



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 29, 2026 – 09:43 AM UTC

PDB ID : 4V99 / pdb_00004v99
Title : The Crystallographic Structure of Panicum Mosaic Virus
Authors : Makino, D.L.; Larson, S.B.; McPherson, A.
Deposited on : 2012-07-04
Resolution : 2.90 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

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>.

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

MolProbity	:	FAILED
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

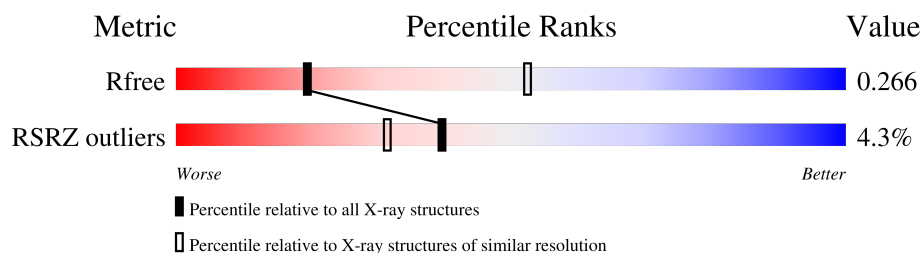
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	180053	2481 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 588120 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 Capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	AB	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	AC	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	AF	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	AG	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	AH	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	AK	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	AL	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	AM	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	AP	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	AQ	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	AR	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	AU	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	AV	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	AW	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	AZ	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Aa	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Ab	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Ae	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Af	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Ag	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Aj	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Ak	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Al	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Ao	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Ap	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Aq	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	At	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Au	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Av	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Ay	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Az	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	A1	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	A4	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	A5	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	A6	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	BA	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	BB	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	BC	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	BF	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	BG	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	BH	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	BK	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	BL	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	BM	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	BP	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	BQ	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	BR	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	BU	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	BV	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	BW	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	BZ	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Ba	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Bb	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Be	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Bf	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Bg	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Bj	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Bk	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Bl	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Bo	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Bp	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Bq	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Bt	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Bu	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Bv	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	By	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Bz	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	B1	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	B4	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	B5	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	B6	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	CA	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	CB	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	CC	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	CF	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	CG	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	CH	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	CK	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	CL	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	CM	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	CP	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	CQ	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	CR	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	CU	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	CV	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	CW	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	CZ	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Ca	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Cb	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Ce	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Cf	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Cg	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Cj	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Ck	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Cl	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Co	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Cp	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Cq	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Ct	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Cu	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Cv	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Cy	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Cz	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	C1	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	C4	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	C5	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	C6	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	DA	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	DB	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	DC	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	DF	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	DG	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	DH	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	DK	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	DL	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	DM	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	DP	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	DQ	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	DR	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	DU	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	DV	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	DW	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	DZ	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Da	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Db	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	De	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Df	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Dg	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Dj	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Dk	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Di	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Do	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Dp	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Dq	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Dt	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Du	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Dv	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Dy	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Dz	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	D1	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	D4	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D5	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	D6	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	EA	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	EB	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	EC	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	EF	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	EG	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	EH	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	EK	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	EL	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	EM	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	EP	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	EQ	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	ER	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	EU	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	EV	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	EW	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	EZ	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Ea	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Eb	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Ee	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Ef	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Eg	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Ej	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Ek	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	El	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Eo	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Ep	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Eq	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Et	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Eu	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Ev	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Ey	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Ez	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	E1	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	E4	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	E5	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	E6	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	FA	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	FB	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	FC	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	FF	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	FG	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	FH	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	FK	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0
1	FL	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	FM	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	FP	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0
1	FQ	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	FR	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	FU	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0
1	FV	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	FW	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	FZ	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0
1	Fa	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	Fb	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	Fe	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0
1	Ff	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	Fg	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	Fj	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0
1	Fk	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	Fl	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	Fo	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Fp	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	Fq	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	Ft	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0
1	Fu	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	Fv	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	Fy	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0
1	Fz	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	F1	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	F4	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0
1	F5	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	F6	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	GA	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0
1	GB	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	GC	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	GF	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0
1	GG	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	GH	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	GK	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0
1	GL	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	GM	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	GP	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	GQ	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	GR	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	GU	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	GV	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	GW	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	GZ	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Ga	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Gb	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Ge	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Gf	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Gg	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Gj	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Gk	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Gl	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Go	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Gp	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Gq	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Gt	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Gu	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Gv	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Gy	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Gz	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	G1	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	G4	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0
1	G5	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	G6	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	HA	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0
1	HB	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	HC	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	HF	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0
1	HG	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	HH	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	HK	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0
1	HL	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	HM	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	HP	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0
1	HQ	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	HR	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	HU	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0
1	HV	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	HW	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	HZ	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Ha	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Hb	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	He	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Hf	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Hg	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Hj	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Hk	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Hi	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Ho	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Hp	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Hq	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Ht	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Hu	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Hv	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Hy	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Hx	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	H1	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	H4	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	H5	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	H6	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	IA	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	IB	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	IC	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	IF	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	IG	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	IH	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	IK	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	IL	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	IM	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	IP	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	IQ	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	IR	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	IU	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	IV	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	IW	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	IZ	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Ia	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Ib	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Ie	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	If	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Ig	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Ij	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Ik	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	Il	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	Io	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0
1	Ip	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	Iq	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	It	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0
1	Iu	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	Iv	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	Iy	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0
1	Iz	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	I1	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	I4	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0
1	I5	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	I6	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	JA	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0
1	JB	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	JC	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	JF	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0
1	JG	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	JH	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	JK	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	JL	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	JM	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	JP	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0
1	JQ	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	JR	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	JU	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0
1	JV	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	JW	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	JZ	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0
1	Ja	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	Jb	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	Je	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0
1	Jf	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	Jg	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	Jj	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0
1	Js	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	Jl	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	Jo	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0
1	Jp	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	Jq	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	Jt	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Ju	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Jv	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Jy	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Jz	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	J1	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	J4	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	J5	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	J6	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			

