	Length	Quality of chain
1	HX	115	
1	HY	115	
1	HZ	115	
1	IA	115	
1	IB	115	
1	IC	115	
1	ID	115	
1	IE	115	
1	IF	115	
1	IG	115	
1	IH	115	
1	II	115	
1	IJ	115	
1	IK	115	
1	IL	115	
1	IM	115	
1	IN	115	
1	IO	115	
1	IP	115	
1	IQ	115	
1	IR	115	
1	IS	115	
1	IT	115	
1	IU	115	
1	IV	115	

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Mol	Chain	Length	Quality of chain
1	IW	115	
1	IX	115	
1	IY	115	
1	IZ	115	
1	JA	115	
1	JB	115	
1	JC	115	
1	JD	115	
1	JE	115	
1	JF	115	
1	JG	115	
1	JH	115	
1	JI	115	
1	JJ	115	
1	JK	115	
1	JL	115	
1	JM	115	
1	JN	115	
1	JO	115	
1	JP	115	
1	JQ	115	
1	JR	115	
1	JS	115	
1	JT	115	
1	JU	115	

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Mol	Chain	Length	Quality of chain
1	JV	115	<div> <div></div> <div>78%</div> <div>21%</div> <div></div> </div>
1	JW	115	<div> <div></div> <div>80%</div> <div>19%</div> <div></div> </div>
1	JX	115	<div> <div>2%</div> <div></div> <div>76%</div> <div>23%</div> <div></div> </div>
1	JY	115	<div> <div></div> <div>79%</div> <div>20%</div> <div></div> </div>
1	JZ	115	<div> <div></div> <div>81%</div> <div>18%</div> <div></div> </div>
1	KA	115	<div> <div>3%</div> <div></div> <div>77%</div> <div>22%</div> <div></div> </div>
1	KB	115	<div> <div></div> <div>78%</div> <div>21%</div> <div></div> </div>
1	KC	115	<div> <div></div> <div>79%</div> <div>20%</div> <div></div> </div>
1	KD	115	<div> <div></div> <div>79%</div> <div>20%</div> <div></div> </div>
1	KE	115	<div> <div></div> <div>79%</div> <div>20%</div> <div></div> </div>
1	KF	115	<div> <div></div> <div>81%</div> <div>18%</div> <div></div> </div>
1	KG	115	<div> <div></div> <div>79%</div> <div>20%</div> <div></div> </div>
1	KH	115	<div> <div></div> <div>72%</div> <div>27%</div> <div></div> </div>
1	KI	115	<div> <div>2%</div> <div></div> <div>78%</div> <div>21%</div> <div></div> </div>
1	KJ	115	<div> <div></div> <div>77%</div> <div>23%</div> <div></div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 231390 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Coat protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	AB	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	AC	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	AD	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	AE	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	AF	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	AG	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	AH	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	AI	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	AJ	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	AK	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	AL	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	AM	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	AN	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	AO	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	AP	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AQ	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	AR	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	AS	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	AT	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	AU	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	AV	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	AW	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	AX	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	AY	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	AZ	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	BA	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	BB	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	BC	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	BD	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	BE	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	BF	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	BG	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	BH	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	BI	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	BJ	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	BK	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	BL	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	BM	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	BN	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	BO	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	BP	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	BQ	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	BR	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	BS	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	BT	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	BU	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	BV	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	BW	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	BX	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	BY	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	BZ	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	CA	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	CB	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	CC	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	CD	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	CE	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	CF	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	CG	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	CH	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	CI	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	CJ	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	CK	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	CL	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	CM	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	CN	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	CO	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	CP	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	CQ	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	CR	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	CS	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	CT	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	CU	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	CV	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	CW	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	CX	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	CY	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	CZ	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	DA	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	DB	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	DC	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	DD	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	DE	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	DF	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	DG	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	DH	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	DI	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	DJ	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	DK	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	DL	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	DM	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	DN	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	DO	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	DP	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	DQ	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	DR	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	DS	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	DT	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	DU	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	DV	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	DW	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	DX	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	DY	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	DZ	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	EA	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	EB	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	EC	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	ED	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	EE	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	EF	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	EG	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	EH	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	EI	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	EJ	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	EK	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	EL	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	EM	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	EN	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	EO	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	EP	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	EQ	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	ER	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	ES	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	ET	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	EU	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	EV	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	EW	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	EX	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	EY	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	EZ	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	FA	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	FB	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	FC	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	FD	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	FE	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	FF	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	FG	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	FH	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	FI	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	FJ	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	FK	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	FL	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	FM	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	FN	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	FO	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	FP	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	FQ	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	FR	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	FS	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	FT	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	FU	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	FV	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	FW	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	FX	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	FY	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	FZ	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	GA	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	GB	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	GC	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	GD	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	GE	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	GF	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	GG	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	GH	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	GI	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	GJ	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	GK	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	GL	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	GM	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	GN	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	GO	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	GP	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	GQ	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	GR	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	GS	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	GT	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	GU	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	GV	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	GW	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	GX	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	GY	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	GZ	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	HA	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	HB	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	HC	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	HD	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	HE	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	HF	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	HG	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	HH	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	HI	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	HJ	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	HK	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	HL	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	HM	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	HN	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	HO	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	HP	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	HQ	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	HR	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	HS	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	HT	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	HU	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	HV	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	HW	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	HX	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	HY	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	HZ	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	IA	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	IB	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	IC	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	ID	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	IE	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	IF	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	IG	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	IH	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	II	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	IJ	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	IK	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	IL	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	IM	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	IN	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	IO	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	IP	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	IQ	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	IR	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	IS	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	IT	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	IU	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	IV	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	IW	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	IX	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	IY	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	IZ	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	JA	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	JB	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	JC	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	JD	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	JE	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	JF	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	JG	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	JH	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	JI	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	JJ	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	JK	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	JL	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	JM	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	JN	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	JO	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	JP	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	JQ	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	JR	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	JS	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	JT	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	JU	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	JV	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	JW	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	JX	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	JY	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	JZ	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	KA	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	KB	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	KC	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	KD	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	KE	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	KF	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	KG	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	KH	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	KI	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			
1	KJ	114	Total	C	N	O	S	0	0	0
			857	545	141	170	1			

### 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 electron 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 dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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: Coat protein

Chain AA: 




- Molecule 1: Coat protein

Chain AB: 




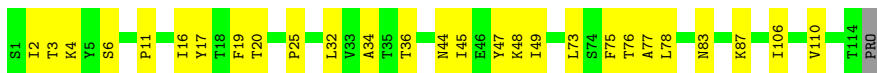
- Molecule 1: Coat protein

Chain AC: 




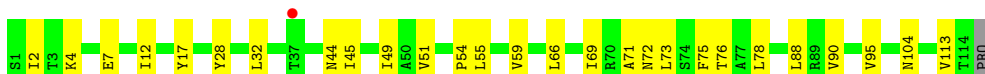
- Molecule 1: Coat protein

Chain AD: 




- Molecule 1: Coat protein

Chain AE: 




- Molecule 1: Coat protein

Chain AF:  74% 25%




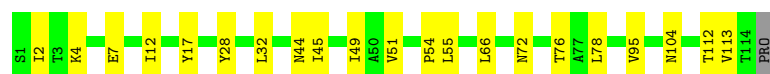
• Molecule 1: Coat protein

Chain AG:  74% 25%




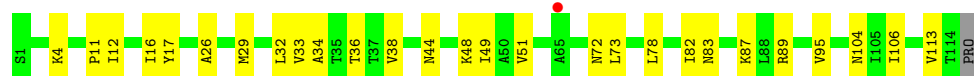
• Molecule 1: Coat protein

Chain AH:  81% 18%




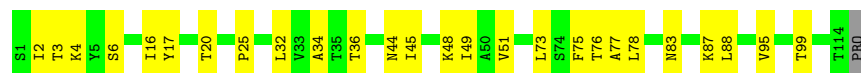
• Molecule 1: Coat protein

Chain AI:  76% 23%




• Molecule 1: Coat protein

Chain AJ:  77% 23%




• Molecule 1: Coat protein

Chain AK:  77% 22%

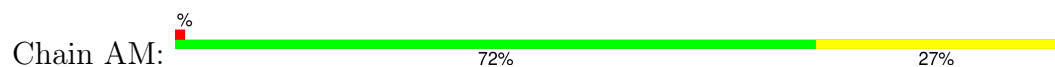


• Molecule 1: Coat protein

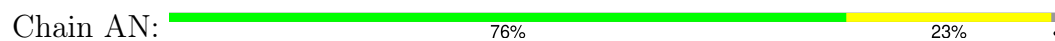
Chain AL:  77% 23%



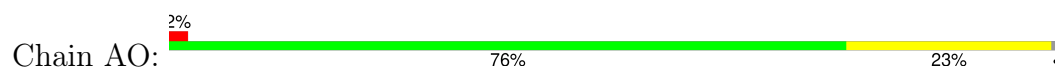
• Molecule 1: Coat protein



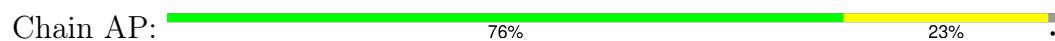
• Molecule 1: Coat protein



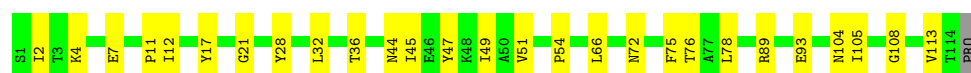
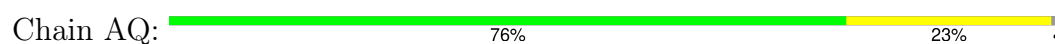
• Molecule 1: Coat protein



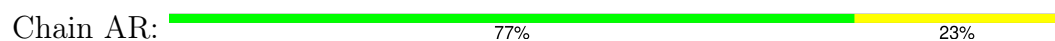
• Molecule 1: Coat protein



• Molecule 1: Coat protein




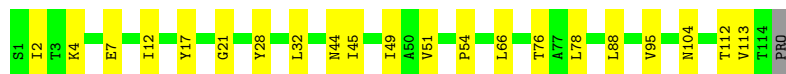
• Molecule 1: Coat protein



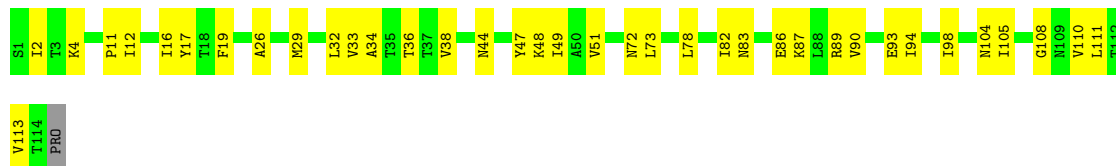
• Molecule 1: Coat protein




## • Molecule 1: Coat protein

Chain AT:  81% 18%


## • Molecule 1: Coat protein

Chain AU:  67% 32%


## • Molecule 1: Coat protein

Chain AV:  78% 21%


## • Molecule 1: Coat protein

Chain AW:  80% 19%


## • Molecule 1: Coat protein

Chain AX:  75% 24%

## • Molecule 1: Coat protein

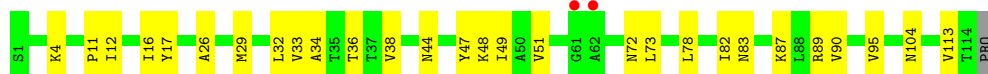
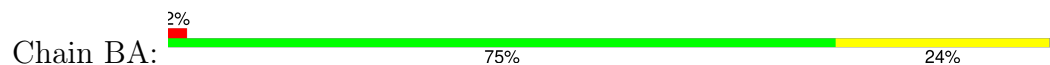
Chain AY:  75% 24%

## • Molecule 1: Coat protein

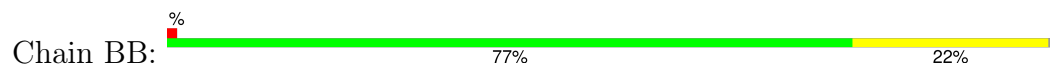
Chain AZ:  80% 19%



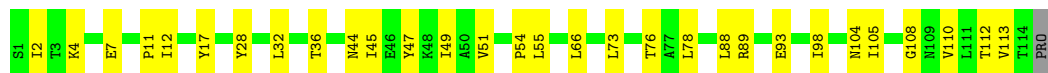
- Molecule 1: Coat protein



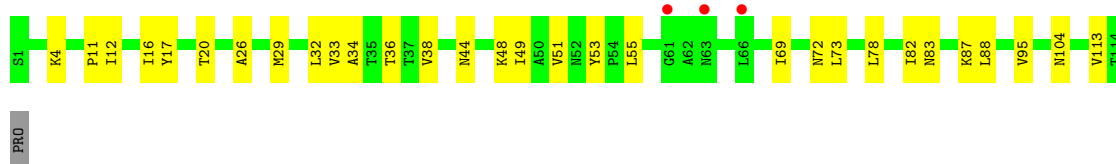
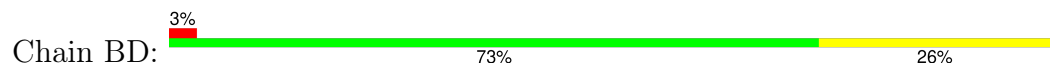
- Molecule 1: Coat protein