- Molecule 2 is a RNA chain called 5'-R(P*UP*UP*AP*AP*UP*AP*UP*UP*UP*UP*UP*AP*UP*UP*UP*UP*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AD	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			
2	AI	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			
2	AN	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			
2	AS	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			
2	AX	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			
2	Ac	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			
2	Ah	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			
2	Am	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			
2	Ar	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			
2	Aw	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			
2	A2	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A7	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	BD	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	BI	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	BN	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	BS	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	BX	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Bc	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Bh	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Bm	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Br	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Bw	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	B2	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	B7	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	CD	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	CI	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	CN	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	CS	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	CX	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Cc	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Ch	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Cm	17	Total 349	C 157	N 46	O 129	P 17	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Cr	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Cw	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	C2	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	C7	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	DD	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	DI	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	DN	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	DS	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	DX	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Dc	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Dh	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Dm	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Dr	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Dw	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	D2	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	D7	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	ED	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	EI	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	EN	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	ES	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	EX	17	Total 349	C 157	N 46	O 129	P 17	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Ec	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Eh	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Em	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Er	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Ew	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	E2	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	E7	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	FD	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	FI	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	FN	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	FS	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	FX	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Fc	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Fh	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Fm	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Fr	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Fw	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	F2	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	F7	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	GD	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	GI	17	Total 349	C 157	N 46	O 129	P 17	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	GN	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	GS	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	GX	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Gc	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Gh	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Gm	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Gr	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Gw	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	G2	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	G7	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	HD	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	HI	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	HN	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	HS	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	HX	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Hc	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Hh	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Hm	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Hr	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Hw	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	H2	17	Total 349	C 157	N 46	O 129	P 17	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H7	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	ID	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	II	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	IN	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	IS	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	IX	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Ic	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Ih	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Im	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Ir	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Iw	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	I2	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	I7	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	JD	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	JI	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	JN	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	JS	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	JX	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Jc	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Jh	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Jm	17	Total 349	C 157	N 46	O 129	P 17	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Jr	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			
2	Jw	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			
2	J2	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			
2	J7	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AA	1	Total	Ca	0	0
			1	1		
3	AF	1	Total	Ca	0	0
			1	1		
3	AL	1	Total	Ca	0	0
			1	1		
3	AP	1	Total	Ca	0	0
			1	1		
3	AU	1	Total	Ca	0	0
			1	1		
3	AZ	1	Total	Ca	0	0
			1	1		
3	Af	1	Total	Ca	0	0
			1	1		
3	Aj	1	Total	Ca	0	0
			1	1		
3	Ao	1	Total	Ca	0	0
			1	1		
3	At	1	Total	Ca	0	0
			1	1		
3	A1	1	Total	Ca	0	0
			1	1		
3	A4	1	Total	Ca	0	0
			1	1		
3	BB	1	Total	Ca	0	0
			1	1		
3	BF	1	Total	Ca	0	0
			1	1		
3	BK	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	BQ	1	Total 1	Ca 1	0	0
3	BU	1	Total 1	Ca 1	0	0
3	BZ	1	Total 1	Ca 1	0	0
3	Be	1	Total 1	Ca 1	0	0
3	Bk	1	Total 1	Ca 1	0	0
3	Bo	1	Total 1	Ca 1	0	0
3	Bt	1	Total 1	Ca 1	0	0
3	By	1	Total 1	Ca 1	0	0
3	B5	1	Total 1	Ca 1	0	0
3	CA	1	Total 1	Ca 1	0	0
3	CG	1	Total 1	Ca 1	0	0
3	CK	1	Total 1	Ca 1	0	0
3	CP	1	Total 1	Ca 1	0	0
3	CU	1	Total 1	Ca 1	0	0
3	CZ	1	Total 1	Ca 1	0	0
3	Ce	1	Total 1	Ca 1	0	0
3	Cj	1	Total 1	Ca 1	0	0
3	Co	1	Total 1	Ca 1	0	0
3	Ct	1	Total 1	Ca 1	0	0
3	Cy	1	Total 1	Ca 1	0	0
3	C4	1	Total 1	Ca 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	DA	1	Total 1	Ca 1	0	0
3	DF	1	Total 1	Ca 1	0	0
3	DK	1	Total 1	Ca 1	0	0
3	DP	1	Total 1	Ca 1	0	0
3	DU	1	Total 1	Ca 1	0	0
3	DZ	1	Total 1	Ca 1	0	0
3	Df	1	Total 1	Ca 1	0	0
3	Dj	1	Total 1	Ca 1	0	0
3	Do	1	Total 1	Ca 1	0	0
3	Dt	1	Total 1	Ca 1	0	0
3	Dy	1	Total 1	Ca 1	0	0
3	D4	1	Total 1	Ca 1	0	0
3	EC	1	Total 1	Ca 1	0	0
3	EF	1	Total 1	Ca 1	0	0
3	EK	1	Total 1	Ca 1	0	0
3	EP	1	Total 1	Ca 1	0	0
3	EU	1	Total 1	Ca 1	0	0
3	EZ	1	Total 1	Ca 1	0	0
3	Ee	1	Total 1	Ca 1	0	0
3	Ek	1	Total 1	Ca 1	0	0
3	Eo	1	Total 1	Ca 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	Et	1	Total 1	Ca 1	0	0
3	Ey	1	Total 1	Ca 1	0	0
3	E4	1	Total 1	Ca 1	0	0
3	FA	1	Total 1	Ca 1	0	0
3	FF	1	Total 1	Ca 1	0	0
3	FK	1	Total 1	Ca 1	0	0
3	FP	1	Total 1	Ca 1	0	0
3	FU	1	Total 1	Ca 1	0	0
3	FZ	1	Total 1	Ca 1	0	0
3	Fe	1	Total 1	Ca 1	0	0
3	Fk	1	Total 1	Ca 1	0	0
3	Fo	1	Total 1	Ca 1	0	0
3	Ft	1	Total 1	Ca 1	0	0
3	F1	1	Total 1	Ca 1	0	0
3	F4	1	Total 1	Ca 1	0	0
3	GA	1	Total 1	Ca 1	0	0
3	GF	1	Total 1	Ca 1	0	0
3	GK	1	Total 1	Ca 1	0	0
3	GP	1	Total 1	Ca 1	0	0
3	GU	1	Total 1	Ca 1	0	0
3	GZ	1	Total 1	Ca 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	Ge	1	Total 1	Ca 1	0	0
3	Gj	1	Total 1	Ca 1	0	0
3	Go	1	Total 1	Ca 1	0	0
3	Gt	1	Total 1	Ca 1	0	0
3	G1	1	Total 1	Ca 1	0	0
3	G4	1	Total 1	Ca 1	0	0
3	HA	1	Total 1	Ca 1	0	0
3	HF	1	Total 1	Ca 1	0	0
3	HK	1	Total 1	Ca 1	0	0
3	HP	1	Total 1	Ca 1	0	0
3	HU	1	Total 1	Ca 1	0	0
3	HZ	1	Total 1	Ca 1	0	0
3	Hg	1	Total 1	Ca 1	0	0
3	Hj	1	Total 1	Ca 1	0	0
3	Ho	1	Total 1	Ca 1	0	0
3	Ht	1	Total 1	Ca 1	0	0
3	Hy	1	Total 1	Ca 1	0	0
3	H4	1	Total 1	Ca 1	0	0
3	IA	1	Total 1	Ca 1	0	0
3	IF	1	Total 1	Ca 1	0	0
3	IK	1	Total 1	Ca 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	IR	1	Total 1	Ca 1	0	0
3	IU	1	Total 1	Ca 1	0	0
3	IZ	1	Total 1	Ca 1	0	0
3	If	1	Total 1	Ca 1	0	0
3	Ij	1	Total 1	Ca 1	0	0
3	Io	1	Total 1	Ca 1	0	0
3	It	1	Total 1	Ca 1	0	0
3	I1	1	Total 1	Ca 1	0	0
3	I4	1	Total 1	Ca 1	0	0
3	JA	1	Total 1	Ca 1	0	0
3	JF	1	Total 1	Ca 1	0	0
3	JL	1	Total 1	Ca 1	0	0
3	JP	1	Total 1	Ca 1	0	0
3	JU	1	Total 1	Ca 1	0	0
3	JZ	1	Total 1	Ca 1	0	0
3	Je	1	Total 1	Ca 1	0	0
3	Jj	1	Total 1	Ca 1	0	0
3	Jo	1	Total 1	Ca 1	0	0
3	Jt	1	Total 1	Ca 1	0	0
3	Jy	1	Total 1	Ca 1	0	0
3	J4	1	Total 1	Ca 1	0	0

MolProbity failed to run properly - this section is therefore empty.

3 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	411.74Å 403.90Å 412.46Å 90.00° 89.65° 90.00°	Depositor
Resolution (Å)	50.01 – 2.90 50.01 – 2.90	Depositor EDS
% Data completeness (in resolution range)	74.9 (50.01-2.90) 74.9 (50.01-2.90)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 2.91Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.251 , 0.285 0.233 , 0.266	Depositor DCC
R_{free} test set	221945 reflections (10.01%)	wwPDB-VP
Wilson B-factor (Å ²)	45.5	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 67.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.025 for -l,k,h 0.034 for -h,-l,-k 0.024 for -h,l,k 0.044 for -k,-h,-l 0.024 for k,h,-l 0.017 for -l,-h,k 0.030 for -k,l,-h 0.038 for l,h,k 0.027 for k,-l,-h 0.035 for h,-k,-l 0.030 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	588120	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 120 ligands modelled in this entry, 120 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers

There are no such residues in this entry.

4.8 Polymer linkage issues

There are no chain breaks in this entry.

5 Fit of model and data ⓘ

5.1 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, 95th 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 ²)	Q<0.9
1	A1	217/242 (89%)	0.19	9 (4%)	41	33	26, 56, 111, 194	0
1	A4	185/242 (76%)	0.15	5 (2%)	56	47	23, 52, 88, 132	0
1	A5	189/242 (78%)	0.12	7 (3%)	45	37	18, 52, 92, 153	0
1	A6	217/242 (89%)	0.14	7 (3%)	50	41	20, 53, 107, 200	0
1	AA	185/242 (76%)	0.11	4 (2%)	62	53	29, 54, 87, 113	0
1	AB	189/242 (78%)	-0.08	5 (2%)	57	48	25, 49, 90, 154	0
1	AC	217/242 (89%)	0.10	7 (3%)	50	41	21, 50, 108, 201	0
1	AF	185/242 (76%)	0.04	2 (1%)	78	71	22, 48, 85, 115	0
1	AG	189/242 (78%)	-0.03	3 (1%)	70	62	17, 42, 85, 140	0
1	AH	217/242 (89%)	0.22	10 (4%)	37	29	21, 50, 114, 203	0
1	AK	185/242 (76%)	0.13	3 (1%)	70	62	17, 51, 88, 123	0
1	AL	189/242 (78%)	-0.02	2 (1%)	78	71	24, 47, 91, 137	0
1	AM	217/242 (89%)	0.14	6 (2%)	55	46	19, 48, 106, 200	0
1	AP	185/242 (76%)	0.02	3 (1%)	70	62	21, 47, 87, 124	0
1	AQ	189/242 (78%)	-0.02	4 (2%)	63	54	17, 47, 87, 127	0
1	AR	217/242 (89%)	0.02	5 (2%)	61	52	17, 48, 103, 199	0
1	AU	185/242 (76%)	0.22	4 (2%)	62	53	36, 61, 96, 124	0
1	AV	189/242 (78%)	0.21	7 (3%)	45	37	35, 58, 91, 154	0
1	AW	217/242 (89%)	0.21	14 (6%)	25	20	27, 58, 108, 201	0
1	AZ	185/242 (76%)	-0.15	2 (1%)	78	71	14, 38, 69, 107	0
1	Aa	189/242 (78%)	-0.20	4 (2%)	63	54	14, 37, 79, 138	0
1	Ab	217/242 (89%)	-0.07	7 (3%)	50	41	16, 43, 107, 197	0
1	Ae	185/242 (76%)	-0.00	4 (2%)	62	53	17, 48, 92, 113	0
1	Af	189/242 (78%)	0.04	5 (2%)	57	48	19, 44, 87, 140	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	Ag	217/242 (89%)	0.04	4 (1%)	67	59	18, 48, 95, 199	0
1	Aj	185/242 (76%)	-0.05	3 (1%)	70	62	15, 48, 82, 114	0
1	Ak	189/242 (78%)	-0.09	2 (1%)	78	71	21, 47, 85, 136	0
1	Al	217/242 (89%)	0.09	5 (2%)	61	52	19, 44, 104, 191	0
1	Ao	185/242 (76%)	0.09	6 (3%)	50	41	20, 46, 79, 105	0
1	Ap	189/242 (78%)	-0.03	2 (1%)	78	71	19, 44, 80, 137	0
1	Aq	217/242 (89%)	0.10	7 (3%)	50	41	16, 46, 100, 197	0
1	At	185/242 (76%)	-0.10	5 (2%)	56	47	19, 45, 81, 112	0
1	Au	189/242 (78%)	-0.14	3 (1%)	70	62	9, 41, 85, 128	0
1	Av	217/242 (89%)	0.13	10 (4%)	37	29	10, 45, 106, 196	0
1	Ay	185/242 (76%)	0.15	4 (2%)	62	53	26, 57, 89, 119	0
1	Az	189/242 (78%)	-0.03	1 (0%)	87	83	27, 54, 96, 132	0
1	B1	217/242 (89%)	-0.02	7 (3%)	50	41	18, 44, 101, 188	0
1	B4	185/242 (76%)	0.23	2 (1%)	78	71	36, 61, 85, 117	0
1	B5	189/242 (78%)	0.08	4 (2%)	63	54	29, 55, 93, 145	0
1	B6	217/242 (89%)	0.15	12 (5%)	30	24	26, 54, 116, 209	0
1	BA	185/242 (76%)	0.22	2 (1%)	78	71	17, 56, 91, 116	0
1	BB	189/242 (78%)	0.13	4 (2%)	63	54	22, 50, 92, 146	0
1	BC	217/242 (89%)	0.19	7 (3%)	50	41	8, 50, 108, 193	0
1	BF	185/242 (76%)	-0.02	1 (0%)	87	83	18, 45, 81, 116	0
1	BG	189/242 (78%)	-0.25	3 (1%)	70	62	10, 38, 85, 127	0
1	BH	217/242 (89%)	-0.04	5 (2%)	61	52	13, 40, 95, 200	0
1	BK	185/242 (76%)	0.13	4 (2%)	62	53	12, 48, 87, 133	0
1	BL	189/242 (78%)	-0.01	1 (0%)	87	83	17, 47, 86, 130	0
1	BM	217/242 (89%)	0.22	11 (5%)	33	26	21, 48, 107, 209	0
1	BP	185/242 (76%)	-0.07	2 (1%)	78	71	22, 48, 84, 109	0
1	BQ	189/242 (78%)	0.03	3 (1%)	70	62	27, 48, 84, 139	0
1	BR	217/242 (89%)	-0.07	5 (2%)	61	52	15, 46, 101, 202	0
1	BU	185/242 (76%)	0.22	5 (2%)	56	47	29, 59, 97, 130	0
1	BV	189/242 (78%)	0.06	3 (1%)	70	62	26, 54, 93, 137	0
1	BW	217/242 (89%)	0.27	9 (4%)	41	33	27, 59, 110, 219	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	BZ	185/242 (76%)	-0.03	4 (2%)	62	53	15, 43, 81, 120	0
1	Ba	189/242 (78%)	-0.09	3 (1%)	70	62	22, 46, 88, 121	0
1	Bb	217/242 (89%)	0.04	8 (3%)	45	37	19, 45, 111, 192	0
1	Be	185/242 (76%)	-0.03	2 (1%)	78	71	17, 44, 83, 112	0
1	Bf	189/242 (78%)	-0.04	6 (3%)	50	41	14, 41, 86, 119	0
1	Bg	217/242 (89%)	0.01	6 (2%)	55	46	18, 45, 105, 176	0
1	Bj	185/242 (76%)	-0.05	2 (1%)	78	71	19, 46, 79, 117	0
1	Bk	189/242 (78%)	-0.01	1 (0%)	87	83	18, 47, 88, 127	0
1	Bl	217/242 (89%)	0.05	7 (3%)	50	41	16, 48, 101, 206	0
1	Bo	185/242 (76%)	0.07	2 (1%)	78	71	20, 50, 77, 121	0
1	Bp	189/242 (78%)	0.03	3 (1%)	70	62	21, 46, 92, 129	0
1	Bq	217/242 (89%)	0.08	6 (2%)	55	46	26, 48, 106, 189	0
1	Bt	185/242 (76%)	0.36	7 (3%)	44	36	33, 60, 94, 120	0
1	Bu	189/242 (78%)	0.12	4 (2%)	63	54	20, 51, 94, 133	0
1	Bv	217/242 (89%)	0.27	11 (5%)	33	26	25, 56, 111, 187	0
1	By	185/242 (76%)	0.03	5 (2%)	56	47	14, 46, 84, 123	0
1	Bz	189/242 (78%)	-0.16	4 (2%)	63	54	14, 40, 80, 139	0
1	C1	217/242 (89%)	-0.05	9 (4%)	41	33	12, 39, 104, 212	0
1	C4	185/242 (76%)	0.19	4 (2%)	62	53	19, 55, 92, 112	0
1	C5	189/242 (78%)	0.10	7 (3%)	45	37	23, 51, 89, 164	0
1	C6	217/242 (89%)	0.24	9 (4%)	41	33	24, 52, 109, 189	0
1	CA	185/242 (76%)	0.17	8 (4%)	40	31	28, 52, 94, 114	0
1	CB	189/242 (78%)	0.12	6 (3%)	50	41	18, 50, 81, 123	0
1	CC	217/242 (89%)	0.21	12 (5%)	30	24	22, 51, 107, 181	0
1	CF	185/242 (76%)	-0.14	5 (2%)	56	47	15, 37, 79, 119	0
1	CG	189/242 (78%)	-0.11	6 (3%)	50	41	9, 36, 82, 131	0
1	CH	217/242 (89%)	-0.09	6 (2%)	55	46	15, 35, 90, 195	0
1	CK	185/242 (76%)	0.16	5 (2%)	56	47	23, 53, 82, 125	0
1	CL	189/242 (78%)	0.05	2 (1%)	78	71	13, 47, 84, 149	0
1	CM	217/242 (89%)	0.27	7 (3%)	50	41	16, 50, 108, 206	0
1	CP	185/242 (76%)	-0.04	5 (2%)	56	47	23, 49, 77, 129	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	CQ	189/242 (78%)	-0.05	7 (3%)	45	37	16, 44, 92, 126	0
1	CR	217/242 (89%)	-0.01	6 (2%)	55	46	24, 50, 106, 195	0
1	CU	185/242 (76%)	0.19	4 (2%)	62	53	28, 56, 91, 117	0
1	CV	189/242 (78%)	0.11	4 (2%)	63	54	21, 52, 92, 144	0
1	CW	217/242 (89%)	0.09	8 (3%)	45	37	21, 51, 107, 194	0
1	CZ	185/242 (76%)	0.11	4 (2%)	62	53	26, 55, 91, 108	0
1	Ca	189/242 (78%)	0.04	1 (0%)	87	83	22, 53, 93, 141	0
1	Cb	217/242 (89%)	0.15	6 (2%)	55	46	15, 50, 106, 197	0