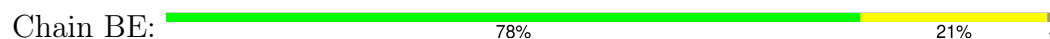
- Molecule 1: Coat protein



- Molecule 1: Coat protein



- Molecule 1: Coat protein




- Molecule 1: Coat protein




- Molecule 1: Coat protein

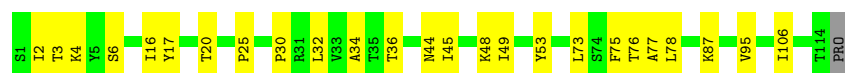


Chain BG:  75% 24%




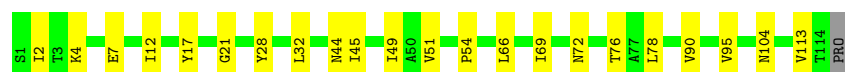
• Molecule 1: Coat protein

Chain BH:  77% 22%




• Molecule 1: Coat protein

Chain BI:  80% 19%




• Molecule 1: Coat protein

Chain BJ:  76% 23%




• Molecule 1: Coat protein

Chain BK:  80% 19%




• Molecule 1: Coat protein

Chain BL:  79% 20%




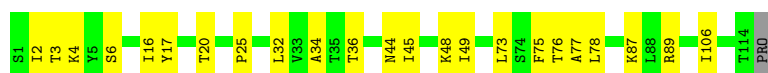
• Molecule 1: Coat protein

Chain BM:  77% 22%




• Molecule 1: Coat protein

Chain BN:  79% 20%




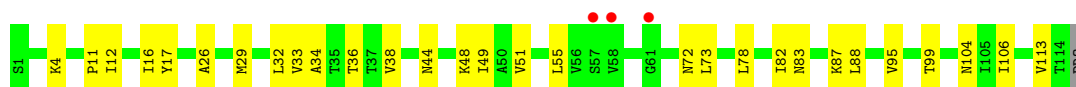
• Molecule 1: Coat protein

Chain BO:  80% 19%




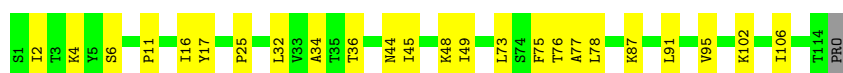
• Molecule 1: Coat protein

Chain BP:  3% 74% 25%




• Molecule 1: Coat protein

Chain BQ:  78% 21%




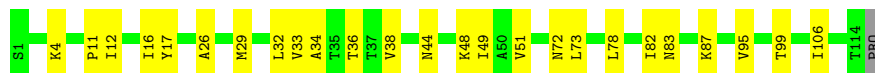
• Molecule 1: Coat protein

Chain BR:  78% 21%




• Molecule 1: Coat protein

Chain BS:  77% 22%




• Molecule 1: Coat protein

Chain BT:  77% 23%




• Molecule 1: Coat protein

Chain BU:  77% 22%




• Molecule 1: Coat protein

Chain BV:  77% 23% 2%




• Molecule 1: Coat protein

Chain BW:  76% 23%




• Molecule 1: Coat protein

Chain BX:  79% 20%



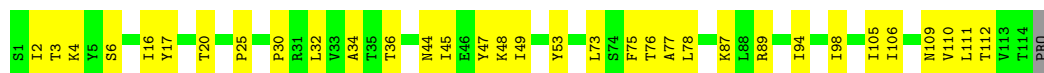
• Molecule 1: Coat protein

Chain BY:  76% 23% %



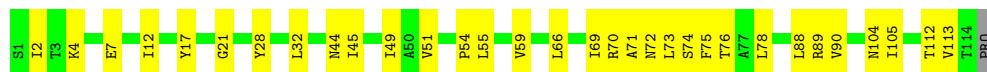
• Molecule 1: Coat protein

Chain BZ:  70% 29%




• Molecule 1: Coat protein

Chain CA:  71% 28%



• Molecule 1: Coat protein

Chain CB:  76% 23%




• Molecule 1: Coat protein

Chain CC:  71% 28%




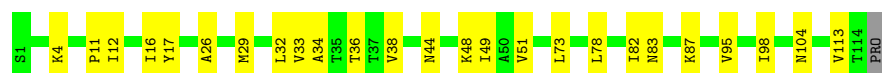
• Molecule 1: Coat protein

Chain CD:  78% 21%




• Molecule 1: Coat protein

Chain CE:  77% 22%



• Molecule 1: Coat protein

Chain CF:  77% 22%



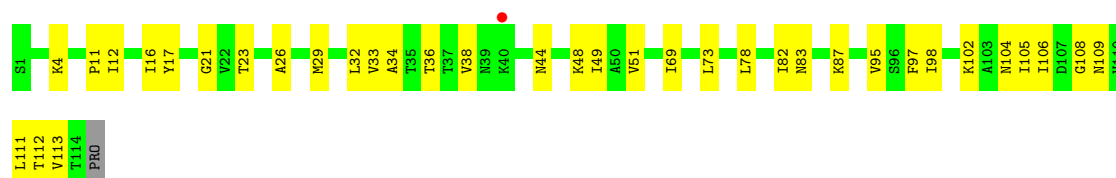
• Molecule 1: Coat protein

Chain CG:  72% 27%




• Molecule 1: Coat protein

Chain CH:  68% 31%




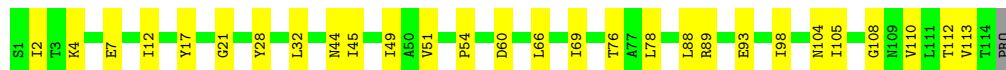
- Molecule 1: Coat protein

Chain CI:  77% 23%




- Molecule 1: Coat protein

Chain CJ:  75% 24%




- Molecule 1: Coat protein

Chain CK:  77% 22%




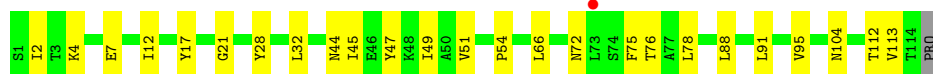
- Molecule 1: Coat protein

Chain CL:  73% 26%



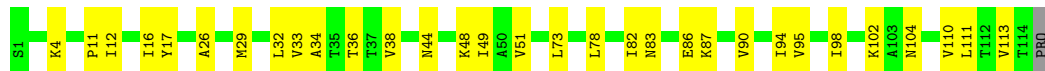
- Molecule 1: Coat protein

Chain CM:  77% 22%




- Molecule 1: Coat protein

Chain CN:  72% 27%




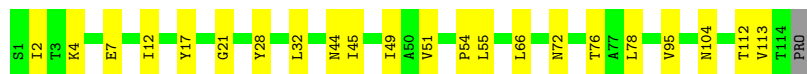
- Molecule 1: Coat protein

Chain CO:  77% 22%




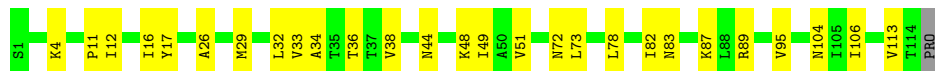
- Molecule 1: Coat protein

Chain CP:  80% 19%




- Molecule 1: Coat protein

Chain CQ:  76% 23%




- Molecule 1: Coat protein

Chain CR:  77% 23%




- Molecule 1: Coat protein

Chain CS:  81% 18%




- Molecule 1: Coat protein

Chain CT:  78% 21%




- Molecule 1: Coat protein

Chain CU:  78% 21%

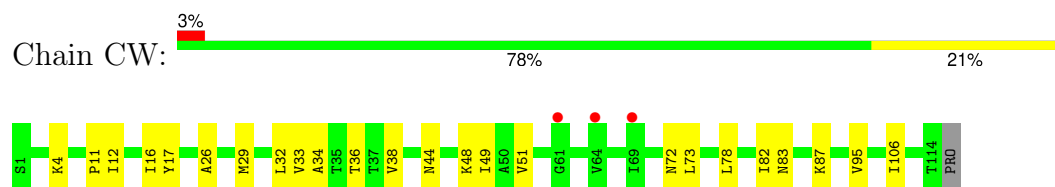


- Molecule 1: Coat protein

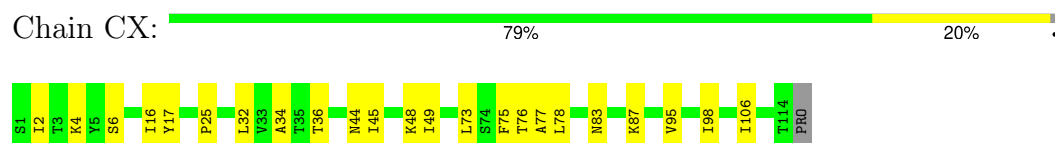
Chain CV:  80% 19%



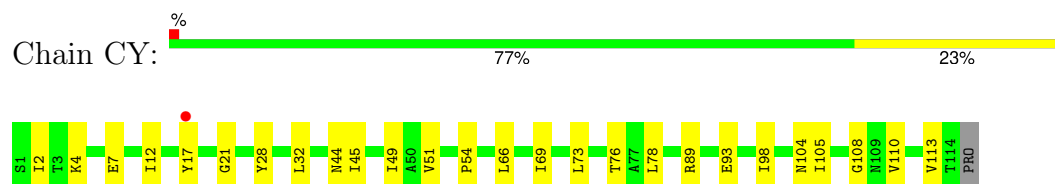
## • Molecule 1: Coat protein



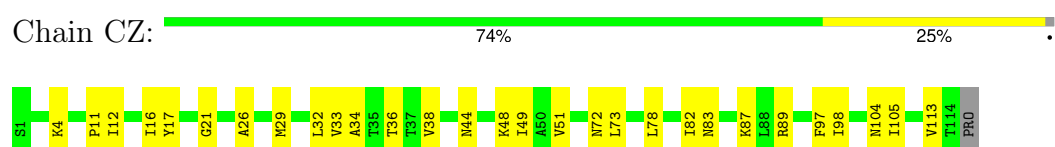
## • Molecule 1: Coat protein



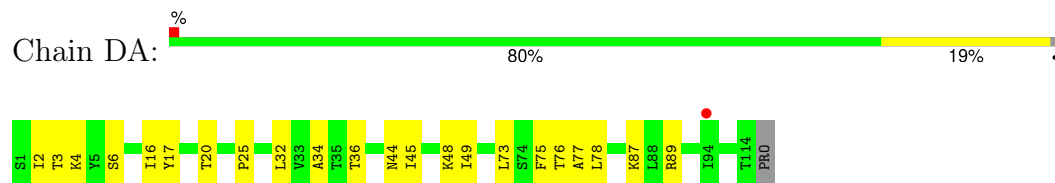
## • Molecule 1: Coat protein



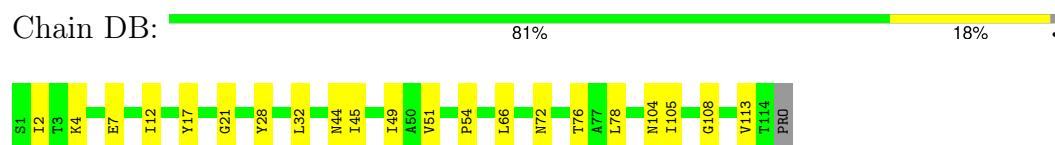
## • Molecule 1: Coat protein



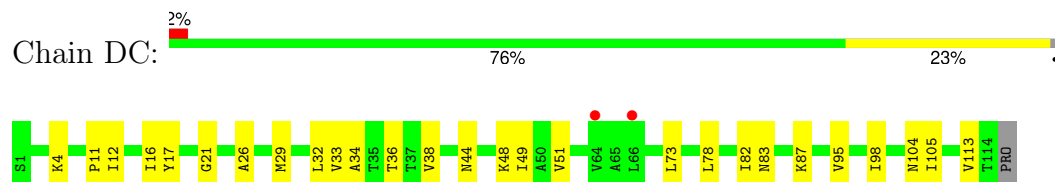
## • Molecule 1: Coat protein




## • Molecule 1: Coat protein



## • Molecule 1: Coat protein




- Molecule 1: Coat protein

Chain DD:  81% 18%




- Molecule 1: Coat protein

Chain DE:  81% 18%




- Molecule 1: Coat protein

Chain DF:  76% 23%




- Molecule 1: Coat protein

Chain DG:  77% 22%




- Molecule 1: Coat protein

Chain DH:  79% 20%




- Molecule 1: Coat protein

Chain DI:  75% 24%




- Molecule 1: Coat protein

Chain DJ:  80% 19%






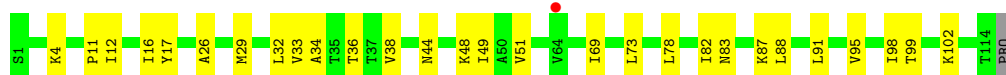
- Molecule 1: Coat protein

Chain DK:  79% 20%




- Molecule 1: Coat protein

Chain DL:  75% 24%




- Molecule 1: Coat protein

Chain DM:  77% 22%




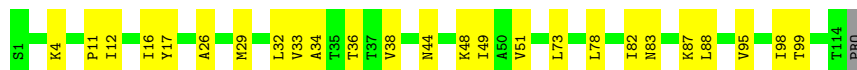
- Molecule 1: Coat protein

Chain DN:  79% 20%




- Molecule 1: Coat protein

Chain DO:  77% 22%




- Molecule 1: Coat protein

Chain DP:  78% 21%

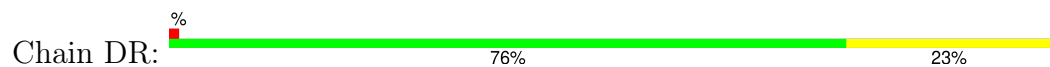


- Molecule 1: Coat protein

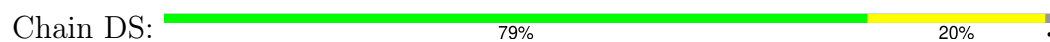
Chain DQ:  77% 22%



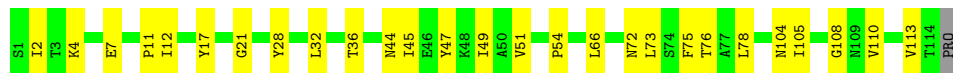
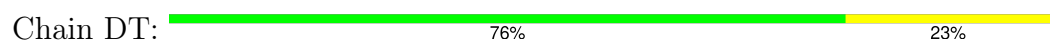
- Molecule 1: Coat protein



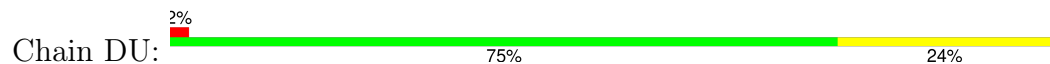
- Molecule 1: Coat protein



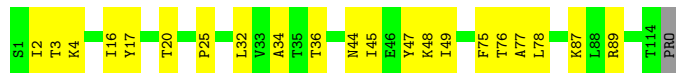
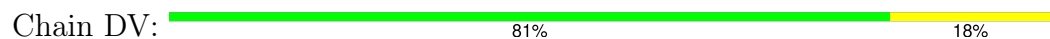
- Molecule 1: Coat protein



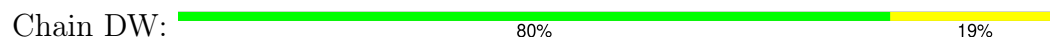
- Molecule 1: Coat protein



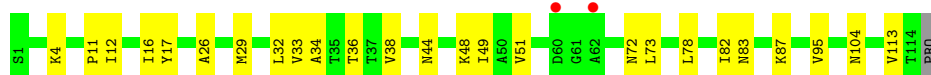
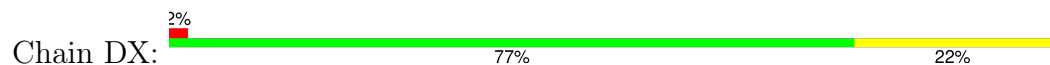
- Molecule 1: Coat protein



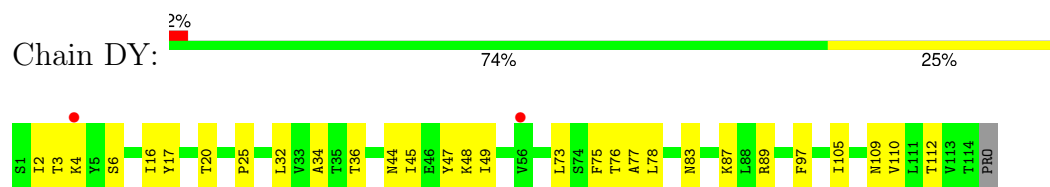
- Molecule 1: Coat protein



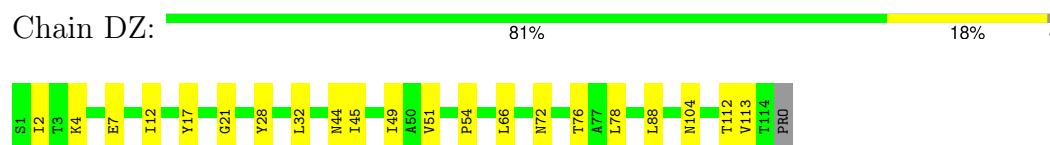
- Molecule 1: Coat protein



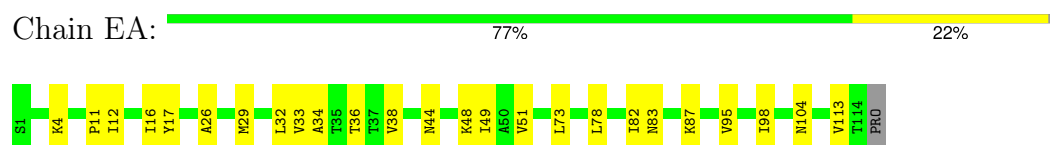
## ● Molecule 1: Coat protein



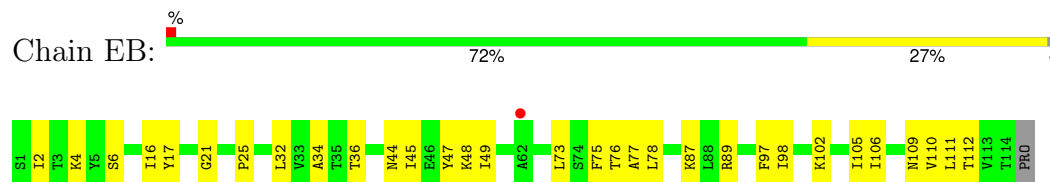
## ● Molecule 1: Coat protein



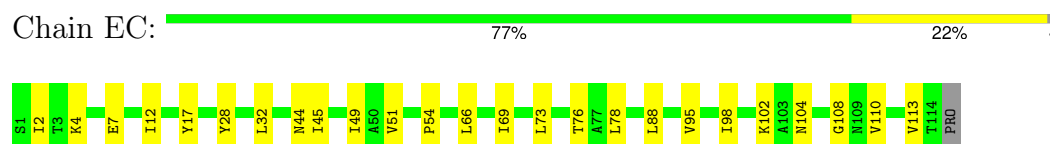
## ● Molecule 1: Coat protein



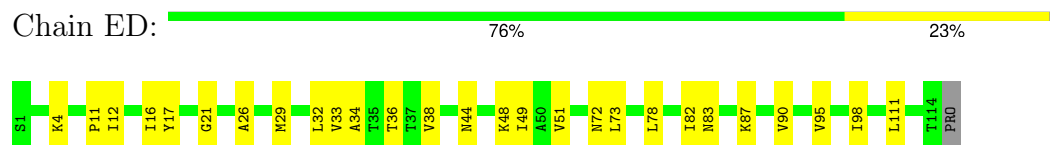
## ● Molecule 1: Coat protein



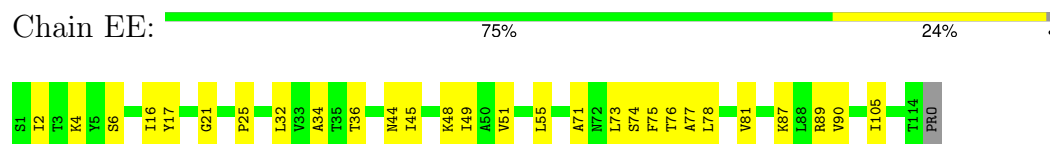
## ● Molecule 1: Coat protein



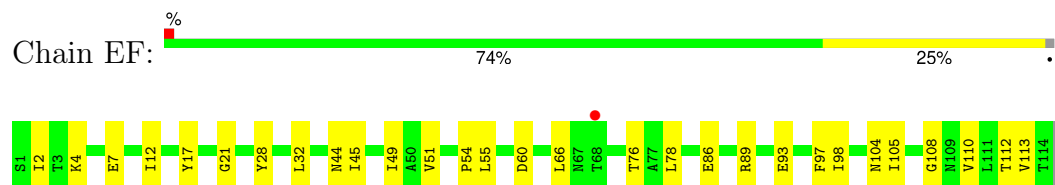
## ● Molecule 1: Coat protein



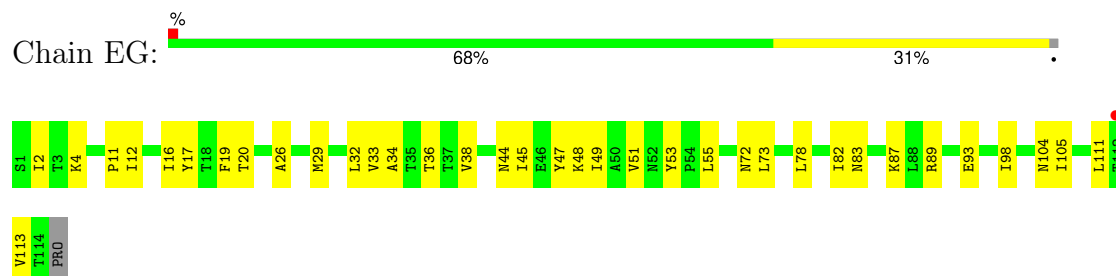
## ● Molecule 1: Coat protein



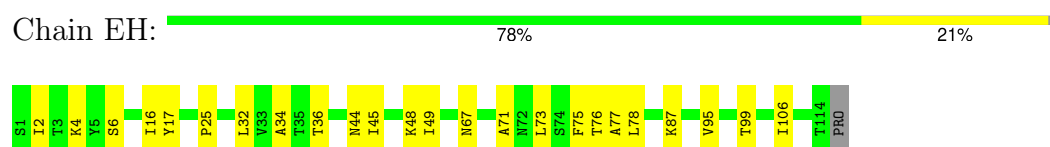
- Molecule 1: Coat protein



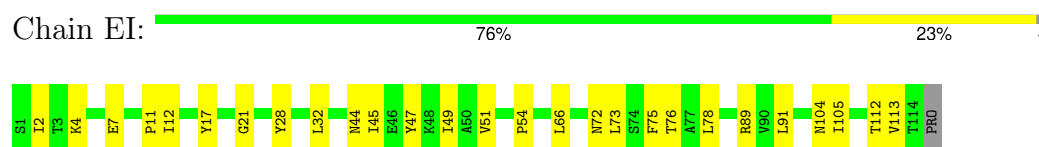
- Molecule 1: Coat protein



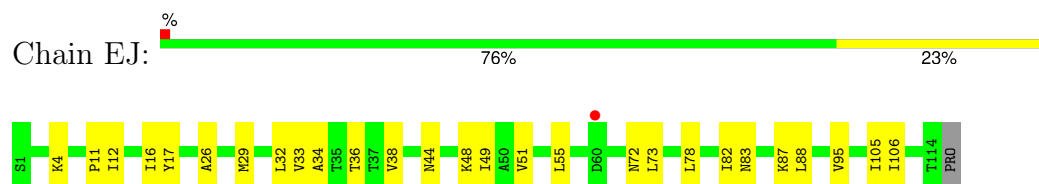
- Molecule 1: Coat protein



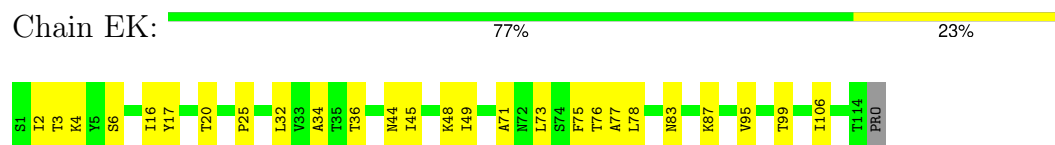
- Molecule 1: Coat protein



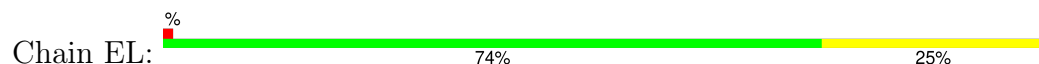
- Molecule 1: Coat protein



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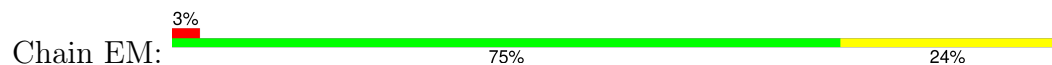


- Molecule 1: Coat protein

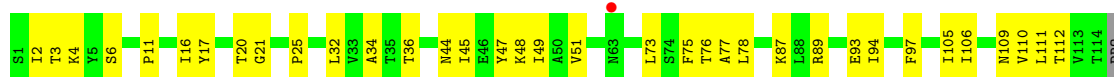




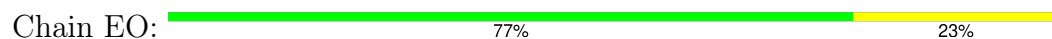
- Molecule 1: Coat protein



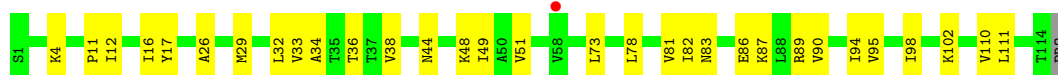
- Molecule 1: Coat protein



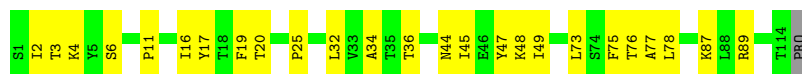
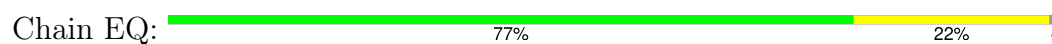
- Molecule 1: Coat protein



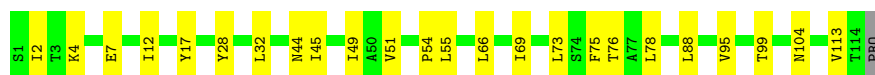
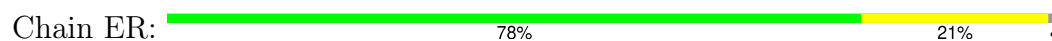
- Molecule 1: Coat protein



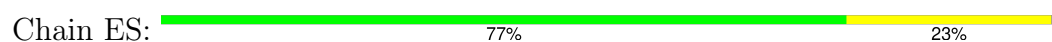
- Molecule 1: Coat protein

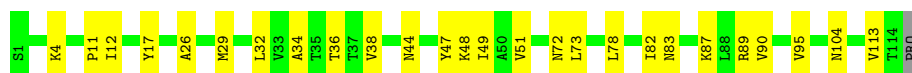


- Molecule 1: Coat protein



- Molecule 1: Coat protein





- Molecule 1: Coat protein

Chain ET: 74% 25%



- Molecule 1: Coat protein

Chain EU: 72% 27%



- Molecule 1: Coat protein

Chain EV: 77% 23%



- Molecule 1: Coat protein

Chain EW: 80% 19%



- Molecule 1: Coat protein

Chain EX: 81% 18%



- Molecule 1: Coat protein

Chain EY: 76% 23%

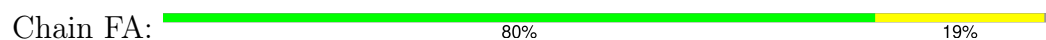


- Molecule 1: Coat protein

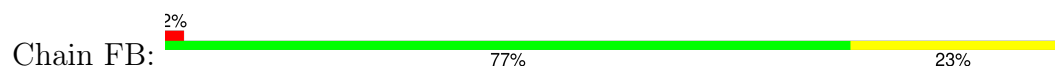
Chain EZ: 81% 18%



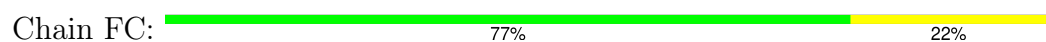
- Molecule 1: Coat protein



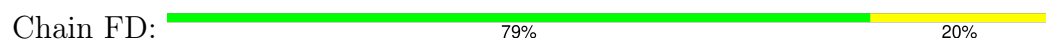
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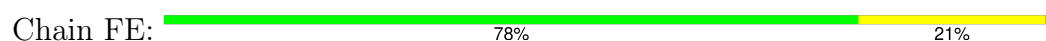
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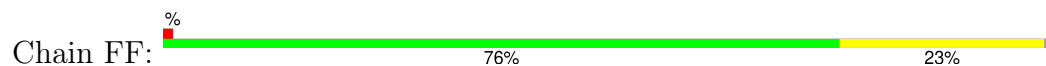
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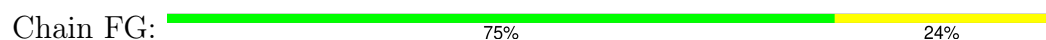
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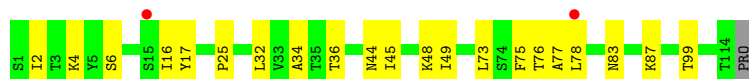
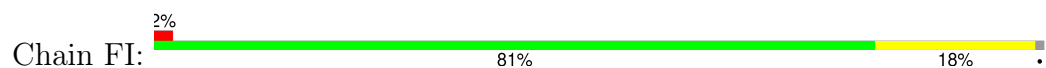




- Molecule 1: Coat protein



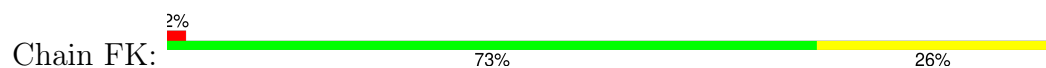
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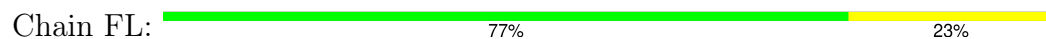
- Molecule 1: Coat protein



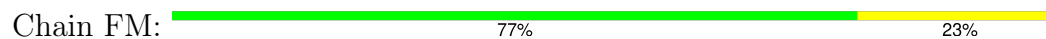
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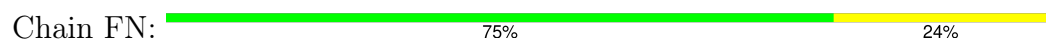
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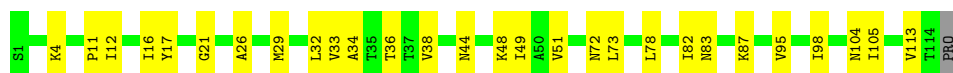
- Molecule 1: Coat protein



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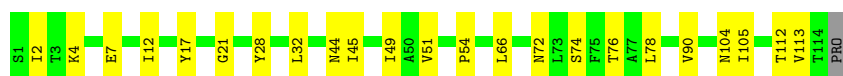
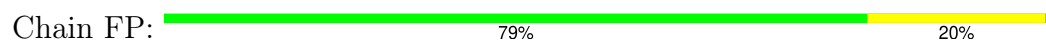




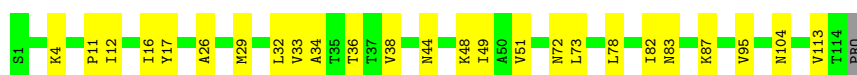
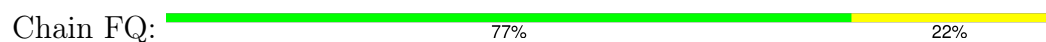
- Molecule 1: Coat protein



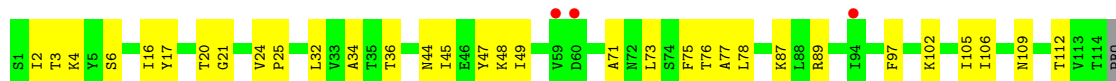
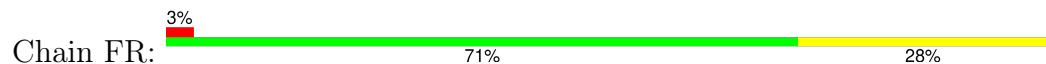
- Molecule 1: Coat protein



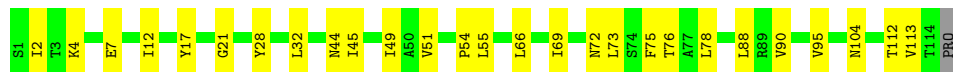
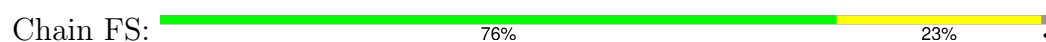
- Molecule 1: Coat protein



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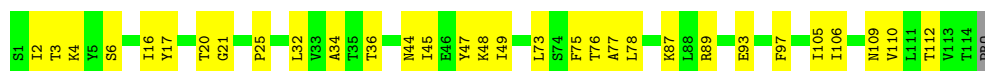


- Molecule 1: Coat protein



- Molecule 1: Coat protein





- Molecule 1: Coat protein

Chain FV: 80% 19%



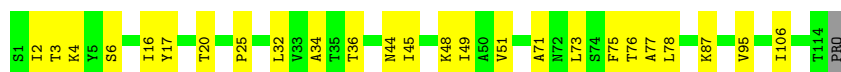
- Molecule 1: Coat protein

Chain FW: 4% 75% 24%



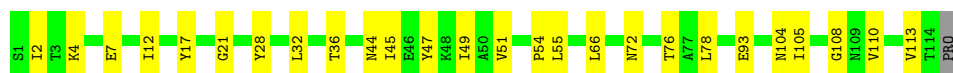
- Molecule 1: Coat protein

Chain FX: 77% 22%



- Molecule 1: Coat protein

Chain FY: 77% 23%



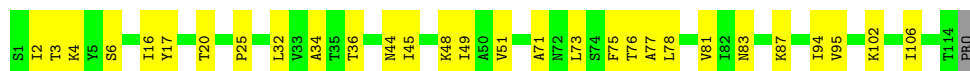
- Molecule 1: Coat protein

Chain FZ: 3% 77% 23%



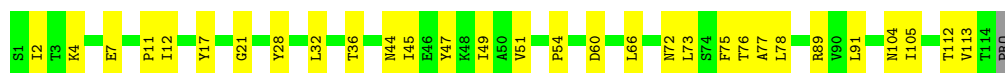
- Molecule 1: Coat protein

Chain GA: 74% 25%

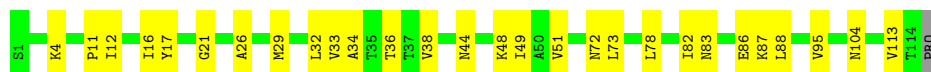
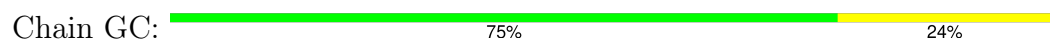


- Molecule 1: Coat protein

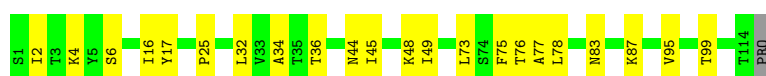
Chain GB: 73% 26%



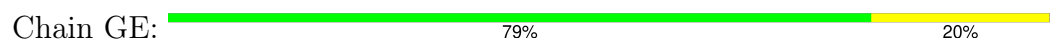
- Molecule 1: Coat protein



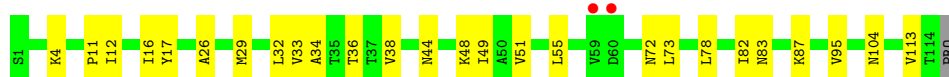
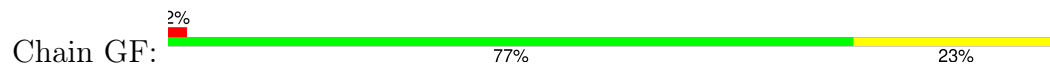
- Molecule 1: Coat protein



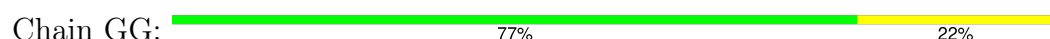
- Molecule 1: Coat protein



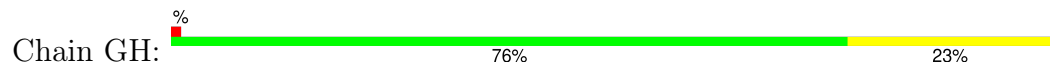
- Molecule 1: Coat protein



- Molecule 1: Coat protein



- Molecule 1: Coat protein

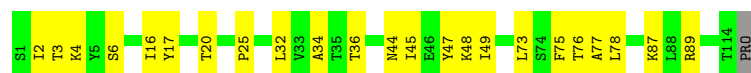
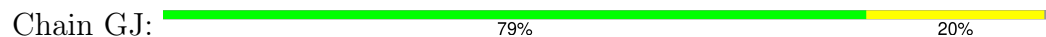


- Molecule 1: Coat protein





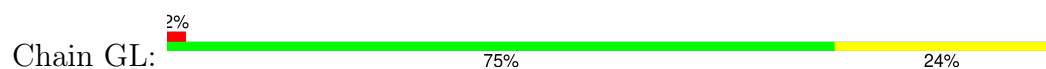
• Molecule 1: Coat protein



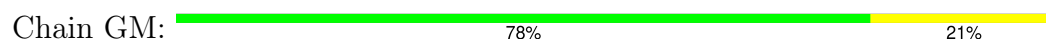
• Molecule 1: Coat protein



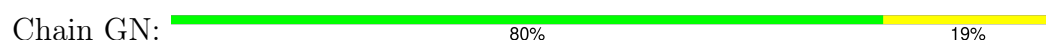
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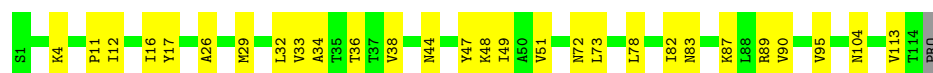
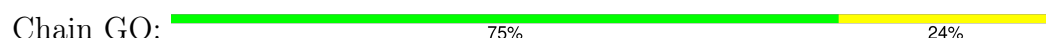
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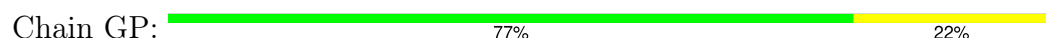
• Molecule 1: Coat protein

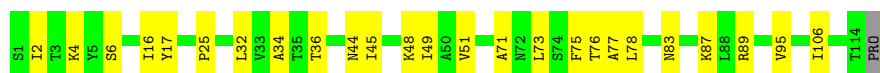


• Molecule 1: Coat protein

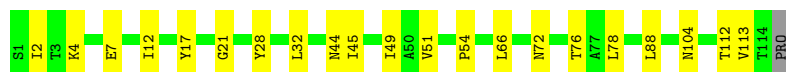
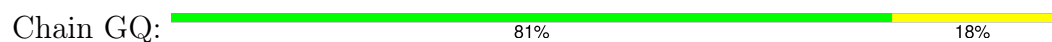


• Molecule 1: Coat protein

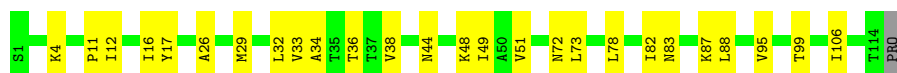
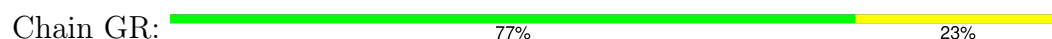




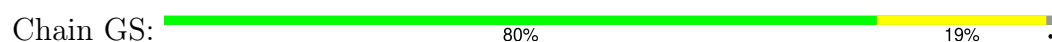
- Molecule 1: Coat protein



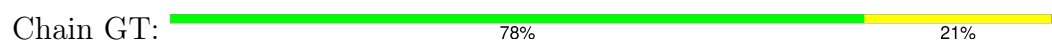
- Molecule 1: Coat protein



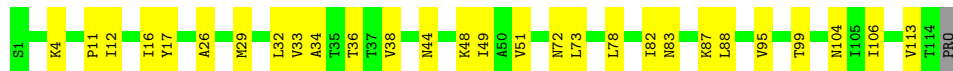
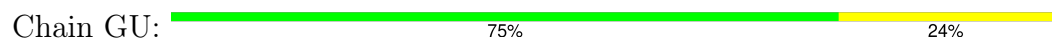
- Molecule 1: Coat protein



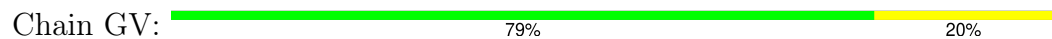
- Molecule 1: Coat protein



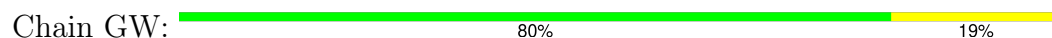
- Molecule 1: Coat protein



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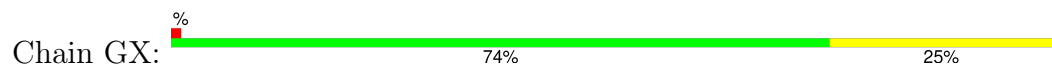


- Molecule 1: Coat protein

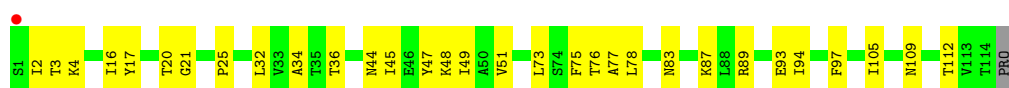




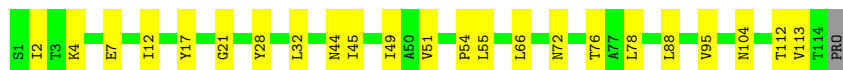
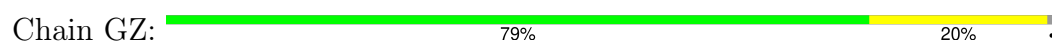
- Molecule 1: Coat protein