1	Ce	185/242 (76%)	0.03	2 (1%)	78	71	17, 49, 82, 117	0
1	Cf	189/242 (78%)	-0.03	2 (1%)	78	71	20, 46, 96, 130	0
1	Cg	217/242 (89%)	0.13	10 (4%)	37	29	16, 50, 104, 215	0
1	Cj	185/242 (76%)	0.09	6 (3%)	50	41	20, 48, 84, 109	0
1	Ck	189/242 (78%)	0.04	6 (3%)	50	41	20, 49, 98, 146	0
1	Cl	217/242 (89%)	0.14	13 (5%)	27	21	20, 46, 105, 204	0
1	Co	185/242 (76%)	0.06	4 (2%)	62	53	24, 49, 77, 110	0
1	Cp	189/242 (78%)	0.00	7 (3%)	45	37	16, 47, 90, 145	0
1	Cq	217/242 (89%)	0.19	8 (3%)	45	37	27, 52, 109, 204	0
1	Ct	185/242 (76%)	-0.03	3 (1%)	70	62	21, 45, 78, 116	0
1	Cu	189/242 (78%)	-0.25	3 (1%)	70	62	11, 39, 89, 136	0
1	Cv	217/242 (89%)	-0.11	7 (3%)	50	41	19, 42, 99, 199	0
1	Cy	185/242 (76%)	-0.22	1 (0%)	87	83	13, 38, 78, 107	0
1	Cz	189/242 (78%)	-0.16	5 (2%)	57	48	12, 34, 82, 123	0
1	D1	217/242 (89%)	-0.01	5 (2%)	61	52	14, 42, 106, 203	0
1	D4	185/242 (76%)	-0.05	2 (1%)	78	71	19, 41, 85, 110	0
1	D5	189/242 (78%)	-0.19	4 (2%)	63	54	12, 35, 78, 121	0
1	D6	217/242 (89%)	-0.06	6 (2%)	55	46	15, 38, 95, 205	0
1	DA	185/242 (76%)	-0.02	4 (2%)	62	53	20, 49, 83, 111	0
1	DB	189/242 (78%)	0.09	6 (3%)	50	41	16, 47, 85, 130	0
1	DC	217/242 (89%)	0.18	11 (5%)	33	26	17, 48, 103, 188	0
1	DF	185/242 (76%)	0.16	4 (2%)	62	53	25, 54, 85, 123	0
1	DG	189/242 (78%)	0.09	5 (2%)	57	48	25, 51, 89, 164	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	DH	217/242 (89%)	0.10	4 (1%)	67	59	22, 53, 106, 186	0
1	DK	185/242 (76%)	-0.09	4 (2%)	62	53	18, 45, 78, 105	0
1	DL	189/242 (78%)	-0.13	2 (1%)	78	71	13, 40, 84, 129	0
1	DM	217/242 (89%)	-0.05	6 (2%)	55	46	15, 43, 105, 207	0
1	DP	185/242 (76%)	0.01	5 (2%)	56	47	26, 52, 91, 123	0
1	DQ	189/242 (78%)	-0.01	4 (2%)	63	54	19, 47, 86, 137	0
1	DR	217/242 (89%)	0.02	5 (2%)	61	52	17, 46, 102, 190	0
1	DU	185/242 (76%)	0.30	6 (3%)	50	41	26, 63, 95, 128	0
1	DV	189/242 (78%)	0.14	5 (2%)	57	48	27, 57, 94, 149	0
1	DW	217/242 (89%)	0.29	11 (5%)	33	26	32, 60, 111, 195	0
1	DZ	185/242 (76%)	0.13	4 (2%)	62	53	22, 50, 94, 123	0
1	Da	189/242 (78%)	0.06	3 (1%)	70	62	18, 46, 89, 134	0
1	Db	217/242 (89%)	0.21	11 (5%)	33	26	19, 49, 102, 207	0
1	De	185/242 (76%)	0.24	5 (2%)	56	47	31, 62, 93, 116	0
1	Df	189/242 (78%)	0.06	6 (3%)	50	41	22, 54, 92, 139	0
1	Dg	217/242 (89%)	0.18	5 (2%)	61	52	24, 56, 108, 184	0
1	Dj	185/242 (76%)	0.04	4 (2%)	62	53	22, 48, 84, 115	0
1	Dk	189/242 (78%)	-0.07	5 (2%)	57	48	14, 41, 88, 147	0
1	Dl	217/242 (89%)	0.08	5 (2%)	61	52	21, 47, 102, 192	0
1	Do	185/242 (76%)	0.22	5 (2%)	56	47	32, 59, 96, 120	0
1	Dp	189/242 (78%)	0.17	6 (3%)	50	41	26, 57, 97, 164	0
1	Dq	217/242 (89%)	0.20	9 (4%)	41	33	24, 56, 111, 193	0
1	Dt	185/242 (76%)	0.08	3 (1%)	70	62	16, 48, 80, 132	0
1	Du	189/242 (78%)	0.12	7 (3%)	45	37	23, 47, 90, 143	0
1	Dv	217/242 (89%)	0.26	5 (2%)	61	52	18, 50, 101, 190	0
1	Dy	185/242 (76%)	-0.18	1 (0%)	87	83	7, 38, 76, 98	0
1	Dz	189/242 (78%)	-0.18	4 (2%)	63	54	16, 38, 75, 130	0
1	E1	217/242 (89%)	-0.04	7 (3%)	50	41	14, 43, 102, 207	0
1	E4	185/242 (76%)	-0.02	3 (1%)	70	62	18, 46, 87, 114	0
1	E5	189/242 (78%)	-0.05	3 (1%)	70	62	15, 43, 84, 124	0
1	E6	217/242 (89%)	0.02	6 (2%)	55	46	16, 44, 106, 194	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	EA	185/242 (76%)	-0.11	2 (1%)	78	71	12, 43, 74, 108	0
1	EB	189/242 (78%)	-0.18	1 (0%)	87	83	12, 41, 81, 122	0
1	EC	217/242 (89%)	0.06	6 (2%)	55	46	18, 43, 98, 186	0
1	EF	185/242 (76%)	0.05	5 (2%)	56	47	22, 52, 90, 126	0
1	EG	189/242 (78%)	0.04	9 (4%)	35	28	21, 51, 92, 151	0
1	EH	217/242 (89%)	0.22	10 (4%)	37	29	24, 55, 114, 189	0
1	EK	185/242 (76%)	0.14	4 (2%)	62	53	25, 54, 89, 122	0
1	EL	189/242 (78%)	0.09	7 (3%)	45	37	27, 53, 95, 126	0
1	EM	217/242 (89%)	0.09	8 (3%)	45	37	21, 52, 108, 195	0
1	EP	185/242 (76%)	-0.04	4 (2%)	62	53	17, 45, 86, 118	0
1	EQ	189/242 (78%)	0.02	2 (1%)	78	71	15, 43, 78, 131	0
1	ER	217/242 (89%)	0.23	14 (6%)	25	20	15, 46, 105, 192	0
1	EU	185/242 (76%)	0.08	3 (1%)	70	62	22, 52, 83, 128	0
1	EV	189/242 (78%)	0.02	5 (2%)	57	48	16, 46, 89, 135	0
1	EW	217/242 (89%)	0.16	6 (2%)	55	46	21, 50, 103, 200	0
1	EZ	185/242 (76%)	0.14	5 (2%)	56	47	30, 53, 85, 118	0
1	Ea	189/242 (78%)	-0.03	3 (1%)	70	62	20, 48, 90, 143	0
1	Eb	217/242 (89%)	0.21	9 (4%)	41	33	16, 50, 105, 190	0
1	Ee	185/242 (76%)	0.16	3 (1%)	70	62	33, 59, 88, 116	0
1	Ef	189/242 (78%)	-0.02	1 (0%)	87	83	21, 54, 93, 136	0
1	Eg	217/242 (89%)	0.20	10 (4%)	37	29	24, 60, 113, 203	0
1	Ej	185/242 (76%)	0.26	6 (3%)	50	41	22, 58, 90, 113	0
1	Ek	189/242 (78%)	0.13	9 (4%)	35	28	29, 57, 94, 139	0
1	El	217/242 (89%)	0.20	9 (4%)	41	33	30, 56, 107, 191	0
1	Eo	185/242 (76%)	-0.01	2 (1%)	78	71	25, 54, 84, 113	0
1	Ep	189/242 (78%)	-0.08	4 (2%)	63	54	20, 46, 89, 162	0
1	Eq	217/242 (89%)	0.05	5 (2%)	61	52	23, 52, 112, 190	0
1	Et	185/242 (76%)	-0.20	4 (2%)	62	53	17, 38, 77, 114	0
1	Eu	189/242 (78%)	-0.20	3 (1%)	70	62	13, 37, 80, 134	0
1	Ev	217/242 (89%)	-0.01	8 (3%)	45	37	12, 38, 97, 197	0
1	Ey	185/242 (76%)	-0.11	2 (1%)	78	71	24, 48, 79, 120	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	Ez	189/242 (78%)	-0.15	2 (1%) 78 71	19, 43, 84, 139	0
1	F1	217/242 (89%)	0.65	19 (8%) 15 13	49, 80, 118, 186	0
1	F4	185/242 (76%)	0.25	5 (2%) 56 47	26, 57, 86, 112	0
1	F5	189/242 (78%)	0.21	7 (3%) 45 37	28, 57, 94, 140	0
1	F6	217/242 (89%)	0.45	14 (6%) 25 20	31, 64, 117, 195	0
1	FA	185/242 (76%)	0.20	5 (2%) 56 47	22, 59, 95, 134	0
1	FB	189/242 (78%)	0.06	5 (2%) 57 48	20, 47, 90, 148	0
1	FC	217/242 (89%)	0.43	14 (6%) 25 20	29, 62, 110, 205	0
1	FF	185/242 (76%)	0.21	4 (2%) 62 53	30, 55, 92, 114	0
1	FG	189/242 (78%)	0.05	4 (2%) 63 54	20, 51, 92, 133	0
1	FH	217/242 (89%)	0.26	7 (3%) 50 41	24, 60, 106, 197	0
1	FK	185/242 (76%)	0.27	6 (3%) 50 41	28, 59, 90, 131	0
1	FL	189/242 (78%)	0.27	7 (3%) 45 37	24, 59, 100, 150	0