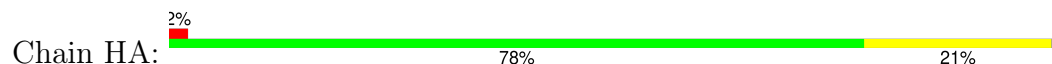
- Molecule 1: Coat protein



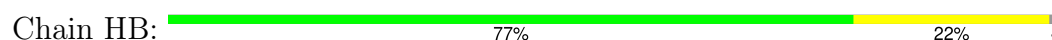
- Molecule 1: Coat protein



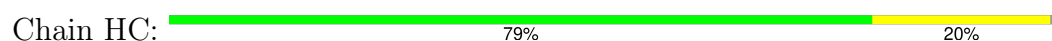
- Molecule 1: Coat protein



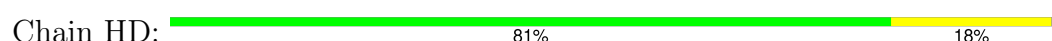
- Molecule 1: Coat protein



- Molecule 1: Coat protein

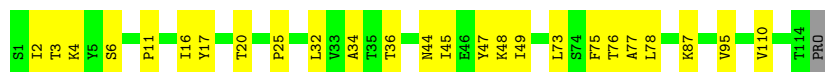
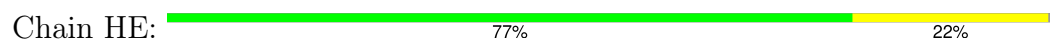


- Molecule 1: Coat protein

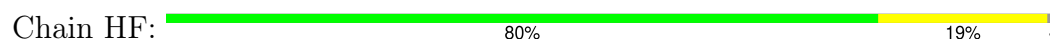




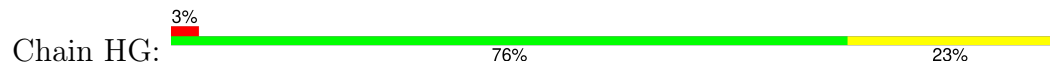
- Molecule 1: Coat protein



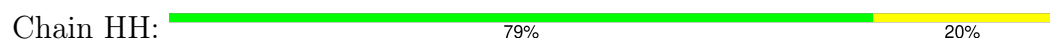
- Molecule 1: Coat protein



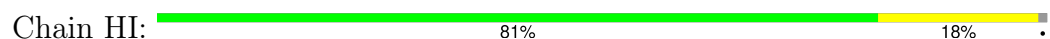
- Molecule 1: Coat protein



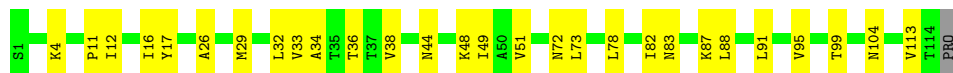
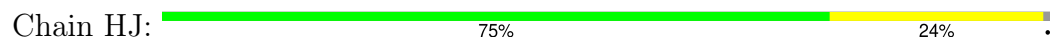
- Molecule 1: Coat protein



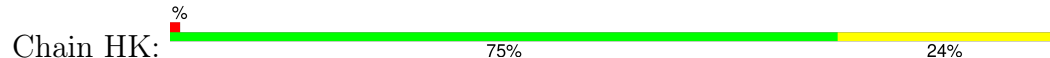
- Molecule 1: Coat protein

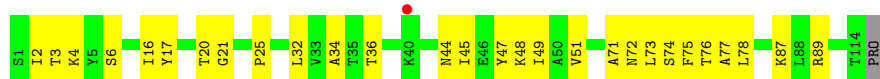


- Molecule 1: Coat protein

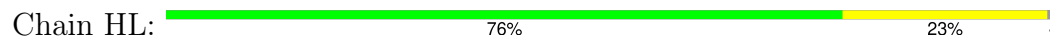


- Molecule 1: Coat protein

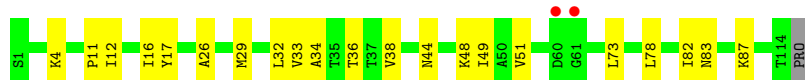
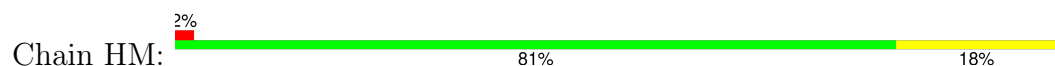




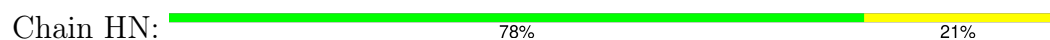
- Molecule 1: Coat protein



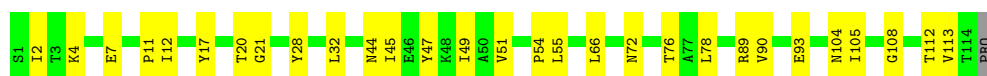
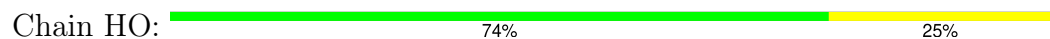
- Molecule 1: Coat protein



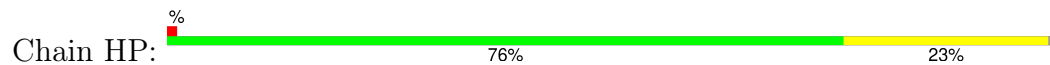
- Molecule 1: Coat protein



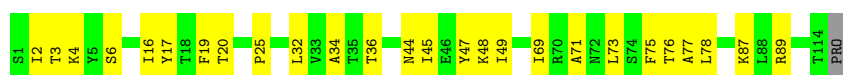
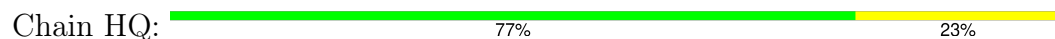
- Molecule 1: Coat protein



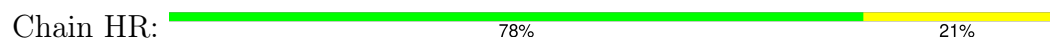
- Molecule 1: Coat protein



- Molecule 1: Coat protein



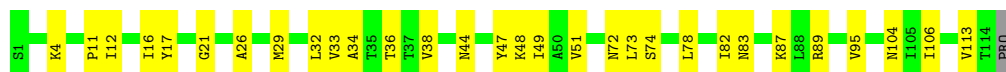
- Molecule 1: Coat protein



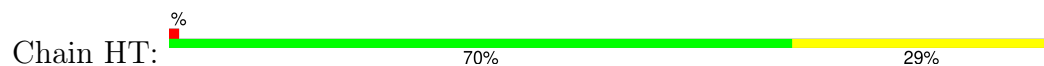




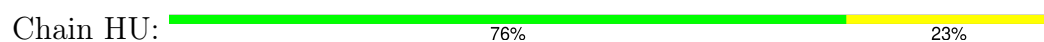
- Molecule 1: Coat protein



- Molecule 1: Coat protein



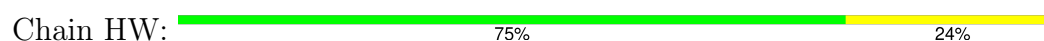
- Molecule 1: Coat protein



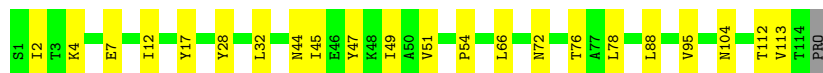
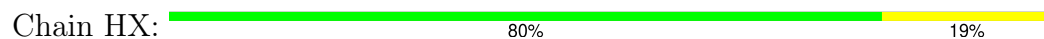
- Molecule 1: Coat protein



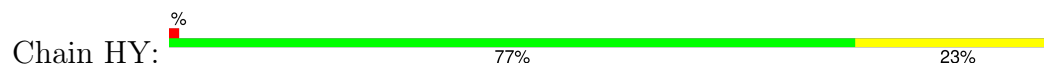
- Molecule 1: Coat protein



- Molecule 1: Coat protein

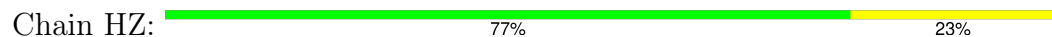


- Molecule 1: Coat protein

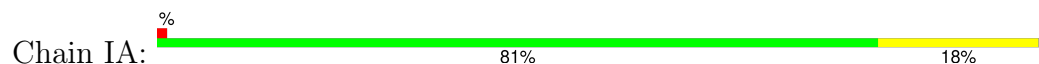




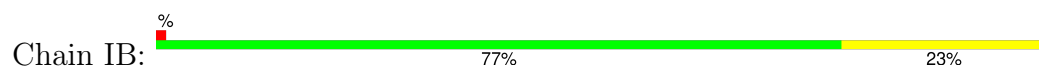
- Molecule 1: Coat protein



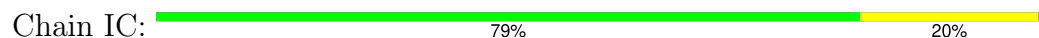
- Molecule 1: Coat protein



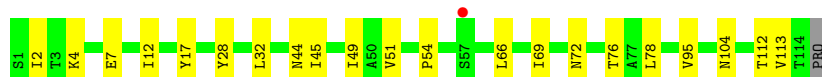
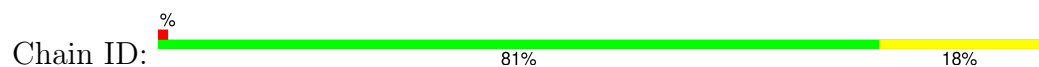
- Molecule 1: Coat protein



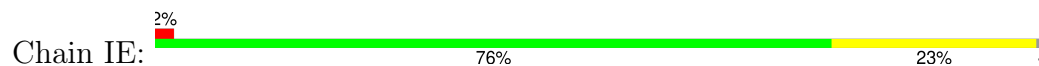
- Molecule 1: Coat protein



- Molecule 1: Coat protein



- Molecule 1: Coat protein




- Molecule 1: Coat protein

Chain IF:  72% 27%




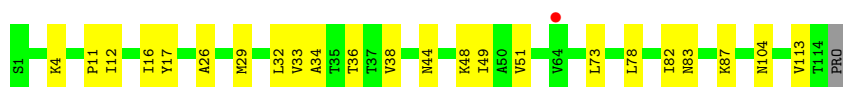
• Molecule 1: Coat protein

Chain IG:  79% 20%




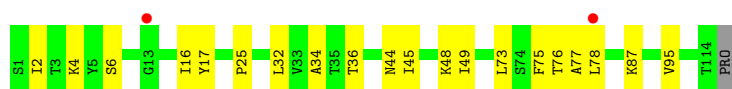
• Molecule 1: Coat protein

Chain IH:  79% 20%




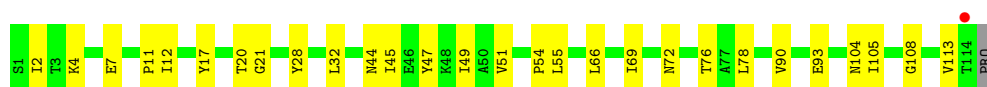
• Molecule 1: Coat protein

Chain II:  82% 17%




• Molecule 1: Coat protein

Chain IJ:  75% 24%




• Molecule 1: Coat protein

Chain IK:  77% 23%



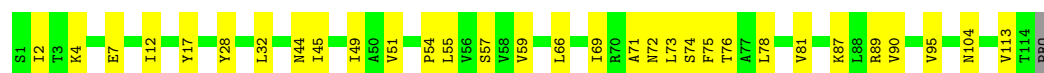
• Molecule 1: Coat protein

Chain IL:  79% 20%




• Molecule 1: Coat protein

Chain IM:  72% 27%




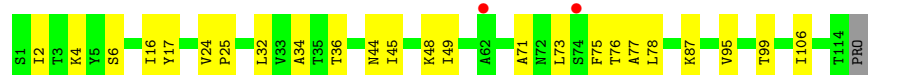
• Molecule 1: Coat protein

Chain IN:  3% 79% 20%




• Molecule 1: Coat protein

Chain IO:  2% 78% 21%




• Molecule 1: Coat protein

Chain IP:  79% 20%




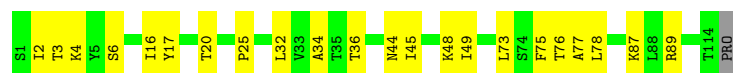
• Molecule 1: Coat protein

Chain IQ:  1% 76% 23%




• Molecule 1: Coat protein

Chain IR:  80% 19%




• Molecule 1: Coat protein

Chain IS:  77% 23%



• Molecule 1: Coat protein

Chain IT:  75% 24%




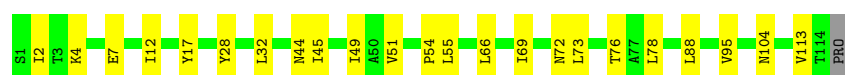
• Molecule 1: Coat protein

Chain IU:  70% 29%




• Molecule 1: Coat protein

Chain IV:  79% 20%




• Molecule 1: Coat protein

Chain IW:  79% 20%




• Molecule 1: Coat protein

Chain IX:  77% 22%



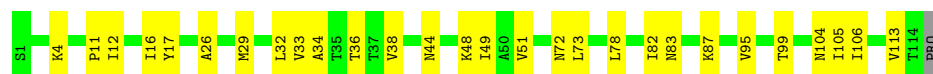
• Molecule 1: Coat protein

Chain IY:  76% 23%



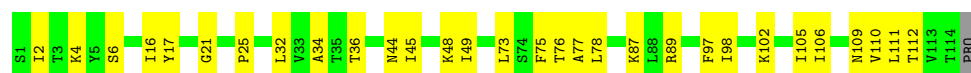
• Molecule 1: Coat protein

Chain IZ:  75% 24%




• Molecule 1: Coat protein

Chain JA:  73% 26%




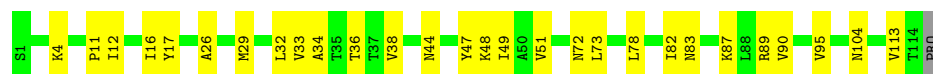
• Molecule 1: Coat protein

Chain JB:  77% 22%




• Molecule 1: Coat protein

Chain JC:  75% 24%



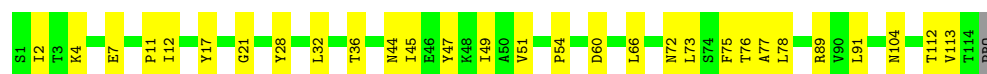
• Molecule 1: Coat protein

Chain JD:  74% 25%




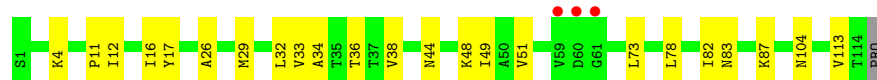
• Molecule 1: Coat protein

Chain JE:  74% 25%




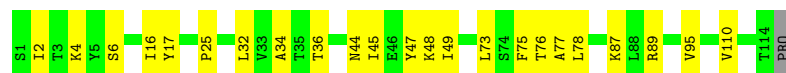
• Molecule 1: Coat protein

Chain JF:  79% 20%




• Molecule 1: Coat protein

Chain JG:  79% 20%




• Molecule 1: Coat protein

Chain JH:  75% 24%




• Molecule 1: Coat protein

Chain JI:  79% 20%




• Molecule 1: Coat protein

Chain JJ:  2% 77% 22%



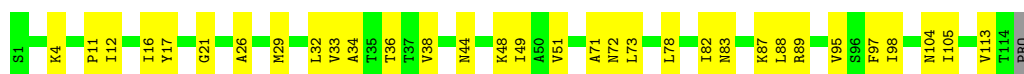
• Molecule 1: Coat protein

Chain JK:  1% 77% 23%




• Molecule 1: Coat protein

Chain JL:  71% 28%



• Molecule 1: Coat protein

Chain JM:  1% 75% 24%

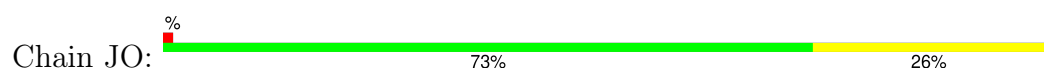


• Molecule 1: Coat protein

Chain JN:  72% 27%



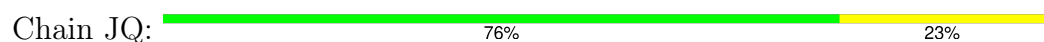
• Molecule 1: Coat protein



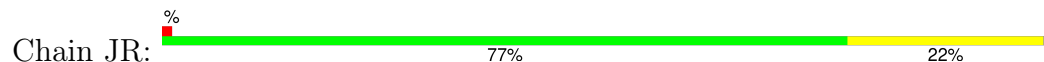
- Molecule 1: Coat protein



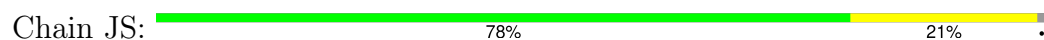
- Molecule 1: Coat protein



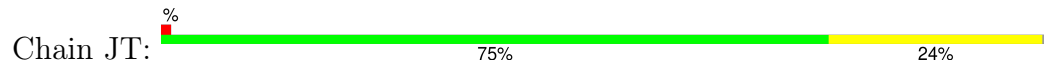
- Molecule 1: Coat protein



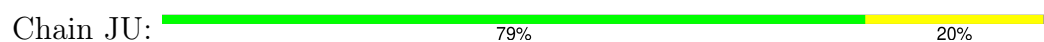
- Molecule 1: Coat protein



- Molecule 1: Coat protein

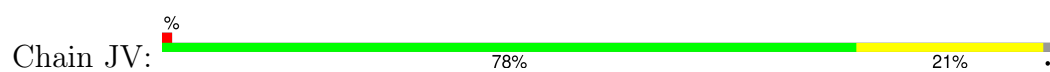


- Molecule 1: Coat protein

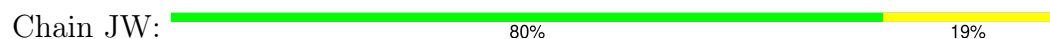


- Molecule 1: Coat protein

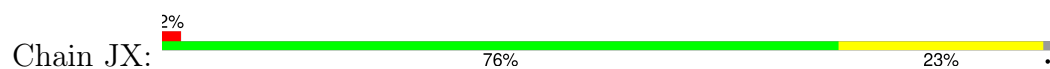




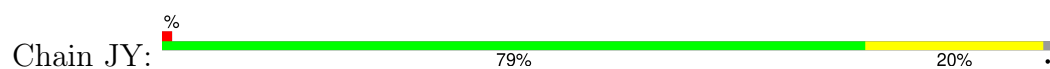
- Molecule 1: Coat protein



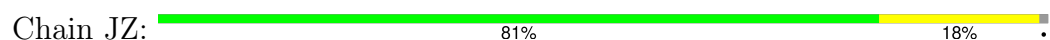
- Molecule 1: Coat protein



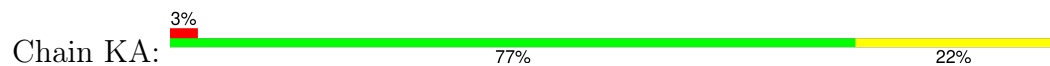
- Molecule 1: Coat protein



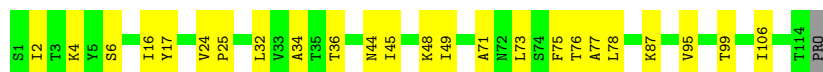
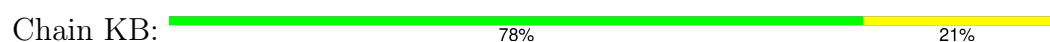
- Molecule 1: Coat protein




- Molecule 1: Coat protein



- Molecule 1: Coat protein




- Molecule 1: Coat protein

Chain KC:  79% 20%




• Molecule 1: Coat protein

Chain KD:  79% 20%




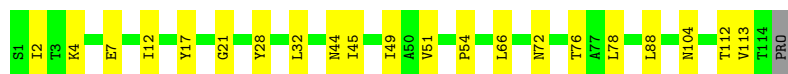
• Molecule 1: Coat protein

Chain KE:  79% 20%




• Molecule 1: Coat protein

Chain KF:  81% 18%



• Molecule 1: Coat protein

Chain KG:  79% 20%




• Molecule 1: Coat protein

Chain KH:  72% 27%

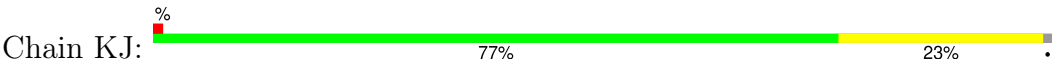


• Molecule 1: Coat protein

Chain KI:  78% 21%



• Molecule 1: Coat protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	432.29Å 307.87Å 679.45Å 90.00° 107.15° 90.00°	Depositor
Resolution (Å)	44.26 – 3.40 44.26 – 3.40	Depositor EDS
% Data completeness (in resolution range)	50.9 (44.26-3.40) 47.5 (44.26-3.40)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.35 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, $R_{free}$	0.268 , 0.270 0.270 , 0.272	Depositor DCC
$R_{free}$ test set	29852 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	61.0	Xtriage
Anisotropy	0.492	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 0.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.054 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	231390	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	AA	0.32	0/868	0.51	0/1188
1	AB	0.33	0/868	0.53	0/1188
1	AC	0.30	0/868	0.50	0/1188
1	AD	0.32	0/868	0.51	0/1188
1	AE	0.33	0/868	0.53	0/1188
1	AF	0.30	0/868	0.50	0/1188
1	AG	0.32	0/868	0.51	0/1188
1	AH	0.33	0/868	0.53	0/1188
1	AI	0.30	0/868	0.50	0/1188
1	AJ	0.32	0/868	0.51	0/1188
1	AK	0.33	0/868	0.53	0/1188
1	AL	0.30	0/868	0.50	0/1188
1	AM	0.32	0/868	0.51	0/1188
1	AN	0.33	0/868	0.54	0/1188
1	AO	0.30	0/868	0.50	0/1188
1	AP	0.32	0/868	0.51	0/1188
1	AQ	0.33	0/868	0.53	0/1188
1	AR	0.30	0/868	0.50	0/1188
1	AS	0.32	0/868	0.51	0/1188
1	AT	0.33	0/868	0.53	0/1188
1	AU	0.30	0/868	0.50	0/1188
1	AV	0.32	0/868	0.51	0/1188
1	AW	0.33	0/868	0.53	0/1188
1	AX	0.30	0/868	0.50	0/1188
1	AY	0.32	0/868	0.51	0/1188
1	AZ	0.33	0/868	0.54	0/1188
1	BA	0.30	0/868	0.50	0/1188
1	BB	0.32	0/868	0.51	0/1188
1	BC	0.33	0/868	0.53	0/1188
1	BD	0.30	0/868	0.50	0/1188
1	BE	0.32	0/868	0.51	0/1188
1	BF	0.33	0/868	0.53	0/1188
1	BG	0.30	0/868	0.50	0/1188
1	BH	0.32	0/868	0.51	0/1188

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	BI	0.33	0/868	0.53	0/1188
1	BJ	0.30	0/868	0.50	0/1188
1	BK	0.32	0/868	0.51	0/1188
1	BL	0.33	0/868	0.53	0/1188
1	BM	0.30	0/868	0.50	0/1188
1	BN	0.32	0/868	0.51	0/1188
1	BO	0.33	0/868	0.54	0/1188
1	BP	0.30	0/868	0.50	0/1188
1	BQ	0.32	0/868	0.51	0/1188
1	BR	0.33	0/868	0.53	0/1188
1	BS	0.30	0/868	0.50	0/1188
1	BT	0.32	0/868	0.51	0/1188
1	BU	0.33	0/868	0.54	0/1188
1	BV	0.30	0/868	0.50	0/1188
1	BW	0.32	0/868	0.51	0/1188
1	BX	0.33	0/868	0.53	0/1188
1	BY	0.30	0/868	0.50	0/1188
1	BZ	0.32	0/868	0.51	0/1188
1	CA	0.33	0/868	0.53	0/1188
1	CB	0.30	0/868	0.50	0/1188
1	CC	0.32	0/868	0.51	0/1188
1	CD	0.33	0/868	0.54	0/1188
1	CE	0.30	0/868	0.50	0/1188
1	CF	0.32	0/868	0.51	0/1188
1	CG	0.33	0/868	0.53	0/1188
1	CH	0.30	0/868	0.50	0/1188
1	CI	0.32	0/868	0.51	0/1188
1	CJ	0.33	0/868	0.54	0/1188
1	CK	0.30	0/868	0.50	0/1188
1	CL	0.32	0/868	0.51	0/1188
1	CM	0.33	0/868	0.53	0/1188
1	CN	0.30	0/868	0.50	0/1188
1	CO	0.32	0/868	0.51	0/1188
1	CP	0.33	0/868	0.53	0/1188
1	CQ	0.30	0/868	0.50	0/1188
1	CR	0.32	0/868	0.51	0/1188
1	CS	0.33	0/868	0.54	0/1188
1	CT	0.30	0/868	0.50	0/1188
1	CU	0.32	0/868	0.51	0/1188
1	CV	0.33	0/868	0.54	0/1188
1	CW	0.30	0/868	0.50	0/1188
1	CX	0.32	0/868	0.51	0/1188
1	CY	0.33	0/868	0.54	0/1188

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	CZ	0.30	0/868	0.50	0/1188
1	DA	0.32	0/868	0.51	0/1188
1	DB	0.33	0/868	0.53	0/1188
1	DC	0.30	0/868	0.50	0/1188
1	DD	0.32	0/868	0.51	0/1188
1	DE	0.33	0/868	0.53	0/1188
1	DF	0.30	0/868	0.50	0/1188
1	DG	0.32	0/868	0.51	0/1188
1	DH	0.33	0/868	0.53	0/1188
1	DI	0.30	0/868	0.50	0/1188
1	DJ	0.32	0/868	0.51	0/1188
1	DK	0.33	0/868	0.53	0/1188
1	DL	0.30	0/868	0.50	0/1188
1	DM	0.32	0/868	0.51	0/1188
1	DN	0.33	0/868	0.53	0/1188
1	DO	0.30	0/868	0.50	0/1188
1	DP	0.32	0/868	0.51	0/1188
1	DQ	0.33	0/868	0.53	0/1188
1	DR	0.30	0/868	0.50	0/1188
1	DS	0.32	0/868	0.51	0/1188
1	DT	0.33	0/868	0.54	0/1188
1	DU	0.30	0/868	0.50	0/1188
1	DV	0.32	0/868	0.51	0/1188
1	DW	0.33	0/868	0.53	0/1188
1	DX	0.30	0/868	0.50	0/1188
1	DY	0.32	0/868	0.51	0/1188
1	DZ	0.33	0/868	0.53	0/1188
1	EA	0.30	0/868	0.50	0/1188
1	EB	0.32	0/868	0.51	0/1188
1	EC	0.33	0/868	0.53	0/1188
1	ED	0.30	0/868	0.50	0/1188
1	EE	0.32	0/868	0.51	0/1188
1	EF	0.33	0/868	0.53	0/1188
1	EG	0.29	0/868	0.50	0/1188
1	EH	0.32	0/868	0.51	0/1188
1	EI	0.33	0/868	0.54	0/1188
1	EJ	0.30	0/868	0.50	0/1188
1	EK	0.32	0/868	0.51	0/1188
1	EL	0.33	0/868	0.53	0/1188
1	EM	0.30	0/868	0.50	0/1188
1	EN	0.32	0/868	0.51	0/1188
1	EO	0.33	0/868	0.54	0/1188
1	EP	0.30	0/868	0.50	0/1188

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	EQ	0.32	0/868	0.51	0/1188
1	ER	0.33	0/868	0.54	0/1188
1	ES	0.30	0/868	0.50	0/1188
1	ET	0.32	0/868	0.51	0/1188
1	EU	0.33	0/868	0.53	0/1188
1	EV	0.30	0/868	0.50	0/1188
1	EW	0.32	0/868	0.51	0/1188
1	EX	0.33	0/868	0.53	0/1188
1	EY	0.30	0/868	0.50	0/1188
1	EZ	0.32	0/868	0.51	0/1188
1	FA	0.33	0/868	0.54	0/1188
1	FB	0.30	0/868	0.50	0/1188
1	FC	0.32	0/868	0.51	0/1188
1	FD	0.33	0/868	0.53	0/1188
1	FE	0.30	0/868	0.50	0/1188
1	FF	0.32	0/868	0.51	0/1188
1	FG	0.33	0/868	0.53	0/1188
1	FH	0.30	0/868	0.50	0/1188
1	FI	0.32	0/868	0.51	0/1188
1	FJ	0.33	0/868	0.53	0/1188
1	FK	0.30	0/868	0.50	0/1188
1	FL	0.32	0/868	0.51	0/1188
1	FM	0.33	0/868	0.54	0/1188
1	FN	0.30	0/868	0.50	0/1188
1	FO	0.32	0/868	0.51	0/1188
1	FP	0.33	0/868	0.54	0/1188
1	FQ	0.30	0/868	0.50	0/1188
1	FR	0.32	0/868	0.51	0/1188
1	FS	0.33	0/868	0.53	0/1188
1	FT	0.30	0/868	0.50	0/1188
1	FU	0.32	0/868	0.51	0/1188
1	FV	0.33	0/868	0.53	0/1188
1	FW	0.30	0/868	0.50	0/1188
1	FX	0.32	0/868	0.51	0/1188
1	FY	0.33	0/868	0.54	0/1188
1	FZ	0.30	0/868	0.50	0/1188
1	GA	0.32	0/868	0.51	0/1188
1	GB	0.33	0/868	0.53	0/1188
1	GC	0.30	0/868	0.50	0/1188
1	GD	0.32	0/868	0.51	0/1188
1	GE	0.33	0/868	0.54	0/1188
1	GF	0.30	0/868	0.50	0/1188
1	GG	0.32	0/868	0.51	0/1188



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	GH	0.33	0/868	0.53	0/1188
1	GI	0.30	0/868	0.50	0/1188
1	GJ	0.32	0/868	0.51	0/1188
1	GK	0.33	0/868	0.53	0/1188
1	GL	0.30	0/868	0.50	0/1188
1	GM	0.32	0/868	0.51	0/1188
1	GN	0.33	0/868	0.53	0/1188
1	GO	0.30	0/868	0.50	0/1188
1	GP	0.32	0/868	0.51	0/1188
1	GQ	0.33	0/868	0.53	0/1188
1	GR	0.30	0/868	0.50	0/1188
1	GS	0.32	0/868	0.51	0/1188
1	GT	0.33	0/868	0.53	0/1188
1	GU	0.30	0/868	0.50	0/1188
1	GV	0.32	0/868	0.51	0/1188
1	GW	0.33	0/868	0.53	0/1188
1	GX	0.30	0/868	0.50	0/1188
1	GY	0.32	0/868	0.51	0/1188
1	GZ	0.33	0/868	0.53	0/1188
1	HA	0.30	0/868	0.50	0/1188
1	HB	0.32	0/868	0.51	0/1188
1	HC	0.33	0/868	0.53	0/1188
1	HD	0.30	0/868	0.50	0/1188
1	HE	0.32	0/868	0.51	0/1188
1	HF	0.33	0/868	0.53	0/1188
1	HG	0.30	0/868	0.50	0/1188
1	HH	0.32	0/868	0.51	0/1188
1	HI	0.33	0/868	0.53	0/1188
1	HJ	0.30	0/868	0.50	0/1188
1	HK	0.32	0/868	0.51	0/1188
1	HL	0.33	0/868	0.54	0/1188
1	HM	0.30	0/868	0.50	0/1188
1	HN	0.32	0/868	0.51	0/1188
1	HO	0.33	0/868	0.53	0/1188
1	HP	0.30	0/868	0.50	0/1188
1	HQ	0.32	0/868	0.51	0/1188
1	HR	0.33	0/868	0.53	0/1188
1	HS	0.30	0/868	0.50	0/1188
1	HT	0.32	0/868	0.51	0/1188
1	HU	0.33	0/868	0.53	0/1188
1	HV	0.30	0/868	0.50	0/1188
1	HW	0.32	0/868	0.51	0/1188
1	HX	0.33	0/868	0.53	0/1188

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	HY	0.30	0/868	0.50	0/1188
1	HZ	0.32	0/868	0.51	0/1188
1	IA	0.33	0/868	0.53	0/1188
1	IB	0.30	0/868	0.50	0/1188
1	IC	0.32	0/868	0.51	0/1188
1	ID	0.33	0/868	0.53	0/1188
1	IE	0.30	0/868	0.50	0/1188
1	IF	0.32	0/868	0.51	0/1188
1	IG	0.33	0/868	0.54	0/1188
1	IH	0.30	0/868	0.50	0/1188
1	II	0.32	0/868	0.51	0/1188
1	IJ	0.33	0/868	0.53	0/1188
1	IK	0.30	0/868	0.50	0/1188
1	IL	0.32	0/868	0.51	0/1188
1	IM	0.33	0/868	0.53	0/1188
1	IN	0.30	0/868	0.50	0/1188
1	IO	0.32	0/868	0.51	0/1188
1	IP	0.33	0/868	0.53	0/1188
1	IQ	0.30	0/868	0.50	0/1188
1	IR	0.32	0/868	0.51	0/1188
1	IS	0.33	0/868	0.53	0/1188
1	IT	0.30	0/868	0.50	0/1188
1	IU	0.32	0/868	0.51	0/1188
1	IV	0.33	0/868	0.53	0/1188
1	IW	0.30	0/868	0.50	0/1188
1	IX	0.32	0/868	0.51	0/1188
1	IY	0.33	0/868	0.53	0/1188
1	IZ	0.30	0/868	0.50	0/1188
1	JA	0.32	0/868	0.51	0/1188
1	JB	0.33	0/868	0.53	0/1188
1	JC	0.30	0/868	0.50	0/1188
1	JD	0.32	0/868	0.51	0/1188
1	JE	0.33	0/868	0.53	0/1188
1	JF	0.30	0/868	0.50	0/1188
1	JG	0.32	0/868	0.51	0/1188
1	JH	0.33	0/868	0.53	0/1188
1	JI	0.30	0/868	0.50	0/1188
1	JJ	0.32	0/868	0.51	0/1188
1	JK	0.33	0/868	0.53	0/1188
1	JL	0.30	0/868	0.50	0/1188
1	JM	0.32	0/868	0.51	0/1188
1	JN	0.33	0/868	0.53	0/1188
1	JO	0.30	0/868	0.50	0/1188

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	JP	0.32	0/868	0.51	0/1188
1	JQ	0.33	0/868	0.54	0/1188
1	JR	0.30	0/868	0.50	0/1188
1	JS	0.32	0/868	0.51	0/1188
1	JT	0.33	0/868	0.53	0/1188
1	JU	0.30	0/868	0.50	0/1188
1	JV	0.32	0/868	0.51	0/1188
1	JW	0.33	0/868	0.54	0/1188
1	JX	0.30	0/868	0.50	0/1188
1	JY	0.32	0/868	0.51	0/1188
1	JZ	0.33	0/868	0.53	0/1188
1	KA	0.30	0/868	0.50	0/1188
1	KB	0.32	0/868	0.51	0/1188
1	KC	0.33	0/868	0.53	0/1188
1	KD	0.30	0/868	0.50	0/1188
1	KE	0.32	0/868	0.51	0/1188
1	KF	0.33	0/868	0.53	0/1188
1	KG	0.30	0/868	0.50	0/1188
1	KH	0.32	0/868	0.51	0/1188
1	KI	0.33	0/868	0.53	0/1188
1	KJ	0.30	0/868	0.50	0/1188
All	All	0.31	0/234360	0.52	0/320760