1	FM	217/242 (89%)	0.25	9 (4%) 41 33	22, 54, 101, 200	0
1	FP	185/242 (76%)	0.66	10 (5%) 31 24	24, 62, 101, 112	0
1	FQ	189/242 (78%)	0.43	4 (2%) 63 54	23, 61, 94, 134	0
1	FR	217/242 (89%)	0.30	13 (5%) 27 21	26, 55, 118, 222	0
1	FU	185/242 (76%)	0.20	5 (2%) 56 47	32, 55, 86, 119	0
1	FV	189/242 (78%)	0.04	4 (2%) 63 54	21, 48, 87, 130	0
1	FW	217/242 (89%)	0.32	8 (3%) 45 37	19, 52, 105, 190	0
1	FZ	185/242 (76%)	0.53	9 (4%) 35 27	42, 78, 106, 129	0
1	Fa	189/242 (78%)	0.46	10 (5%) 32 25	34, 70, 104, 156	0
1	Fb	217/242 (89%)	0.43	11 (5%) 33 26	41, 70, 117, 212	0
1	Fe	185/242 (76%)	1.16	33 (17%) 4 3	63, 97, 124, 151	0
1	Ff	189/242 (78%)	0.99	27 (14%) 6 5	52, 93, 121, 163	0
1	Fg	217/242 (89%)	1.06	36 (16%) 4 3	58, 92, 134, 190	0
1	Fj	185/242 (76%)	0.84	15 (8%) 18 15	38, 74, 107, 128	0
1	Fk	189/242 (78%)	0.82	16 (8%) 16 14	35, 75, 111, 141	0
1	Fl	217/242 (89%)	0.95	28 (12%) 7 6	41, 79, 127, 203	0
1	Fo	185/242 (76%)	0.24	7 (3%) 44 36	26, 54, 92, 120	0
1	Fp	189/242 (78%)	0.22	6 (3%) 50 41	14, 49, 93, 134	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	Fq	217/242 (89%)	0.14	7 (3%) 50 41	11, 50, 103, 203	0
1	Ft	185/242 (76%)	0.21	2 (1%) 78 71	27, 55, 92, 127	0
1	Fu	189/242 (78%)	0.05	4 (2%) 63 54	24, 51, 88, 140	0
1	Fv	217/242 (89%)	0.17	9 (4%) 41 33	20, 53, 102, 187	0
1	Fy	185/242 (76%)	0.78	15 (8%) 18 15	59, 90, 117, 135	0
1	Fz	189/242 (78%)	0.34	9 (4%) 35 28	40, 76, 113, 150	0
1	G1	217/242 (89%)	0.45	16 (7%) 20 17	34, 66, 116, 201	0
1	G4	185/242 (76%)	0.93	19 (10%) 12 10	57, 89, 114, 148	0
1	G5	189/242 (78%)	0.84	18 (9%) 14 11	45, 83, 114, 159	0
1	G6	217/242 (89%)	0.77	21 (9%) 13 11	38, 73, 126, 187	0
1	GA	185/242 (76%)	0.32	7 (3%) 44 36	20, 57, 92, 118	0
1	GB	189/242 (78%)	0.27	4 (2%) 63 54	28, 59, 96, 125	0
1	GC	217/242 (89%)	0.24	4 (1%) 67 59	23, 58, 113, 202	0
1	GF	185/242 (76%)	0.31	6 (3%) 50 41	20, 56, 83, 116	0
1	GG	189/242 (78%)	0.23	8 (4%) 40 32	22, 53, 94, 132	0
1	GH	217/242 (89%)	0.15	8 (3%) 45 37	25, 54, 105, 188	0
1	GK	185/242 (76%)	0.80	13 (7%) 22 18	61, 90, 117, 142	0
1	GL	189/242 (78%)	0.77	13 (6%) 23 18	52, 84, 119, 165	0
1	GM	217/242 (89%)	0.52	11 (5%) 33 26	42, 77, 118, 205	0
1	GP	185/242 (76%)	0.23	8 (4%) 40 31	20, 55, 91, 125	0
1	GQ	189/242 (78%)	0.37	7 (3%) 45 37	26, 58, 93, 117	0
1	GR	217/242 (89%)	0.38	12 (5%) 30 24	25, 55, 106, 199	0
1	GU	185/242 (76%)	0.12	5 (2%) 56 47	26, 55, 87, 128	0
1	GV	189/242 (78%)	-0.02	5 (2%) 57 48	15, 46, 88, 131	0
1	GW	217/242 (89%)	0.10	5 (2%) 61 52	23, 48, 102, 194	0
1	GZ	185/242 (76%)	0.55	8 (4%) 40 31	26, 67, 96, 131	0
1	Ga	189/242 (78%)	0.28	7 (3%) 45 37	20, 55, 99, 172	0
1	Gb	217/242 (89%)	0.29	10 (4%) 37 29	32, 61, 109, 200	0
1	Ge	185/242 (76%)	0.69	9 (4%) 35 27	33, 67, 100, 126	0
1	Gf	189/242 (78%)	0.95	25 (13%) 7 6	28, 70, 108, 147	0
1	Gg	217/242 (89%)	0.72	14 (6%) 25 20	34, 69, 117, 199	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	Gj	185/242 (76%)	0.98	27 (14%) 6 4	51, 89, 118, 144	0
1	Gk	189/242 (78%)	0.73	18 (9%) 14 11	53, 82, 114, 143	0
1	Gl	217/242 (89%)	0.61	10 (4%) 37 29	38, 75, 119, 194	0
1	Go	185/242 (76%)	1.00	17 (9%) 14 12	62, 92, 120, 144	0
1	Gp	189/242 (78%)	0.92	17 (8%) 15 13	56, 95, 124, 162	0
1	Gq	217/242 (89%)	0.96	27 (12%) 8 7	57, 91, 129, 191	0
1	Gt	185/242 (76%)	0.26	3 (1%) 70 62	25, 56, 90, 118	0
1	Gu	189/242 (78%)	0.12	5 (2%) 57 48	24, 51, 89, 145	0
1	Gv	217/242 (89%)	0.19	8 (3%) 45 37	24, 53, 105, 199	0
1	Gy	185/242 (76%)	0.44	9 (4%) 35 27	35, 64, 98, 129	0
1	Gz	189/242 (78%)	0.23	1 (0%) 87 83	34, 63, 97, 153	0
1	H1	217/242 (89%)	0.62	14 (6%) 25 20	32, 69, 116, 189	0
1	H4	185/242 (76%)	0.92	14 (7%) 20 16	56, 91, 125, 144	0
1	H5	189/242 (78%)	1.04	23 (12%) 8 7	57, 93, 122, 143	0
1	H6	217/242 (89%)	1.02	22 (10%) 12 10	55, 92, 133, 193	0
1	HA	185/242 (76%)	0.35	6 (3%) 50 41	41, 71, 100, 130	0
1	HB	189/242 (78%)	0.36	7 (3%) 45 37	34, 67, 106, 131	0
1	HC	217/242 (89%)	0.69	20 (9%) 14 12	46, 78, 133, 205	0
1	HF	185/242 (76%)	0.49	9 (4%) 35 27	40, 70, 98, 130	0
1	HG	189/242 (78%)	0.22	6 (3%) 50 41	32, 58, 99, 136	0
1	HH	217/242 (89%)	0.31	8 (3%) 45 37	26, 60, 105, 206	0
1	HK	185/242 (76%)	0.30	4 (2%) 62 53	30, 62, 97, 119	0
1	HL	189/242 (78%)	0.15	2 (1%) 78 71	24, 52, 93, 141	0
1	HM	217/242 (89%)	0.41	12 (5%) 30 24	25, 64, 112, 190	0
1	HP	185/242 (76%)	0.67	14 (7%) 20 16	23, 66, 103, 127	0
1	HQ	189/242 (78%)	0.20	5 (2%) 57 48	21, 54, 99, 137	0
1	HR	217/242 (89%)	0.48	14 (6%) 25 20	24, 62, 118, 186	0
1	HU	185/242 (76%)	0.29	4 (2%) 62 53	27, 60, 89, 126	0
1	HV	189/242 (78%)	0.33	8 (4%) 40 32	31, 60, 104, 142	0
1	HW	217/242 (89%)	0.42	11 (5%) 33 26	38, 67, 112, 183	0
1	HZ	185/242 (76%)	0.37	4 (2%) 62 53	36, 66, 93, 130	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	Ha	189/242 (78%)	0.16	5 (2%) 57 48	26, 57, 95, 154	0
1	Hb	217/242 (89%)	0.40	11 (5%) 33 26	33, 65, 107, 199	0
1	He	185/242 (76%)	1.11	29 (15%) 5 4	55, 96, 127, 153	0
1	Hf	189/242 (78%)	1.00	23 (12%) 8 7	50, 88, 122, 171	0
1	Hg	217/242 (89%)	0.94	24 (11%) 10 9	54, 94, 131, 203	0
1	Hj	185/242 (76%)	0.67	8 (4%) 40 31	51, 88, 110, 134	0
1	Hk	189/242 (78%)	0.45	8 (4%) 40 32	35, 73, 112, 169	0
1	Hl	217/242 (89%)	0.57	12 (5%) 30 24	39, 71, 121, 178	0
1	Ho	185/242 (76%)	0.29	5 (2%) 56 47	37, 65, 100, 127	0
1	Hp	189/242 (78%)	0.16	4 (2%) 63 54	32, 61, 96, 139	0
1	Hq	217/242 (89%)	0.26	7 (3%) 50 41	31, 62, 106, 201	0
1	Ht	185/242 (76%)	0.64	14 (7%) 20 16	27, 67, 98, 131	0
1	Hu	189/242 (78%)	0.51	11 (5%) 29 22	23, 62, 106, 162	0
1	Hv	217/242 (89%)	0.42	14 (6%) 25 20	25, 57, 111, 205	0
1	Hy	185/242 (76%)	0.47	9 (4%) 35 27	37, 68, 108, 132	0
1	Hx	189/242 (78%)	0.40	10 (5%) 32 25	25, 62, 101, 141	0