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	857	0	885	20	0
1	AB	857	0	885	21	0
1	AC	857	0	885	19	0
1	AD	857	0	885	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AE	857	0	885	28	0
1	AF	857	0	885	23	0
1	AG	857	0	885	33	0
1	AH	857	0	885	19	0
1	AI	857	0	885	21	0
1	AJ	857	0	885	24	0
1	AK	857	0	885	25	0
1	AL	857	0	885	19	0
1	AM	857	0	885	33	0
1	AN	857	0	885	31	0
1	AO	857	0	885	21	0
1	AP	857	0	885	26	0
1	AQ	857	0	885	34	0
1	AR	857	0	885	22	0
1	AS	857	0	885	36	0
1	AT	857	0	885	18	0
1	AU	857	0	885	39	0
1	AV	857	0	885	33	0
1	AW	857	0	885	21	0
1	AX	857	0	885	25	0
1	AY	857	0	885	30	0
1	AZ	857	0	885	19	0
1	BA	857	0	885	22	0
1	BB	857	0	885	23	0
1	BC	857	0	885	32	0
1	BD	857	0	885	36	0
1	BE	857	0	885	23	0
1	BF	857	0	885	30	0
1	BG	857	0	885	22	0
1	BH	857	0	885	22	0
1	BI	857	0	885	18	0
1	BJ	857	0	885	20	0
1	BK	857	0	885	20	0
1	BL	857	0	885	22	0
1	BM	857	0	885	23	0
1	BN	857	0	885	21	0
1	BO	857	0	885	19	0
1	BP	857	0	885	23	0
1	BQ	857	0	885	27	0
1	BR	857	0	885	22	0
1	BS	857	0	885	23	0
1	BT	857	0	885	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BU	857	0	885	23	0
1	BV	857	0	885	20	0
1	BW	857	0	885	28	0
1	BX	857	0	885	21	0
1	BY	857	0	885	28	0
1	BZ	857	0	885	34	0
1	CA	857	0	885	32	0
1	CB	857	0	885	22	0
1	CC	857	0	885	35	0
1	CD	857	0	885	23	0
1	CE	857	0	885	18	0
1	CF	857	0	885	22	0
1	CG	857	0	885	36	0
1	CH	857	0	885	34	0
1	CI	857	0	885	25	0
1	CJ	857	0	885	27	0
1	CK	857	0	885	22	0
1	CL	857	0	885	38	0
1	CM	857	0	885	25	0
1	CN	857	0	885	26	0
1	CO	857	0	885	29	0
1	CP	857	0	885	19	0
1	CQ	857	0	885	20	0
1	CR	857	0	885	27	0
1	CS	857	0	885	18	0
1	CT	857	0	885	20	0
1	CU	857	0	885	23	0
1	CV	857	0	885	18	0
1	CW	857	0	885	20	0
1	CX	857	0	885	22	0
1	CY	857	0	885	27	0
1	CZ	857	0	885	24	0
1	DA	857	0	885	19	0
1	DB	857	0	885	20	0
1	DC	857	0	885	22	0
1	DD	857	0	885	19	0
1	DE	857	0	885	17	0
1	DF	857	0	885	24	0
1	DG	857	0	885	26	0
1	DH	857	0	885	21	0
1	DI	857	0	885	25	0
1	DJ	857	0	885	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	DK	857	0	885	21	0
1	DL	857	0	885	30	0
1	DM	857	0	885	26	0
1	DN	857	0	885	26	0
1	DO	857	0	885	19	0
1	DP	857	0	885	23	0
1	DQ	857	0	885	26	0
1	DR	857	0	885	22	0
1	DS	857	0	885	20	0
1	DT	857	0	885	30	0
1	DU	857	0	885	21	0
1	DV	857	0	885	23	0
1	DW	857	0	885	18	0
1	DX	857	0	885	18	0
1	DY	857	0	885	31	0
1	DZ	857	0	885	18	0
1	EA	857	0	885	21	0
1	EB	857	0	885	34	0
1	EC	857	0	885	26	0
1	ED	857	0	885	21	0
1	EE	857	0	885	33	0
1	EF	857	0	885	32	0
1	EG	857	0	885	40	0
1	EH	857	0	885	26	0
1	EI	857	0	885	29	0
1	EJ	857	0	885	24	0
1	EK	857	0	885	26	0
1	EL	857	0	885	32	0
1	EM	857	0	885	23	0
1	EN	857	0	885	45	0
1	EO	857	0	885	25	0
1	EP	857	0	885	34	0
1	EQ	857	0	885	29	0
1	ER	857	0	885	24	0
1	ES	857	0	885	21	0
1	ET	857	0	885	30	0
1	EU	857	0	885	34	0
1	EV	857	0	885	21	0
1	EW	857	0	885	20	0
1	EX	857	0	885	19	0
1	EY	857	0	885	24	0
1	EZ	857	0	885	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	FA	857	0	885	19	0
1	FB	857	0	885	22	0
1	FC	857	0	885	24	0
1	FD	857	0	885	21	0
1	FE	857	0	885	24	0
1	FF	857	0	885	24	0
1	FG	857	0	885	26	0
1	FH	857	0	885	19	0
1	FI	857	0	885	20	0
1	FJ	857	0	885	43	0
1	FK	857	0	885	27	0
1	FL	857	0	885	22	0
1	FM	857	0	885	27	0
1	FN	857	0	885	21	0
1	FO	857	0	885	28	0
1	FP	857	0	885	20	0
1	FQ	857	0	885	18	0
1	FR	857	0	885	34	0
1	FS	857	0	885	24	0
1	FT	857	0	885	34	0
1	FU	857	0	885	36	0
1	FV	857	0	885	21	0
1	FW	857	0	885	24	0
1	FX	857	0	885	24	0
1	FY	857	0	885	29	0
1	FZ	857	0	885	25	0
1	GA	857	0	885	29	0
1	GB	857	0	885	34	0
1	GC	857	0	885	21	0
1	GD	857	0	885	21	0
1	GE	857	0	885	22	0
1	GF	857	0	885	20	0
1	GG	857	0	885	29	0
1	GH	857	0	885	25	0
1	GI	857	0	885	20	0
1	GJ	857	0	885	23	0
1	GK	857	0	885	34	0
1	GL	857	0	885	24	0
1	GM	857	0	885	20	0
1	GN	857	0	885	21	0
1	GO	857	0	885	21	0
1	GP	857	0	885	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	GQ	857	0	885	18	0
1	GR	857	0	885	24	0
1	GS	857	0	885	22	0
1	GT	857	0	885	24	0
1	GU	857	0	885	24	0
1	GV	857	0	885	22	0
1	GW	857	0	885	21	0
1	GX	857	0	885	29	0
1	GY	857	0	885	38	0
1	GZ	857	0	885	19	0
1	HA	857	0	885	18	0
1	HB	857	0	885	24	0
1	HC	857	0	885	20	0
1	HD	857	0	885	13	0
1	HE	857	0	885	28	0
1	HF	857	0	885	20	0
1	HG	857	0	885	23	0
1	HH	857	0	885	23	0
1	HI	857	0	885	18	0
1	HJ	857	0	885	25	0
1	HK	857	0	885	27	0
1	HL	857	0	885	26	0
1	HM	857	0	885	15	0
1	HN	857	0	885	24	0
1	HO	857	0	885	37	0
1	HP	857	0	885	21	0
1	HQ	857	0	885	29	0
1	HR	857	0	885	23	0
1	HS	857	0	885	26	0
1	HT	857	0	885	45	0
1	HU	857	0	885	28	0
1	HV	857	0	885	31	0
1	HW	857	0	885	27	0
1	HX	857	0	885	23	0
1	HY	857	0	885	20	0
1	HZ	857	0	885	26	0
1	IA	857	0	885	19	0
1	IB	857	0	885	21	0
1	IC	857	0	885	21	0
1	ID	857	0	885	17	0
1	IE	857	0	885	24	0
1	IF	857	0	885	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	IG	857	0	885	23	0
1	IH	857	0	885	15	0
1	II	857	0	885	18	0
1	IJ	857	0	885	30	0
1	IK	857	0	885	21	0
1	IL	857	0	885	20	0
1	IM	857	0	885	45	0
1	IN	857	0	885	15	0
1	IO	857	0	885	24	0
1	IP	857	0	885	26	0
1	IQ	857	0	885	20	0
1	IR	857	0	885	21	0
1	IS	857	0	885	27	0
1	IT	857	0	885	24	0
1	IU	857	0	885	36	0
1	IV	857	0	885	21	0
1	IW	857	0	885	15	0
1	IX	857	0	885	25	0
1	IY	857	0	885	25	0
1	IZ	857	0	885	25	0
1	JA	857	0	885	33	0
1	JB	857	0	885	23	0
1	JC	857	0	885	21	0
1	JD	857	0	885	32	0
1	JE	857	0	885	33	0
1	JF	857	0	885	14	0
1	JG	857	0	885	27	0
1	JH	857	0	885	30	0
1	JI	857	0	885	16	0
1	JJ	857	0	885	21	0
1	JK	857	0	885	28	0
1	JL	857	0	885	26	0
1	JM	857	0	885	31	0
1	JN	857	0	885	31	0
1	JO	857	0	885	31	0
1	JP	857	0	885	32	0
1	JQ	857	0	885	31	0
1	JR	857	0	885	19	0
1	JS	857	0	885	22	0
1	JT	857	0	885	36	0
1	JU	857	0	885	16	0
1	JV	857	0	885	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	JW	857	0	885	18	0
1	JX	857	0	885	21	0
1	JY	857	0	885	20	0
1	JZ	857	0	885	19	0
1	KA	857	0	885	22	0
1	KB	857	0	885	25	0
1	KC	857	0	885	23	0
1	KD	857	0	885	15	0
1	KE	857	0	885	20	0
1	KF	857	0	885	18	0
1	KG	857	0	885	15	0
1	KH	857	0	885	38	0
1	KI	857	0	885	23	0
1	KJ	857	0	885	20	0
All	All	231390	0	238950	5039	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 5039 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DL:95:VAL:HG13	1:GX:95:VAL:HG13	1.54	0.86
1:AU:111:LEU:HG	1:EG:11:PRO:HA	1.55	0.86
1:HJ:95:VAL:HG13	1:IZ:95:VAL:HG13	1.60	0.83
1:AX:95:VAL:HG13	1:EJ:95:VAL:HG13	1.60	0.82
1:CI:4:LYS:HE2	1:GH:112:THR:HG21	1.64	0.80

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	AA	112/115 (97%)	112 (100%)	0	0	100	100
1	AB	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	AC	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	AD	112/115 (97%)	112 (100%)	0	0	100	100
1	AE	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	AF	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	AG	112/115 (97%)	112 (100%)	0	0	100	100
1	AH	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	AI	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	AJ	112/115 (97%)	112 (100%)	0	0	100	100
1	AK	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	AL	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	AM	112/115 (97%)	112 (100%)	0	0	100	100
1	AN	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	AO	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	AP	112/115 (97%)	112 (100%)	0	0	100	100
1	AQ	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	AR	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	AS	112/115 (97%)	112 (100%)	0	0	100	100
1	AT	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	AU	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	AV	112/115 (97%)	112 (100%)	0	0	100	100
1	AW	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	AX	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	AY	112/115 (97%)	112 (100%)	0	0	100	100
1	AZ	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	BA	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	BB	112/115 (97%)	112 (100%)	0	0	100	100
1	BC	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	BD	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	BE	112/115 (97%)	112 (100%)	0	0	100	100
1	BF	112/115 (97%)	111 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BG	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	BH	112/115 (97%)	112 (100%)	0	0	100	100
1	BI	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	BJ	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	BK	112/115 (97%)	112 (100%)	0	0	100	100
1	BL	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	BM	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	BN	112/115 (97%)	112 (100%)	0	0	100	100
1	BO	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	BP	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	BQ	112/115 (97%)	112 (100%)	0	0	100	100
1	BR	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	BS	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	BT	112/115 (97%)	112 (100%)	0	0	100	100
1	BU	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	BV	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	BW	112/115 (97%)	112 (100%)	0	0	100	100
1	BX	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	BY	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	BZ	112/115 (97%)	112 (100%)	0	0	100	100
1	CA	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	CB	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	CC	112/115 (97%)	112 (100%)	0	0	100	100
1	CD	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	CE	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	CF	112/115 (97%)	112 (100%)	0	0	100	100
1	CG	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	CH	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	CI	112/115 (97%)	112 (100%)	0	0	100	100
1	CJ	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	CK	112/115 (97%)	110 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CL	112/115 (97%)	112 (100%)	0	0	100	100
1	CM	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	CN	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	CO	112/115 (97%)	112 (100%)	0	0	100	100
1	CP	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	CQ	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	CR	112/115 (97%)	112 (100%)	0	0	100	100
1	CS	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	CT	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	CU	112/115 (97%)	112 (100%)	0	0	100	100
1	CV	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	CW	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	CX	112/115 (97%)	112 (100%)	0	0	100	100
1	CY	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	CZ	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	DA	112/115 (97%)	112 (100%)	0	0	100	100
1	DB	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	DC	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	DD	112/115 (97%)	112 (100%)	0	0	100	100
1	DE	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	DF	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	DG	112/115 (97%)	112 (100%)	0	0	100	100
1	DH	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	DI	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	DJ	112/115 (97%)	112 (100%)	0	0	100	100
1	DK	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	DL	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	DM	112/115 (97%)	112 (100%)	0	0	100	100
1	DN	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	DO	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	DP	112/115 (97%)	112 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	DQ	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	DR	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	DS	112/115 (97%)	112 (100%)	0	0	100	100
1	DT	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	DU	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	DV	112/115 (97%)	112 (100%)	0	0	100	100
1	DW	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	DX	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	DY	112/115 (97%)	112 (100%)	0	0	100	100
1	DZ	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	EA	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	EB	112/115 (97%)	112 (100%)	0	0	100	100
1	EC	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	ED	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	EE	112/115 (97%)	112 (100%)	0	0	100	100
1	EF	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	EG	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	EH	112/115 (97%)	112 (100%)	0	0	100	100
1	EI	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	EJ	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	EK	112/115 (97%)	112 (100%)	0	0	100	100
1	EL	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	EM	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	EN	112/115 (97%)	112 (100%)	0	0	100	100
1	EO	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	EP	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	EQ	112/115 (97%)	112 (100%)	0	0	100	100
1	ER	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	ES	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	ET	112/115 (97%)	112 (100%)	0	0	100	100
1	EU	112/115 (97%)	111 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	EV	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	EW	112/115 (97%)	112 (100%)	0	0	100	100
1	EX	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	EY	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	EZ	112/115 (97%)	112 (100%)	0	0	100	100
1	FA	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	FB	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	FC	112/115 (97%)	112 (100%)	0	0	100	100
1	FD	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	FE	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	FF	112/115 (97%)	112 (100%)	0	0	100	100
1	FG	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	FH	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	FI	112/115 (97%)	112 (100%)	0	0	100	100
1	FJ	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	FK	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	FL	112/115 (97%)	112 (100%)	0	0	100	100
1	FM	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	FN	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	FO	112/115 (97%)	112 (100%)	0	0	100	100
1	FP	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	FQ	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	FR	112/115 (97%)	112 (100%)	0	0	100	100
1	FS	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	FT	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	FU	112/115 (97%)	112 (100%)	0	0	100	100
1	FV	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	FW	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	FX	112/115 (97%)	112 (100%)	0	0	100	100
1	FY	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	FZ	112/115 (97%)	110 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	GA	112/115 (97%)	112 (100%)	0	0	100	100
1	GB	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	GC	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	GD	112/115 (97%)	112 (100%)	0	0	100	100
1	GE	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	GF	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	GG	112/115 (97%)	112 (100%)	0	0	100	100
1	GH	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	GI	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	GJ	112/115 (97%)	112 (100%)	0	0	100	100
1	GK	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	GL	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	GM	112/115 (97%)	112 (100%)	0	0	100	100
1	GN	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	GO	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	GP	112/115 (97%)	112 (100%)	0	0	100	100
1	GQ	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	GR	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	GS	112/115 (97%)	112 (100%)	0	0	100	100
1	GT	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	GU	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	GV	112/115 (97%)	112 (100%)	0	0	100	100
1	GW	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	GX	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	GY	112/115 (97%)	112 (100%)	0	0	100	100
1	GZ	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	HA	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	HB	112/115 (97%)	112 (100%)	0	0	100	100
1	HC	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	HD	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	HE	112/115 (97%)	112 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	HF	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	HG	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	HH	112/115 (97%)	112 (100%)	0	0	100	100
1	HI	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	HJ	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	HK	112/115 (97%)	112 (100%)	0	0	100	100
1	HL	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	HM	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	HN	112/115 (97%)	112 (100%)	0	0	100	100
1	HO	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	HP	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	HQ	112/115 (97%)	112 (100%)	0	0	100	100
1	HR	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	HS	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	HT	112/115 (97%)	112 (100%)	0	0	100	100
1	HU	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	HV	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	HW	112/115 (97%)	112 (100%)	0	0	100	100
1	HX	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	HY	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	HZ	112/115 (97%)	112 (100%)	0	0	100	100
1	IA	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	IB	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	IC	112/115 (97%)	112 (100%)	0	0	100	100
1	ID	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	IE	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	IF	112/115 (97%)	112 (100%)	0	0	100	100
1	IG	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	IH	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	II	112/115 (97%)	112 (100%)	0	0	100	100
1	IJ	112/115 (97%)	111 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	IK	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	IL	112/115 (97%)	112 (100%)	0	0	100	100
1	IM	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	IN	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	IO	112/115 (97%)	112 (100%)	0	0	100	100
1	IP	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	IQ	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	IR	112/115 (97%)	112 (100%)	0	0	100	100
1	IS	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	IT	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	IU	112/115 (97%)	112 (100%)	0	0	100	100
1	IV	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	IW	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	IX	112/115 (97%)	112 (100%)	0	0	100	100
1	IY	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	IZ	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	JA	112/115 (97%)	112 (100%)	0	0	100	100
1	JB	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	JC	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	JD	112/115 (97%)	112 (100%)	0	0	100	100
1	JE	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	JF	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	JG	112/115 (97%)	112 (100%)	0	0	100	100
1	JH	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	JI	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	JJ	112/115 (97%)	112 (100%)	0	0	100	100
1	JK	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	JL	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	JM	112/115 (97%)	112 (100%)	0	0	100	100
1	JN	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	JO	112/115 (97%)	110 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	JP	112/115 (97%)	112 (100%)	0	0	100	100
1	JQ	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	JR	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	JS	112/115 (97%)	112 (100%)	0	0	100	100
1	JT	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	JU	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	JV	112/115 (97%)	112 (100%)	0	0	100	100
1	JW	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	JX	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	JY	112/115 (97%)	112 (100%)	0	0	100	100
1	JZ	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	KA	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	KB	112/115 (97%)	112 (100%)	0	0	100	100
1	KC	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	KD	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	KE	112/115 (97%)	112 (100%)	0	0	100	100
1	KF	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	KG	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	KH	112/115 (97%)	112 (100%)	0	0	100	100
1	KI	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
1	KJ	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
All	All	30240/31050 (97%)	29970 (99%)	270 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	AA	97/98 (99%)	97 (100%)	0	100	100
1	AB	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	AC	97/98 (99%)	97 (100%)	0	100	100
1	AD	97/98 (99%)	97 (100%)	0	100	100
1	AE	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	AF	97/98 (99%)	97 (100%)	0	100	100
1	AG	97/98 (99%)	97 (100%)	0	100	100
1	AH	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	AI	97/98 (99%)	97 (100%)	0	100	100
1	AJ	97/98 (99%)	97 (100%)	0	100	100
1	AK	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	AL	97/98 (99%)	97 (100%)	0	100	100
1	AM	97/98 (99%)	97 (100%)	0	100	100
1	AN	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	AO	97/98 (99%)	97 (100%)	0	100	100
1	AP	97/98 (99%)	97 (100%)	0	100	100
1	AQ	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	AR	97/98 (99%)	97 (100%)	0	100	100
1	AS	97/98 (99%)	97 (100%)	0	100	100
1	AT	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	AU	97/98 (99%)	97 (100%)	0	100	100
1	AV	97/98 (99%)	97 (100%)	0	100	100
1	AW	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	AX	97/98 (99%)	97 (100%)	0	100	100
1	AY	97/98 (99%)	97 (100%)	0	100	100
1	AZ	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	BA	97/98 (99%)	97 (100%)	0	100	100
1	BB	97/98 (99%)	97 (100%)	0	100	100
1	BC	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	BD	97/98 (99%)	97 (100%)	0	100	100
1	BE	97/98 (99%)	97 (100%)	0	100	100
1	BF	97/98 (99%)	96 (99%)	1 (1%)	76	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BG	97/98 (99%)	97 (100%)	0	100	100
1	BH	97/98 (99%)	97 (100%)	0	100	100
1	BI	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	BJ	97/98 (99%)	97 (100%)	0	100	100
1	BK	97/98 (99%)	97 (100%)	0	100	100
1	BL	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	BM	97/98 (99%)	97 (100%)	0	100	100
1	BN	97/98 (99%)	97 (100%)	0	100	100
1	BO	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	BP	97/98 (99%)	97 (100%)	0	100	100
1	BQ	97/98 (99%)	97 (100%)	0	100	100
1	BR	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	BS	97/98 (99%)	97 (100%)	0	100	100
1	BT	97/98 (99%)	97 (100%)	0	100	100
1	BU	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	BV	97/98 (99%)	97 (100%)	0	100	100
1	BW	97/98 (99%)	97 (100%)	0	100	100
1	BX	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	BY	97/98 (99%)	97 (100%)	0	100	100
1	BZ	97/98 (99%)	97 (100%)	0	100	100
1	CA	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	CB	97/98 (99%)	97 (100%)	0	100	100
1	CC	97/98 (99%)	97 (100%)	0	100	100
1	CD	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	CE	97/98 (99%)	97 (100%)	0	100	100
1	CF	97/98 (99%)	97 (100%)	0	100	100
1	CG	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	CH	97/98 (99%)	97 (100%)	0	100	100
1	CI	97/98 (99%)	97 (100%)	0	100	100
1	CJ	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	CK	97/98 (99%)	97 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CL	97/98 (99%)	97 (100%)	0	100	100
1	CM	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	CN	97/98 (99%)	97 (100%)	0	100	100
1	CO	97/98 (99%)	97 (100%)	0	100	100
1	CP	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	CQ	97/98 (99%)	97 (100%)	0	100	100
1	CR	97/98 (99%)	97 (100%)	0	100	100
1	CS	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	CT	97/98 (99%)	97 (100%)	0	100	100
1	CU	97/98 (99%)	97 (100%)	0	100	100
1	CV	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	CW	97/98 (99%)	97 (100%)	0	100	100
1	CX	97/98 (99%)	97 (100%)	0	100	100
1	CY	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	CZ	97/98 (99%)	97 (100%)	0	100	100
1	DA	97/98 (99%)	97 (100%)	0	100	100
1	DB	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	DC	97/98 (99%)	97 (100%)	0	100	100
1	DD	97/98 (99%)	97 (100%)	0	100	100
1	DE	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	DF	97/98 (99%)	97 (100%)	0	100	100
1	DG	97/98 (99%)	97 (100%)	0	100	100
1	DH	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	DI	97/98 (99%)	97 (100%)	0	100	100
1	DJ	97/98 (99%)	97 (100%)	0	100	100
1	DK	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	DL	97/98 (99%)	97 (100%)	0	100	100
1	DM	97/98 (99%)	97 (100%)	0	100	100
1	DN	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	DO	97/98 (99%)	97 (100%)	0	100	100
1	DP	97/98 (99%)	97 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	DQ	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	DR	97/98 (99%)	97 (100%)	0	100	100
1	DS	97/98 (99%)	97 (100%)	0	100	100
1	DT	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	DU	97/98 (99%)	97 (100%)	0	100	100
1	DV	97/98 (99%)	97 (100%)	0	100	100
1	DW	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	DX	97/98 (99%)	97 (100%)	0	100	100
1	DY	97/98 (99%)	97 (100%)	0	100	100
1	DZ	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	EA	97/98 (99%)	97 (100%)	0	100	100
1	EB	97/98 (99%)	97 (100%)	0	100	100
1	EC	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	ED	97/98 (99%)	97 (100%)	0	100	100
1	EE	97/98 (99%)	97 (100%)	0	100	100
1	EF	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	EG	97/98 (99%)	97 (100%)	0	100	100
1	EH	97/98 (99%)	97 (100%)	0	100	100
1	EI	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	EJ	97/98 (99%)	97 (100%)	0	100	100
1	EK	97/98 (99%)	97 (100%)	0	100	100
1	EL	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	EM	97/98 (99%)	97 (100%)	0	100	100
1	EN	97/98 (99%)	97 (100%)	0	100	100
1	EO	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	EP	97/98 (99%)	97 (100%)	0	100	100
1	EQ	97/98 (99%)	97 (100%)	0	100	100
1	ER	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	ES	97/98 (99%)	97 (100%)	0	100	100
1	ET	97/98 (99%)	97 (100%)	0	100	100
1	EU	97/98 (99%)	96 (99%)	1 (1%)	76	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	EV	97/98 (99%)	97 (100%)	0	100	100
1	EW	97/98 (99%)	97 (100%)	0	100	100
1	EX	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	EY	97/98 (99%)	97 (100%)	0	100	100
1	EZ	97/98 (99%)	97 (100%)	0	100	100
1	FA	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	FB	97/98 (99%)	97 (100%)	0	100	100
1	FC	97/98 (99%)	97 (100%)	0	100	100
1	FD	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	FE	97/98 (99%)	97 (100%)	0	100	100
1	FF	97/98 (99%)	97 (100%)	0	100	100
1	FG	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	FH	97/98 (99%)	97 (100%)	0	100	100
1	FI	97/98 (99%)	97 (100%)	0	100	100
1	FJ	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	FK	97/98 (99%)	97 (100%)	0	100	100
1	FL	97/98 (99%)	97 (100%)	0	100	100
1	FM	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	FN	97/98 (99%)	97 (100%)	0	100	100
1	FO	97/98 (99%)	97 (100%)	0	100	100
1	FP	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	FQ	97/98 (99%)	97 (100%)	0	100	100
1	FR	97/98 (99%)	97 (100%)	0	100	100
1	FS	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	FT	97/98 (99%)	97 (100%)	0	100	100
1	FU	97/98 (99%)	97 (100%)	0	100	100
1	FV	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	FW	97/98 (99%)	97 (100%)	0	100	100
1	FX	97/98 (99%)	97 (100%)	0	100	100
1	FY	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	FZ	97/98 (99%)	97 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	GA	97/98 (99%)	97 (100%)	0	100	100
1	GB	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	GC	97/98 (99%)	97 (100%)	0	100	100
1	GD	97/98 (99%)	97 (100%)	0	100	100
1	GE	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	GF	97/98 (99%)	97 (100%)	0	100	100
1	GG	97/98 (99%)	97 (100%)	0	100	100
1	GH	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	GI	97/98 (99%)	97 (100%)	0	100	100
1	GJ	97/98 (99%)	97 (100%)	0	100	100
1	GK	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	GL	97/98 (99%)	97 (100%)	0	100	100
1	GM	97/98 (99%)	97 (100%)	0	100	100
1	GN	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	GO	97/98 (99%)	97 (100%)	0	100	100
1	GP	97/98 (99%)	97 (100%)	0	100	100
1	GQ	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	GR	97/98 (99%)	97 (100%)	0	100	100
1	GS	97/98 (99%)	97 (100%)	0	100	100
1	GT	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	GU	97/98 (99%)	97 (100%)	0	100	100
1	GV	97/98 (99%)	97 (100%)	0	100	100
1	GW	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	GX	97/98 (99%)	97 (100%)	0	100	100
1	GY	97/98 (99%)	97 (100%)	0	100	100
1	GZ	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	HA	97/98 (99%)	97 (100%)	0	100	100
1	HB	97/98 (99%)	97 (100%)	0	100	100
1	HC	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	HD	97/98 (99%)	97 (100%)	0	100	100
1	HE	97/98 (99%)	97 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	HF	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	HG	97/98 (99%)	97 (100%)	0	100	100
1	HH	97/98 (99%)	97 (100%)	0	100	100
1	HI	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	HJ	97/98 (99%)	97 (100%)	0	100	100
1	HK	97/98 (99%)	97 (100%)	0	100	100
1	HL	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	HM	97/98 (99%)	97 (100%)	0	100	100
1	HN	97/98 (99%)	97 (100%)	0	100	100
1	HO	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	HP	97/98 (99%)	97 (100%)	0	100	100
1	HQ	97/98 (99%)	97 (100%)	0	100	100
1	HR	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	HS	97/98 (99%)	97 (100%)	0	100	100
1	HT	97/98 (99%)	97 (100%)	0	100	100
1	HU	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	HV	97/98 (99%)	97 (100%)	0	100	100
1	HW	97/98 (99%)	97 (100%)	0	100	100
1	HX	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	HY	97/98 (99%)	97 (100%)	0	100	100
1	HZ	97/98 (99%)	97 (100%)	0	100	100
1	IA	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	IB	97/98 (99%)	97 (100%)	0	100	100
1	IC	97/98 (99%)	97 (100%)	0	100	100
1	ID	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	IE	97/98 (99%)	97 (100%)	0	100	100
1	IF	97/98 (99%)	97 (100%)	0	100	100
1	IG	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	IH	97/98 (99%)	97 (100%)	0	100	100
1	II	97/98 (99%)	97 (100%)	0	100	100
1	IJ	97/98 (99%)	96 (99%)	1 (1%)	76	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	IK	97/98 (99%)	97 (100%)	0	100	100
1	IL	97/98 (99%)	97 (100%)	0	100	100
1	IM	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	IN	97/98 (99%)	97 (100%)	0	100	100
1	IO	97/98 (99%)	97 (100%)	0	100	100
1	IP	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	IQ	97/98 (99%)	97 (100%)	0	100	100
1	IR	97/98 (99%)	97 (100%)	0	100	100
1	IS	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	IT	97/98 (99%)	97 (100%)	0	100	100
1	IU	97/98 (99%)	97 (100%)	0	100	100
1	IV	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	IW	97/98 (99%)	97 (100%)	0	100	100
1	IX	97/98 (99%)	97 (100%)	0	100	100
1	IY	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	IZ	97/98 (99%)	97 (100%)	0	100	100
1	JA	97/98 (99%)	97 (100%)	0	100	100
1	JB	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	JC	97/98 (99%)	97 (100%)	0	100	100
1	JD	97/98 (99%)	97 (100%)	0	100	100
1	JE	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	JF	97/98 (99%)	97 (100%)	0	100	100
1	JG	97/98 (99%)	97 (100%)	0	100	100
1	JH	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	JI	97/98 (99%)	97 (100%)	0	100	100
1	JJ	97/98 (99%)	97 (100%)	0	100	100
1	JK	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	JL	97/98 (99%)	97 (100%)	0	100	100
1	JM	97/98 (99%)	97 (100%)	0	100	100
1	JN	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	JO	97/98 (99%)	97 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	JP	97/98 (99%)	97 (100%)	0	100	100
1	JQ	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	JR	97/98 (99%)	97 (100%)	0	100	100
1	JS	97/98 (99%)	97 (100%)	0	100	100
1	JT	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	JU	97/98 (99%)	97 (100%)	0	100	100
1	JV	97/98 (99%)	97 (100%)	0	100	100
1	JW	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	JX	97/98 (99%)	97 (100%)	0	100	100
1	JY	97/98 (99%)	97 (100%)	0	100	100
1	JZ	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	KA	97/98 (99%)	97 (100%)	0	100	100
1	KB	97/98 (99%)	97 (100%)	0	100	100
1	KC	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	KD	97/98 (99%)	97 (100%)	0	100	100
1	KE	97/98 (99%)	97 (100%)	0	100	100
1	KF	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	KG	97/98 (99%)	97 (100%)	0	100	100
1	KH	97/98 (99%)	97 (100%)	0	100	100
1	KI	97/98 (99%)	96 (99%)	1 (1%)	76	88
1	KJ	97/98 (99%)	97 (100%)	0	100	100
All	All	26190/26460 (99%)	26100 (100%)	90 (0%)	92	97