1	I1	217/242 (89%)	0.47	15 (6%) 23 18	23, 63, 112, 193	0
1	I4	185/242 (76%)	0.69	9 (4%) 35 27	29, 67, 97, 116	0
1	I5	189/242 (78%)	0.29	8 (4%) 40 32	31, 58, 97, 146	0
1	I6	217/242 (89%)	0.66	15 (6%) 23 18	30, 69, 117, 212	0
1	IA	185/242 (76%)	0.88	12 (6%) 25 20	67, 98, 122, 151	0
1	IB	189/242 (78%)	0.84	22 (11%) 9 8	53, 89, 127, 196	0
1	IC	217/242 (89%)	1.04	28 (12%) 7 6	56, 98, 138, 201	0
1	IF	185/242 (76%)	0.32	8 (4%) 40 31	34, 68, 102, 130	0
1	IG	189/242 (78%)	0.44	10 (5%) 32 25	46, 73, 104, 142	0
1	IH	217/242 (89%)	0.45	13 (5%) 27 21	42, 71, 118, 184	0
1	IK	185/242 (76%)	0.21	2 (1%) 78 71	35, 60, 90, 127	0
1	IL	189/242 (78%)	0.10	7 (3%) 45 37	22, 50, 90, 138	0
1	IM	217/242 (89%)	0.24	6 (2%) 55 46	27, 58, 112, 188	0
1	IP	185/242 (76%)	0.28	7 (3%) 44 36	36, 68, 101, 128	0
1	IQ	189/242 (78%)	0.29	4 (2%) 63 54	39, 65, 102, 162	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	IR	217/242 (89%)	0.41	10 (4%) 37 29	40, 69, 111, 186	0
1	IU	185/242 (76%)	0.30	8 (4%) 40 31	21, 55, 88, 116	0
1	IV	189/242 (78%)	0.02	3 (1%) 70 62	18, 48, 81, 134	0
1	IW	217/242 (89%)	0.34	13 (5%) 27 21	21, 52, 107, 195	0
1	IZ	185/242 (76%)	0.26	4 (2%) 62 53	21, 58, 87, 123	0
1	Ia	189/242 (78%)	0.05	6 (3%) 50 41	17, 46, 86, 144	0
1	Ib	217/242 (89%)	0.21	10 (4%) 37 29	23, 50, 105, 194	0
1	Ie	185/242 (76%)	0.71	11 (5%) 28 22	53, 85, 115, 136	0
1	If	189/242 (78%)	0.48	10 (5%) 32 25	37, 71, 116, 154	0
1	Ig	217/242 (89%)	0.50	11 (5%) 33 26	34, 70, 116, 193	0
1	Ij	185/242 (76%)	1.00	20 (10%) 11 9	56, 89, 121, 143	0
1	Ik	189/242 (78%)	0.87	21 (11%) 10 9	34, 76, 114, 152	0
1	Il	217/242 (89%)	0.95	28 (12%) 7 6	40, 85, 123, 212	0
1	Io	185/242 (76%)	0.27	10 (5%) 31 24	26, 56, 94, 123	0
1	Ip	189/242 (78%)	0.09	4 (2%) 63 54	21, 51, 90, 140	0
1	Iq	217/242 (89%)	0.37	13 (5%) 27 21	26, 58, 112, 189	0
1	It	185/242 (76%)	0.21	5 (2%) 56 47	29, 59, 94, 132	0
1	Iu	189/242 (78%)	0.20	7 (3%) 45 37	21, 53, 102, 135	0
1	Iv	217/242 (89%)	0.16	5 (2%) 61 52	26, 54, 103, 186	0
1	Iy	185/242 (76%)	0.35	3 (1%) 70 62	44, 73, 104, 132	0
1	Iz	189/242 (78%)	0.34	7 (3%) 45 37	37, 67, 105, 162	0
1	J1	217/242 (89%)	0.67	16 (7%) 20 17	23, 66, 107, 195	0
1	J4	185/242 (76%)	1.04	26 (14%) 6 5	43, 83, 113, 139	0
1	J5	189/242 (78%)	0.90	22 (11%) 9 8	27, 73, 118, 145	0
1	J6	217/242 (89%)	0.88	22 (10%) 12 10	34, 74, 126, 198	0
1	JA	185/242 (76%)	0.88	14 (7%) 20 16	35, 70, 105, 127	0
1	JB	189/242 (78%)	0.73	15 (7%) 18 15	32, 65, 110, 139	0
1	JC	217/242 (89%)	0.89	22 (10%) 12 10	31, 74, 118, 188	0
1	JF	185/242 (76%)	0.75	14 (7%) 20 16	39, 73, 109, 134	0
1	JG	189/242 (78%)	0.58	10 (5%) 32 25	24, 70, 109, 153	0
1	JH	217/242 (89%)	0.85	25 (11%) 9 8	42, 77, 115, 192	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	JK	185/242 (76%)	1.04	25 (13%) 7 5	63, 97, 126, 150	0
1	JL	189/242 (78%)	0.72	12 (6%) 26 20	52, 87, 125, 168	0
1	JM	217/242 (89%)	0.95	17 (7%) 19 16	62, 98, 136, 192	0
1	JP	185/242 (76%)	0.92	22 (11%) 9 7	58, 90, 114, 148	0
1	JQ	189/242 (78%)	0.46	9 (4%) 35 28	44, 77, 116, 137	0
1	JR	217/242 (89%)	0.73	13 (5%) 27 21	47, 85, 125, 215	0
1	JU	185/242 (76%)	0.39	9 (4%) 35 27	38, 69, 105, 133	0
1	JV	189/242 (78%)	0.51	4 (2%) 63 54	35, 67, 102, 152	0
1	JW	217/242 (89%)	0.56	12 (5%) 30 24	42, 79, 121, 215	0
1	JZ	185/242 (76%)	0.41	6 (3%) 50 41	38, 68, 101, 131	0
1	Ja	189/242 (78%)	0.56	9 (4%) 35 28	41, 76, 108, 163	0
1	Jb	217/242 (89%)	0.51	16 (7%) 20 17	36, 69, 115, 195	0
1	Je	185/242 (76%)	0.24	4 (2%) 62 53	29, 57, 92, 124	0
1	Jf	189/242 (78%)	0.28	6 (3%) 50 41	28, 58, 98, 135	0
1	Jg	217/242 (89%)	0.23	8 (3%) 45 37	19, 51, 99, 197	0
1	Jj	185/242 (76%)	0.07	5 (2%) 56 47	22, 49, 80, 117	0
1	Jk	189/242 (78%)	0.05	6 (3%) 50 41	14, 44, 91, 123	0
1	Jl	217/242 (89%)	0.06	5 (2%) 61 52	17, 44, 92, 208	0
1	Jo	185/242 (76%)	0.22	4 (2%) 62 53	31, 59, 91, 124	0
1	Jp	189/242 (78%)	0.17	1 (0%) 87 83	31, 62, 101, 130	0
1	Jq	217/242 (89%)	0.21	7 (3%) 50 41	24, 54, 108, 199	0
1	Jt	185/242 (76%)	0.55	11 (5%) 28 22	36, 73, 106, 129	0
1	Ju	189/242 (78%)	0.56	9 (4%) 35 28	34, 69, 102, 152	0
1	Jv	217/242 (89%)	0.53	15 (6%) 23 18	34, 68, 121, 185	0
1	Jy	185/242 (76%)	0.74	15 (8%) 18 15	36, 71, 108, 126	0
1	Jz	189/242 (78%)	0.87	20 (10%) 11 9	34, 73, 110, 141	0
2	A2	17/17 (100%)	1.26	1 (5%) 28 22	159, 199, 279, 304	0
2	A7	17/17 (100%)	1.40	2 (11%) 9 7	154, 204, 269, 286	0
2	AD	17/17 (100%)	1.02	1 (5%) 28 22	157, 204, 281, 286	0
2	AI	17/17 (100%)	1.17	1 (5%) 28 22	164, 188, 256, 267	0
2	AN	17/17 (100%)	1.06	1 (5%) 28 22	159, 190, 274, 277	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	AS	17/17 (100%)	0.94	0 100 100	154, 202, 274, 275	0
2	AX	17/17 (100%)	0.88	0 100 100	164, 193, 269, 273	0
2	Ac	17/17 (100%)	1.13	1 (5%) 28 22	141, 188, 262, 275	0
2	Ah	17/17 (100%)	0.85	0 100 100	154, 193, 271, 272	0
2	Am	17/17 (100%)	1.19	1 (5%) 28 22	137, 213, 264, 277	0
2	Ar	17/17 (100%)	1.29	2 (11%) 9 7	149, 198, 271, 283	0
2	Aw	17/17 (100%)	1.27	2 (11%) 9 7	163, 197, 284, 286	0
2	B2	17/17 (100%)	1.15	2 (11%) 9 7	162, 190, 261, 267	0
2	B7	17/17 (100%)	1.00	1 (5%) 28 22	177, 200, 254, 265	0
2	BD	17/17 (100%)	1.07	2 (11%) 9 7	160, 209, 274, 279	0
2	BI	17/17 (100%)	1.11	1 (5%) 28 22	156, 207, 280, 280	0
2	BN	17/17 (100%)	1.22	1 (5%) 28 22	156, 200, 262, 264	0
2	BS	17/17 (100%)	1.15	1 (5%) 28 22	159, 208, 260, 270	0
2	BX	17/17 (100%)	0.88	0 100 100	174, 199, 274, 277	0
2	Bc	17/17 (100%)	0.96	1 (5%) 28 22	165, 199, 272, 280	0
2	Bh	17/17 (100%)	1.06	1 (5%) 28 22	163, 199, 271, 273	0
2	Bm	17/17 (100%)	1.14	1 (5%) 28 22	154, 202, 276, 289	0
2	Br	17/17 (100%)	1.06	1 (5%) 28 22	144, 200, 289, 290	0
2	Bw	17/17 (100%)	0.94	1 (5%) 28 22	154, 195, 277, 282	0