5 of 90 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	GQ	66	LEU
1	IG	66	LEU
1	GW	66	LEU
1	HO	66	LEU
1	IS	66	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	HD	83	ASN
1	JS	83	ASN
1	HT	83	ASN
1	KD	83	ASN
1	JI	83	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AA	114/115 (99%)	-0.09	0 100 100	44, 67, 100, 129	0
1	AB	114/115 (99%)	0.02	0 100 100	39, 66, 99, 114	0
1	AC	114/115 (99%)	-0.07	1 (0%) 84 83	40, 68, 111, 175	0
1	AD	114/115 (99%)	0.11	0 100 100	44, 67, 100, 129	0
1	AE	114/115 (99%)	-0.04	1 (0%) 84 83	39, 66, 99, 114	0
1	AF	114/115 (99%)	0.08	0 100 100	40, 68, 111, 175	0
1	AG	114/115 (99%)	0.05	0 100 100	44, 67, 100, 129	0
1	AH	114/115 (99%)	-0.06	0 100 100	39, 66, 99, 114	0
1	AI	114/115 (99%)	0.01	1 (0%) 84 83	40, 68, 111, 175	0
1	AJ	114/115 (99%)	0.01	0 100 100	44, 67, 100, 129	0
1	AK	114/115 (99%)	-0.11	0 100 100	39, 66, 99, 114	0
1	AL	114/115 (99%)	0.04	2 (1%) 68 67	40, 68, 111, 175	0
1	AM	114/115 (99%)	0.06	1 (0%) 84 83	44, 67, 100, 129	0
1	AN	114/115 (99%)	-0.01	0 100 100	39, 66, 99, 114	0
1	AO	114/115 (99%)	0.12	2 (1%) 68 67	40, 68, 111, 175	0
1	AP	114/115 (99%)	-0.15	0 100 100	44, 67, 100, 129	0
1	AQ	114/115 (99%)	-0.14	0 100 100	39, 66, 99, 114	0
1	AR	114/115 (99%)	-0.06	0 100 100	40, 68, 111, 175	0
1	AS	114/115 (99%)	0.12	0 100 100	44, 67, 100, 129	0
1	AT	114/115 (99%)	0.19	0 100 100	39, 66, 99, 114	0
1	AU	114/115 (99%)	0.19	0 100 100	40, 68, 111, 175	0
1	AV	114/115 (99%)	0.20	0 100 100	44, 67, 100, 129	0
1	AW	114/115 (99%)	0.10	0 100 100	39, 66, 99, 114	0
1	AX	114/115 (99%)	0.10	1 (0%) 84 83	40, 68, 111, 175	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AY	114/115 (99%)	0.11	0 100 100	44, 67, 100, 129	0
1	AZ	114/115 (99%)	0.18	1 (0%) 84 83	39, 66, 99, 114	0
1	BA	114/115 (99%)	0.27	2 (1%) 68 67	40, 68, 111, 175	0
1	BB	114/115 (99%)	0.06	1 (0%) 84 83	44, 67, 100, 129	0
1	BC	114/115 (99%)	0.09	0 100 100	39, 66, 99, 114	0
1	BD	114/115 (99%)	0.27	3 (2%) 56 54	40, 68, 111, 175	0
1	BE	114/115 (99%)	0.05	0 100 100	44, 67, 100, 129	0
1	BF	114/115 (99%)	-0.01	0 100 100	39, 66, 99, 114	0
1	BG	114/115 (99%)	-0.03	0 100 100	40, 68, 111, 175	0
1	BH	114/115 (99%)	-0.06	0 100 100	44, 67, 100, 129	0
1	BI	114/115 (99%)	-0.05	0 100 100	39, 66, 99, 114	0
1	BJ	114/115 (99%)	0.07	1 (0%) 84 83	40, 68, 111, 175	0
1	BK	114/115 (99%)	-0.04	0 100 100	44, 67, 100, 129	0
1	BL	114/115 (99%)	-0.09	0 100 100	39, 66, 99, 114	0
1	BM	114/115 (99%)	0.06	1 (0%) 84 83	40, 68, 111, 175	0
1	BN	114/115 (99%)	-0.06	0 100 100	44, 67, 100, 129	0
1	BO	114/115 (99%)	-0.02	0 100 100	39, 66, 99, 114	0
1	BP	114/115 (99%)	0.06	3 (2%) 56 54	40, 68, 111, 175	0
1	BQ	114/115 (99%)	-0.02	0 100 100	44, 67, 100, 129	0
1	BR	114/115 (99%)	-0.11	0 100 100	39, 66, 99, 114	0
1	BS	114/115 (99%)	-0.12	0 100 100	40, 68, 111, 175	0
1	BT	114/115 (99%)	-0.13	0 100 100	44, 67, 100, 129	0
1	BU	114/115 (99%)	-0.17	0 100 100	39, 66, 99, 114	0
1	BV	114/115 (99%)	-0.02	2 (1%) 68 67	40, 68, 111, 175	0
1	BW	114/115 (99%)	-0.05	0 100 100	44, 67, 100, 129	0
1	BX	114/115 (99%)	0.06	0 100 100	39, 66, 99, 114	0
1	BY	114/115 (99%)	0.23	1 (0%) 84 83	40, 68, 111, 175	0
1	BZ	114/115 (99%)	0.01	0 100 100	44, 67, 100, 129	0
1	CA	114/115 (99%)	-0.11	0 100 100	39, 66, 99, 114	0
1	CB	114/115 (99%)	0.04	0 100 100	40, 68, 111, 175	0
1	CC	114/115 (99%)	-0.12	0 100 100	44, 67, 100, 129	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	CD	114/115 (99%)	-0.10	0 100 100	39, 66, 99, 114	0
1	CE	114/115 (99%)	-0.02	0 100 100	40, 68, 111, 175	0
1	CF	114/115 (99%)	0.08	0 100 100	44, 67, 100, 129	0
1	CG	114/115 (99%)	0.12	1 (0%) 84 83	39, 66, 99, 114	0
1	CH	114/115 (99%)	0.16	1 (0%) 84 83	40, 68, 111, 175	0
1	CI	114/115 (99%)	-0.04	0 100 100	44, 67, 100, 129	0
1	CJ	114/115 (99%)	-0.04	0 100 100	39, 66, 99, 114	0
1	CK	114/115 (99%)	0.03	1 (0%) 84 83	40, 68, 111, 175	0
1	CL	114/115 (99%)	0.05	1 (0%) 84 83	44, 67, 100, 129	0
1	CM	114/115 (99%)	0.11	1 (0%) 84 83	39, 66, 99, 114	0
1	CN	114/115 (99%)	0.11	0 100 100	40, 68, 111, 175	0
1	CO	114/115 (99%)	-0.12	0 100 100	44, 67, 100, 129	0
1	CP	114/115 (99%)	-0.11	0 100 100	39, 66, 99, 114	0
1	CQ	114/115 (99%)	-0.00	0 100 100	40, 68, 111, 175	0
1	CR	114/115 (99%)	0.03	0 100 100	44, 67, 100, 129	0
1	CS	114/115 (99%)	-0.09	0 100 100	39, 66, 99, 114	0
1	CT	114/115 (99%)	-0.07	1 (0%) 84 83	40, 68, 111, 175	0
1	CU	114/115 (99%)	0.04	1 (0%) 84 83	44, 67, 100, 129	0
1	CV	114/115 (99%)	-0.02	0 100 100	39, 66, 99, 114	0
1	CW	114/115 (99%)	0.13	3 (2%) 56 54	40, 68, 111, 175	0
1	CX	114/115 (99%)	0.07	0 100 100	44, 67, 100, 129	0
1	CY	114/115 (99%)	0.04	1 (0%) 84 83	39, 66, 99, 114	0
1	CZ	114/115 (99%)	0.04	0 100 100	40, 68, 111, 175	0
1	DA	114/115 (99%)	0.00	1 (0%) 84 83	44, 67, 100, 129	0
1	DB	114/115 (99%)	0.03	0 100 100	39, 66, 99, 114	0
1	DC	114/115 (99%)	0.18	2 (1%) 68 67	40, 68, 111, 175	0
1	DD	114/115 (99%)	0.00	0 100 100	44, 67, 100, 129	0
1	DE	114/115 (99%)	-0.03	0 100 100	39, 66, 99, 114	0
1	DF	114/115 (99%)	-0.06	0 100 100	40, 68, 111, 175	0
1	DG	114/115 (99%)	-0.02	0 100 100	44, 67, 100, 129	0
1	DH	114/115 (99%)	-0.01	1 (0%) 84 83	39, 66, 99, 114	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	DI	114/115 (99%)	0.04	2 (1%) 68 67	40, 68, 111, 175	0
1	DJ	114/115 (99%)	-0.08	0 100 100	44, 67, 100, 129	0
1	DK	114/115 (99%)	-0.10	0 100 100	39, 66, 99, 114	0
1	DL	114/115 (99%)	-0.02	1 (0%) 84 83	40, 68, 111, 175	0
1	DM	114/115 (99%)	0.00	0 100 100	44, 67, 100, 129	0
1	DN	114/115 (99%)	-0.06	1 (0%) 84 83	39, 66, 99, 114	0
1	DO	114/115 (99%)	-0.09	0 100 100	40, 68, 111, 175	0
1	DP	114/115 (99%)	0.07	0 100 100	44, 67, 100, 129	0
1	DQ	114/115 (99%)	0.01	0 100 100	39, 66, 99, 114	0
1	DR	114/115 (99%)	0.10	1 (0%) 84 83	40, 68, 111, 175	0
1	DS	114/115 (99%)	-0.11	0 100 100	44, 67, 100, 129	0
1	DT	114/115 (99%)	-0.11	0 100 100	39, 66, 99, 114	0
1	DU	114/115 (99%)	0.07	2 (1%) 68 67	40, 68, 111, 175	0
1	DV	114/115 (99%)	-0.01	0 100 100	44, 67, 100, 129	0
1	DW	114/115 (99%)	-0.03	0 100 100	39, 66, 99, 114	0
1	DX	114/115 (99%)	0.05	2 (1%) 68 67	40, 68, 111, 175	0
1	DY	114/115 (99%)	0.03	2 (1%) 68 67	44, 67, 100, 129	0
1	DZ	114/115 (99%)	0.02	0 100 100	39, 66, 99, 114	0
1	EA	114/115 (99%)	0.02	0 100 100	40, 68, 111, 175	0
1	EB	114/115 (99%)	-0.06	1 (0%) 84 83	44, 67, 100, 129	0
1	EC	114/115 (99%)	-0.10	0 100 100	39, 66, 99, 114	0
1	ED	114/115 (99%)	-0.04	0 100 100	40, 68, 111, 175	0
1	EE	114/115 (99%)	0.06	0 100 100	44, 67, 100, 129	0
1	EF	114/115 (99%)	0.17	1 (0%) 84 83	39, 66, 99, 114	0
1	EG	114/115 (99%)	0.28	1 (0%) 84 83	40, 68, 111, 175	0
1	EH	114/115 (99%)	0.13	0 100 100	44, 67, 100, 129	0
1	EI	114/115 (99%)	0.21	0 100 100	39, 66, 99, 114	0
1	EJ	114/115 (99%)	0.17	1 (0%) 84 83	40, 68, 111, 175	0
1	EK	114/115 (99%)	0.18	0 100 100	44, 67, 100, 129	0
1	EL	114/115 (99%)	0.03	1 (0%) 84 83	39, 66, 99, 114	0
1	EM	114/115 (99%)	0.34	4 (3%) 44 43	40, 68, 111, 175	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	EN	114/115 (99%)	0.19	1 (0%) 84 83	44, 67, 100, 129	0
1	EO	114/115 (99%)	0.16	0 100 100	39, 66, 99, 114	0
1	EP	114/115 (99%)	0.19	1 (0%) 84 83	40, 68, 111, 175	0
1	EQ	114/115 (99%)	-0.04	0 100 100	44, 67, 100, 129	0
1	ER	114/115 (99%)	0.08	0 100 100	39, 66, 99, 114	0
1	ES	114/115 (99%)	-0.00	0 100 100	40, 68, 111, 175	0
1	ET	114/115 (99%)	-0.00	0 100 100	44, 67, 100, 129	0
1	EU	114/115 (99%)	-0.06	0 100 100	39, 66, 99, 114	0
1	EV	114/115 (99%)	0.11	0 100 100	40, 68, 111, 175	0
1	EW	114/115 (99%)	0.09	0 100 100	44, 67, 100, 129	0
1	EX	114/115 (99%)	0.08	0 100 100	39, 66, 99, 114	0
1	EY	114/115 (99%)	0.19	1 (0%) 84 83	40, 68, 111, 175	0
1	EZ	114/115 (99%)	-0.01	0 100 100	44, 67, 100, 129	0
1	FA	114/115 (99%)	0.03	0 100 100	39, 66, 99, 114	0
1	FB	114/115 (99%)	0.07	2 (1%) 68 67	40, 68, 111, 175	0
1	FC	114/115 (99%)	0.04	0 100 100	44, 67, 100, 129	0
1	FD	114/115 (99%)	-0.08	0 100 100	39, 66, 99, 114	0
1	FE	114/115 (99%)	0.02	0 100 100	40, 68, 111, 175	0
1	FF	114/115 (99%)	-0.14	1 (0%) 84 83	44, 67, 100, 129	0
1	FG	114/115 (99%)	-0.17	0 100 100	39, 66, 99, 114	0
1	FH	114/115 (99%)	-0.05	0 100 100	40, 68, 111, 175	0
1	FI	114/115 (99%)	0.14	2 (1%) 68 67	44, 67, 100, 129	0
1	FJ	114/115 (99%)	0.13	1 (0%) 84 83	39, 66, 99, 114	0
1	FK	114/115 (99%)	0.18	2 (1%) 68 67	40, 68, 111, 175	0
1	FL	114/115 (99%)	-0.01	0 100 100	44, 67, 100, 129	0
1	FM	114/115 (99%)	-0.05	0 100 100	39, 66, 99, 114	0
1	FN	114/115 (99%)	0.05	0 100 100	40, 68, 111, 175	0
1	FO	114/115 (99%)	-0.09	0 100 100	44, 67, 100, 129	0
1	FP	114/115 (99%)	-0.18	0 100 100	39, 66, 99, 114	0
1	FQ	114/115 (99%)	-0.08	0 100 100	40, 68, 111, 175	0
1	FR	114/115 (99%)	0.12	3 (2%) 56 54	44, 67, 100, 129	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	FS	114/115 (99%)	0.05	0 100 100	39, 66, 99, 114	0
1	FT	114/115 (99%)	0.03	0 100 100	40, 68, 111, 175	0
1	FU	114/115 (99%)	-0.10	0 100 100	44, 67, 100, 129	0
1	FV	114/115 (99%)	-0.05	0 100 100	39, 66, 99, 114	0
1	FW	114/115 (99%)	0.00	5 (4%) 34 34	40, 68, 111, 175	0
1	FX	114/115 (99%)	0.06	0 100 100	44, 67, 100, 129	0
1	FY	114/115 (99%)	-0.07	0 100 100	39, 66, 99, 114	0
1	FZ	114/115 (99%)	0.19	3 (2%) 56 54	40, 68, 111, 175	0
1	GA	114/115 (99%)	-0.08	0 100 100	44, 67, 100, 129	0
1	GB	114/115 (99%)	-0.14	0 100 100	39, 66, 99, 114	0
1	GC	114/115 (99%)	-0.00	0 100 100	40, 68, 111, 175	0
1	GD	114/115 (99%)	-0.05	0 100 100	44, 67, 100, 129	0
1	GE	114/115 (99%)	0.02	0 100 100	39, 66, 99, 114	0
1	GF	114/115 (99%)	-0.01	2 (1%) 68 67	40, 68, 111, 175	0
1	GG	114/115 (99%)	-0.10	0 100 100	44, 67, 100, 129	0
1	GH	114/115 (99%)	0.09	1 (0%) 84 83	39, 66, 99, 114	0
1	GI	114/115 (99%)	0.11	2 (1%) 68 67	40, 68, 111, 175	0
1	GJ	114/115 (99%)	0.05	0 100 100	44, 67, 100, 129	0
1	GK	114/115 (99%)	-0.06	0 100 100	39, 66, 99, 114	0
1	GL	114/115 (99%)	0.12	2 (1%) 68 67	40, 68, 111, 175	0
1	GM	114/115 (99%)	0.04	0 100 100	44, 67, 100, 129	0
1	GN	114/115 (99%)	0.06	0 100 100	39, 66, 99, 114	0
1	GO	114/115 (99%)	-0.03	0 100 100	40, 68, 111, 175	0
1	GP	114/115 (99%)	-0.04	0 100 100	44, 67, 100, 129	0
1	GQ	114/115 (99%)	-0.09	0 100 100	39, 66, 99, 114	0
1	GR	114/115 (99%)	0.06	0 100 100	40, 68, 111, 175	0
1	GS	114/115 (99%)	-0.12	0 100 100	44, 67, 100, 129	0
1	GT	114/115 (99%)	-0.17	0 100 100	39, 66, 99, 114	0
1	GU	114/115 (99%)	-0.02	0 100 100	40, 68, 111, 175	0
1	GV	114/115 (99%)	-0.09	0 100 100	44, 67, 100, 129	0
1	GW	114/115 (99%)	-0.00	0 100 100	39, 66, 99, 114	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	GX	114/115 (99%)	-0.10	1 (0%) 84 83	40, 68, 111, 175	0
1	GY	114/115 (99%)	-0.14	1 (0%) 84 83	44, 67, 100, 129	0
1	GZ	114/115 (99%)	-0.11	0 100 100	39, 66, 99, 114	0
1	HA	114/115 (99%)	-0.03	2 (1%) 68 67	40, 68, 111, 175	0
1	HB	114/115 (99%)	-0.13	0 100 100	44, 67, 100, 129	0
1	HC	114/115 (99%)	-0.18	0 100 100	39, 66, 99, 114	0
1	HD	114/115 (99%)	-0.10	0 100 100	40, 68, 111, 175	0
1	HE	114/115 (99%)	-0.12	0 100 100	44, 67, 100, 129	0
1	HF	114/115 (99%)	-0.04	0 100 100	39, 66, 99, 114	0
1	HG	114/115 (99%)	-0.06	3 (2%) 56 54	40, 68, 111, 175	0
1	HH	114/115 (99%)	-0.13	0 100 100	44, 67, 100, 129	0
1	HI	114/115 (99%)	-0.18	0 100 100	39, 66, 99, 114	0
1	HJ	114/115 (99%)	-0.06	0 100 100	40, 68, 111, 175	0
1	HK	114/115 (99%)	-0.03	1 (0%) 84 83	44, 67, 100, 129	0
1	HL	114/115 (99%)	0.05	0 100 100	39, 66, 99, 114	0
1	HM	114/115 (99%)	0.18	2 (1%) 68 67	40, 68, 111, 175	0
1	HN	114/115 (99%)	-0.15	0 100 100	44, 67, 100, 129	0
1	HO	114/115 (99%)	-0.20	0 100 100	39, 66, 99, 114	0
1	HP	114/115 (99%)	-0.06	1 (0%) 84 83	40, 68, 111, 175	0
1	HQ	114/115 (99%)	-0.02	0 100 100	44, 67, 100, 129	0
1	HR	114/115 (99%)	-0.25	0 100 100	39, 66, 99, 114	0
1	HS	114/115 (99%)	-0.09	0 100 100	40, 68, 111, 175	0
1	HT	114/115 (99%)	-0.14	1 (0%) 84 83	44, 67, 100, 129	0
1	HU	114/115 (99%)	-0.21	0 100 100	39, 66, 99, 114	0
1	HV	114/115 (99%)	0.05	0 100 100	40, 68, 111, 175	0
1	HW	114/115 (99%)	-0.10	0 100 100	44, 67, 100, 129	0
1	HX	114/115 (99%)	-0.18	0 100 100	39, 66, 99, 114	0
1	HY	114/115 (99%)	0.01	1 (0%) 84 83	40, 68, 111, 175	0
1	HZ	114/115 (99%)	0.07	0 100 100	44, 67, 100, 129	0
1	IA	114/115 (99%)	0.10	1 (0%) 84 83	39, 66, 99, 114	0
1	IB	114/115 (99%)	0.13	1 (0%) 84 83	40, 68, 111, 175	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	IC	114/115 (99%)	-0.09	0 100 100	44, 67, 100, 129	0
1	ID	114/115 (99%)	-0.08	1 (0%) 84 83	39, 66, 99, 114	0
1	IE	114/115 (99%)	0.05	2 (1%) 68 67	40, 68, 111, 175	0
1	IF	114/115 (99%)	0.13	0 100 100	44, 67, 100, 129	0
1	IG	114/115 (99%)	0.17	0 100 100	39, 66, 99, 114	0
1	IH	114/115 (99%)	0.09	1 (0%) 84 83	40, 68, 111, 175	0
1	II	114/115 (99%)	0.06	2 (1%) 68 67	44, 67, 100, 129	0
1	IJ	114/115 (99%)	0.06	1 (0%) 84 83	39, 66, 99, 114	0
1	IK	114/115 (99%)	0.07	1 (0%) 84 83	40, 68, 111, 175	0
1	IL	114/115 (99%)	-0.16	0 100 100	44, 67, 100, 129	0
1	IM	114/115 (99%)	-0.18	0 100 100	39, 66, 99, 114	0
1	IN	114/115 (99%)	0.02	3 (2%) 56 54	40, 68, 111, 175	0
1	IO	114/115 (99%)	0.00	2 (1%) 68 67	44, 67, 100, 129	0
1	IP	114/115 (99%)	-0.19	0 100 100	39, 66, 99, 114	0
1	IQ	114/115 (99%)	-0.01	1 (0%) 84 83	40, 68, 111, 175	0
1	IR	114/115 (99%)	-0.01	0 100 100	44, 67, 100, 129	0
1	IS	114/115 (99%)	-0.11	0 100 100	39, 66, 99, 114	0
1	IT	114/115 (99%)	-0.13	0 100 100	40, 68, 111, 175	0
1	IU	114/115 (99%)	0.17	1 (0%) 84 83	44, 67, 100, 129	0
1	IV	114/115 (99%)	-0.08	0 100 100	39, 66, 99, 114	0
1	IW	114/115 (99%)	0.06	2 (1%) 68 67	40, 68, 111, 175	0
1	IX	114/115 (99%)	-0.14	0 100 100	44, 67, 100, 129	0
1	IY	114/115 (99%)	-0.15	0 100 100	39, 66, 99, 114	0
1	IZ	114/115 (99%)	-0.05	0 100 100	40, 68, 111, 175	0
1	JA	114/115 (99%)	-0.03	0 100 100	44, 67, 100, 129	0
1	JB	114/115 (99%)	-0.15	1 (0%) 84 83	39, 66, 99, 114	0
1	JC	114/115 (99%)	-0.10	0 100 100	40, 68, 111, 175	0
1	JD	114/115 (99%)	0.12	2 (1%) 68 67	44, 67, 100, 129	0
1	JE	114/115 (99%)	-0.04	0 100 100	39, 66, 99, 114	0
1	JF	114/115 (99%)	0.00	3 (2%) 56 54	40, 68, 111, 175	0
1	JG	114/115 (99%)	0.03	0 100 100	44, 67, 100, 129	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	JH	114/115 (99%)	-0.05	0 100 100	39, 66, 99, 114	0
1	JI	114/115 (99%)	0.01	0 100 100	40, 68, 111, 175	0
1	JJ	114/115 (99%)	-0.06	2 (1%) 68 67	44, 67, 100, 129	0
1	JK	114/115 (99%)	-0.18	1 (0%) 84 83	39, 66, 99, 114	0
1	JL	114/115 (99%)	-0.04	0 100 100	40, 68, 111, 175	0
1	JM	114/115 (99%)	-0.06	1 (0%) 84 83	44, 67, 100, 129	0
1	JN	114/115 (99%)	-0.12	0 100 100	39, 66, 99, 114	0
1	JO	114/115 (99%)	-0.06	1 (0%) 84 83	40, 68, 111, 175	0
1	JP	114/115 (99%)	-0.15	0 100 100	44, 67, 100, 129	0
1	JQ	114/115 (99%)	-0.14	0 100 100	39, 66, 99, 114	0
1	JR	114/115 (99%)	0.03	1 (0%) 84 83	40, 68, 111, 175	0
1	JS	114/115 (99%)	-0.07	0 100 100	44, 67, 100, 129	0
1	JT	114/115 (99%)	-0.04	1 (0%) 84 83	39, 66, 99, 114	0
1	JU	114/115 (99%)	0.03	0 100 100	40, 68, 111, 175	0
1	JV	114/115 (99%)	0.07	1 (0%) 84 83	44, 67, 100, 129	0
1	JW	114/115 (99%)	-0.11	0 100 100	39, 66, 99, 114	0
1	JX	114/115 (99%)	0.16	2 (1%) 68 67	40, 68, 111, 175	0
1	JY	114/115 (99%)	-0.04	1 (0%) 84 83	44, 67, 100, 129	0
1	JZ	114/115 (99%)	-0.09	0 100 100	39, 66, 99, 114	0
1	KA	114/115 (99%)	-0.06	3 (2%) 56 54	40, 68, 111, 175	0
1	KB	114/115 (99%)	-0.01	0 100 100	44, 67, 100, 129	0
1	KC	114/115 (99%)	0.04	0 100 100	39, 66, 99, 114	0
1	KD	114/115 (99%)	0.10	1 (0%) 84 83	40, 68, 111, 175	0
1	KE	114/115 (99%)	-0.10	1 (0%) 84 83	44, 67, 100, 129	0
1	KF	114/115 (99%)	-0.06	0 100 100	39, 66, 99, 114	0
1	KG	114/115 (99%)	-0.03	0 100 100	40, 68, 111, 175	0
1	KH	114/115 (99%)	-0.07	0 100 100	44, 67, 100, 129	0
1	KI	114/115 (99%)	0.07	2 (1%) 68 67	39, 66, 99, 114	0
1	KJ	114/115 (99%)	0.17	1 (0%) 84 83	40, 68, 111, 175	0
All	All	30780/31050 (99%)	-0.00	145 (0%) 91 90	39, 67, 105, 175	0

The worst 5 of 145 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DI	61	GLY	5.7
1	FB	60	ASP	5.7
1	HM	61	GLY	5.6
1	EJ	60	ASP	5.1
1	HY	61	GLY	5.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.