2	C2	17/17 (100%)	1.34	4 (23%) 2 2	144, 205, 267, 273	0
2	C7	17/17 (100%)	1.22	0 100 100	164, 209, 267, 273	0
2	CD	17/17 (100%)	1.07	0 100 100	158, 202, 277, 281	0
2	CI	17/17 (100%)	1.24	1 (5%) 28 22	159, 206, 278, 289	0
2	CN	17/17 (100%)	1.44	4 (23%) 2 2	168, 187, 268, 276	0
2	CS	17/17 (100%)	0.91	1 (5%) 28 22	157, 199, 273, 276	0
2	CX	17/17 (100%)	1.14	0 100 100	162, 189, 274, 293	0
2	Cc	17/17 (100%)	1.13	1 (5%) 28 22	161, 205, 260, 270	0
2	Ch	17/17 (100%)	1.18	1 (5%) 28 22	151, 201, 273, 279	0
2	Cm	17/17 (100%)	1.14	1 (5%) 28 22	152, 201, 267, 268	0
2	Cr	17/17 (100%)	1.05	1 (5%) 28 22	152, 206, 261, 272	0
2	Cw	17/17 (100%)	1.13	1 (5%) 28 22	160, 193, 274, 284	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	D2	17/17 (100%)	1.32	2 (11%) 9 7	152, 201, 267, 269	0
2	D7	17/17 (100%)	1.21	1 (5%) 28 22	152, 194, 266, 269	0
2	DD	17/17 (100%)	1.14	2 (11%) 9 7	161, 204, 270, 283	0
2	DI	17/17 (100%)	1.16	2 (11%) 9 7	164, 212, 272, 278	0
2	DN	17/17 (100%)	1.25	2 (11%) 9 7	162, 207, 268, 275	0
2	DS	17/17 (100%)	1.09	1 (5%) 28 22	168, 199, 259, 264	0
2	DX	17/17 (100%)	0.94	0 100 100	176, 203, 267, 271	0
2	Dc	17/17 (100%)	1.20	3 (17%) 4 3	159, 209, 267, 279	0
2	Dh	17/17 (100%)	1.35	4 (23%) 2 2	164, 208, 269, 280	0
2	Dm	17/17 (100%)	1.24	1 (5%) 28 22	148, 199, 269, 272	0
2	Dr	17/17 (100%)	1.15	1 (5%) 28 22	157, 207, 277, 281	0
2	Dw	17/17 (100%)	1.09	1 (5%) 28 22	152, 191, 275, 293	0
2	E2	17/17 (100%)	1.19	1 (5%) 28 22	156, 193, 283, 293	0
2	E7	17/17 (100%)	1.12	0 100 100	156, 195, 271, 287	0
2	ED	17/17 (100%)	1.05	1 (5%) 28 22	152, 188, 275, 277	0
2	EI	17/17 (100%)	0.99	0 100 100	160, 206, 260, 264	0
2	EN	17/17 (100%)	1.15	1 (5%) 28 22	156, 192, 258, 286	0
2	ES	17/17 (100%)	1.18	2 (11%) 9 7	162, 204, 265, 279	0
2	EX	17/17 (100%)	1.28	2 (11%) 9 7	158, 195, 272, 273	0
2	Ec	17/17 (100%)	0.99	0 100 100	157, 196, 258, 270	0
2	Eh	17/17 (100%)	1.31	3 (17%) 4 3	172, 198, 263, 268	0
2	Em	17/17 (100%)	0.94	1 (5%) 28 22	147, 194, 261, 261	0
2	Er	17/17 (100%)	0.97	0 100 100	159, 202, 272, 280	0
2	Ew	17/17 (100%)	0.91	0 100 100	150, 183, 263, 264	0
2	F2	17/17 (100%)	1.03	0 100 100	194, 214, 267, 274	0
2	F7	17/17 (100%)	1.25	3 (17%) 4 3	159, 205, 277, 288	0
2	FD	17/17 (100%)	1.15	1 (5%) 28 22	167, 208, 268, 288	0
2	FI	17/17 (100%)	1.10	0 100 100	170, 198, 262, 266	0
2	FN	17/17 (100%)	1.25	0 100 100	163, 208, 292, 304	0
2	FS	17/17 (100%)	1.23	1 (5%) 28 22	174, 204, 274, 289	0
2	FX	17/17 (100%)	1.30	2 (11%) 9 7	158, 198, 284, 293	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	Fc	17/17 (100%)	1.18	1 (5%) 28 22	179, 218, 269, 281	0
2	Fh	17/17 (100%)	1.20	1 (5%) 28 22	180, 240, 287, 293	0
2	Fm	17/17 (100%)	1.10	1 (5%) 28 22	181, 216, 278, 291	0
2	Fr	17/17 (100%)	1.13	0 100 100	167, 200, 274, 280	0
2	Fw	17/17 (100%)	1.24	1 (5%) 28 22	165, 214, 286, 290	0
2	G2	17/17 (100%)	1.21	2 (11%) 9 7	170, 212, 259, 261	0
2	G7	17/17 (100%)	1.20	3 (17%) 4 3	189, 209, 259, 271	0
2	GD	17/17 (100%)	1.15	0 100 100	168, 211, 280, 286	0
2	GI	17/17 (100%)	1.15	0 100 100	163, 209, 263, 277	0
2	GN	17/17 (100%)	1.11	1 (5%) 28 22	185, 217, 288, 291	0
2	GS	17/17 (100%)	1.05	1 (5%) 28 22	184, 209, 263, 275	0
2	GX	17/17 (100%)	1.24	1 (5%) 28 22	166, 203, 273, 303	0
2	Gc	17/17 (100%)	1.13	2 (11%) 9 7	165, 211, 270, 276	0
2	Gh	17/17 (100%)	1.29	2 (11%) 9 7	162, 216, 260, 260	0
2	Gm	17/17 (100%)	1.03	1 (5%) 28 22	191, 213, 278, 289	0
2	Gr	17/17 (100%)	1.15	0 100 100	192, 219, 275, 295	0
2	Gw	17/17 (100%)	1.19	2 (11%) 9 7	165, 218, 280, 284	0
2	H2	17/17 (100%)	1.10	1 (5%) 28 22	173, 207, 289, 293	0
2	H7	17/17 (100%)	1.07	2 (11%) 9 7	195, 214, 276, 279	0
2	HD	17/17 (100%)	1.20	2 (11%) 9 7	177, 229, 281, 286	0
2	HI	17/17 (100%)	1.21	1 (5%) 28 22	173, 194, 258, 289	0
2	HN	17/17 (100%)	1.42	2 (11%) 9 7	167, 214, 281, 292	0
2	HS	17/17 (100%)	1.15	1 (5%) 28 22	174, 213, 281, 294	0
2	HX	17/17 (100%)	1.19	1 (5%) 28 22	158, 206, 276, 283	0
2	Hc	17/17 (100%)	1.15	1 (5%) 28 22	173, 208, 274, 293	0
2	Hh	17/17 (100%)	1.08	2 (11%) 9 7	196, 227, 270, 292	0
2	Hm	17/17 (100%)	1.31	2 (11%) 9 7	191, 215, 278, 297	0
2	Hr	17/17 (100%)	1.54	3 (17%) 4 3	170, 214, 284, 291	0
2	Hw	17/17 (100%)	1.41	4 (23%) 2 2	170, 214, 272, 286	0
2	I2	17/17 (100%)	1.07	0 100 100	173, 227, 265, 269	0
2	I7	17/17 (100%)	1.29	2 (11%) 9 7	169, 209, 277, 284	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	ID	17/17 (100%)	1.03	1 (5%) 28 22	197, 230, 270, 282	0
2	II	17/17 (100%)	1.29	1 (5%) 28 22	181, 209, 283, 298	0
2	IN	17/17 (100%)	1.33	1 (5%) 28 22	170, 195, 279, 286	0
2	IS	17/17 (100%)	1.17	1 (5%) 28 22	180, 207, 271, 276	0
2	IX	17/17 (100%)	1.42	2 (11%) 9 7	168, 215, 279, 286	0
2	Ic	17/17 (100%)	1.05	2 (11%) 9 7	165, 214, 265, 278	0
2	Ih	17/17 (100%)	1.13	0 100 100	176, 208, 264, 275	0
2	Im	17/17 (100%)	1.09	1 (5%) 28 22	193, 215, 278, 294	0
2	Ir	17/17 (100%)	1.03	1 (5%) 28 22	175, 206, 269, 274	0
2	Iw	17/17 (100%)	0.78	0 100 100	167, 208, 273, 276	0
2	J2	17/17 (100%)	1.29	2 (11%) 9 7	187, 220, 287, 302	0
2	J7	17/17 (100%)	1.26	2 (11%) 9 7	181, 227, 279, 294	0
2	JD	17/17 (100%)	1.19	0 100 100	169, 211, 260, 265	0
2	JI	17/17 (100%)	1.27	2 (11%) 9 7	179, 213, 269, 274	0
2	JN	17/17 (100%)	1.02	0 100 100	193, 227, 264, 264	0
2	JS	17/17 (100%)	1.18	2 (11%) 9 7	203, 222, 276, 276	0
2	JX	17/17 (100%)	1.02	0 100 100	175, 221, 275, 281	0
2	Jc	17/17 (100%)	1.21	1 (5%) 28 22	177, 215, 290, 291	0
2	Jh	17/17 (100%)	1.10	1 (5%) 28 22	156, 200, 280, 285	0
2	Jm	17/17 (100%)	1.23	2 (11%) 9 7	165, 207, 294, 298	0
2	Jr	17/17 (100%)	1.09	0 100 100	165, 208, 270, 278	0
2	Jw	17/17 (100%)	1.24	2 (11%) 9 7	180, 215, 280, 291	0
All	All	72960/89160 (81%)	0.29	3113 (4%) 40 31	7, 58, 123, 304	0

The worst 5 of 3113 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	If	52	GLN	8.5
1	Cz	52	GLN	7.5
1	BM	237	ILE	7.0
1	Av	25	ALA	6.8
1	IW	25	ALA	6.6

5.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CA	Jt	301	1/1	0.64	0.23	154,154,154,154	0
3	CA	Hy	301	1/1	0.65	0.21	138,138,138,138	0
3	CA	I4	301	1/1	0.66	0.26	147,147,147,147	0
3	CA	If	301	1/1	0.73	0.19	124,124,124,124	0
3	CA	Ij	301	1/1	0.78	0.15	130,130,130,130	0
3	CA	JL	301	1/1	0.79	0.11	141,141,141,141	0
3	CA	Ce	301	1/1	0.80	0.30	113,113,113,113	0
3	CA	Eo	301	1/1	0.82	0.19	105,105,105,105	0
3	CA	C4	301	1/1	0.83	0.20	127,127,127,127	0
3	CA	Ge	301	1/1	0.83	0.28	121,121,121,121	0
3	CA	JP	301	1/1	0.84	0.29	143,143,143,143	0
3	CA	G1	301	1/1	0.85	0.14	103,103,103,103	0
3	CA	IF	301	1/1	0.85	0.14	111,111,111,111	0
3	CA	IR	301	1/1	0.86	0.18	119,119,119,119	0
3	CA	J4	301	1/1	0.86	0.10	110,110,110,110	0
3	CA	Fe	301	1/1	0.87	0.17	123,123,123,123	0
3	CA	G4	301	1/1	0.87	0.09	109,109,109,109	0
3	CA	F1	301	1/1	0.88	0.13	102,102,102,102	0
3	CA	I1	301	1/1	0.88	0.21	117,117,117,117	0
3	CA	EF	301	1/1	0.88	0.26	112,112,112,112	0
3	CA	JA	301	1/1	0.88	0.20	109,109,109,109	0
3	CA	Je	301	1/1	0.89	0.25	112,112,112,112	0
3	CA	Gt	301	1/1	0.89	0.09	92,92,92,92	0
3	CA	JU	301	1/1	0.89	0.14	100,100,100,100	0
3	CA	Ht	301	1/1	0.90	0.11	88,88,88,88	0
3	CA	Et	301	1/1	0.90	0.12	71,71,71,71	0
3	CA	JF	301	1/1	0.90	0.12	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CA	H4	301	1/1	0.90	0.19	115,115,115,115	0
3	CA	Gj	301	1/1	0.90	0.20	126,126,126,126	0
3	CA	B5	301	1/1	0.90	0.17	95,95,95,95	0
3	CA	CU	301	1/1	0.90	0.11	96,96,96,96	0
3	CA	F4	301	1/1	0.90	0.12	95,95,95,95	0
3	CA	Ho	301	1/1	0.90	0.16	95,95,95,95	0
3	CA	Fk	301	1/1	0.91	0.13	96,96,96,96	0
3	CA	Do	301	1/1	0.91	0.14	87,87,87,87	0
3	CA	Ao	301	1/1	0.91	0.14	93,93,93,93	0
3	CA	IZ	301	1/1	0.91	0.18	94,94,94,94	0
3	CA	HZ	301	1/1	0.91	0.14	88,88,88,88	0
3	CA	JZ	301	1/1	0.91	0.16	109,109,109,109	0
3	CA	GF	301	1/1	0.91	0.21	105,105,105,105	0
3	CA	FA	301	1/1	0.91	0.15	94,94,94,94	0
3	CA	EU	301	1/1	0.91	0.18	109,109,109,109	0
3	CA	GA	301	1/1	0.92	0.12	90,90,90,90	0
3	CA	IK	301	1/1	0.92	0.16	105,105,105,105	0
3	CA	EC	301	1/1	0.92	0.17	90,90,90,90	0
3	CA	GP	301	1/1	0.92	0.10	91,91,91,91	0
3	CA	By	301	1/1	0.92	0.14	90,90,90,90	0
3	CA	AP	301	1/1	0.92	0.10	81,81,81,81	0
3	CA	Ee	301	1/1	0.92	0.13	102,102,102,102	0
3	CA	Af	301	1/1	0.92	0.17	105,105,105,105	0
3	CA	AF	301	1/1	0.92	0.16	92,92,92,92	0
3	CA	HK	301	1/1	0.92	0.14	88,88,88,88	0
3	CA	A4	301	1/1	0.92	0.14	81,81,81,81	0
3	CA	Hj	301	1/1	0.92	0.07	104,104,104,104	0
3	CA	DK	301	1/1	0.92	0.17	101,101,101,101	0
3	CA	DP	301	1/1	0.92	0.09	67,67,67,67	0
3	CA	DU	301	1/1	0.92	0.27	113,113,113,113	0
3	CA	Bk	301	1/1	0.92	0.12	90,90,90,90	0
3	CA	Jy	301	1/1	0.92	0.13	123,123,123,123	0
3	CA	IA	301	1/1	0.92	0.18	115,115,115,115	0
3	CA	Io	301	1/1	0.93	0.10	85,85,85,85	0
3	CA	EK	301	1/1	0.93	0.09	89,89,89,89	0
3	CA	Co	301	1/1	0.93	0.15	86,86,86,86	0
3	CA	Bo	301	1/1	0.93	0.11	74,74,74,74	0
3	CA	GZ	301	1/1	0.93	0.17	104,104,104,104	0
3	CA	DF	301	1/1	0.93	0.15	94,94,94,94	0
3	CA	Bt	301	1/1	0.93	0.08	90,90,90,90	0
3	CA	BB	301	1/1	0.93	0.21	114,114,114,114	0
3	CA	BF	301	1/1	0.93	0.12	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CA	CP	301	1/1	0.93	0.14	71,71,71,71	0
3	CA	Jo	301	1/1	0.93	0.14	105,105,105,105	0
3	CA	BU	301	1/1	0.93	0.12	110,110,110,110	0
3	CA	AL	301	1/1	0.93	0.20	85,85,85,85	0
3	CA	Hg	301	1/1	0.93	0.09	102,102,102,102	0
3	CA	Df	301	1/1	0.94	0.06	74,74,74,74	0
3	CA	Cj	301	1/1	0.94	0.13	87,87,87,87	0
3	CA	CG	301	1/1	0.94	0.12	79,79,79,79	0
3	CA	CK	301	1/1	0.94	0.10	105,105,105,105	0
3	CA	AU	301	1/1	0.94	0.16	102,102,102,102	0
3	CA	HA	301	1/1	0.94	0.11	93,93,93,93	0
3	CA	HF	301	1/1	0.94	0.12	101,101,101,101	0
3	CA	AA	301	1/1	0.94	0.12	75,75,75,75	0
3	CA	CZ	301	1/1	0.94	0.12	84,84,84,84	0
3	CA	BK	301	1/1	0.94	0.21	96,96,96,96	0
3	CA	GU	301	1/1	0.94	0.13	84,84,84,84	0
3	CA	DZ	301	1/1	0.94	0.11	68,68,68,68	0
3	CA	Ft	301	1/1	0.95	0.10	88,88,88,88	0
3	CA	BZ	301	1/1	0.95	0.21	97,97,97,97	0
3	CA	It	301	1/1	0.95	0.06	102,102,102,102	0
3	CA	Be	301	1/1	0.95	0.07	53,53,53,53	0
3	CA	Dt	301	1/1	0.95	0.07	76,76,76,76	0
3	CA	Dy	301	1/1	0.95	0.13	65,65,65,65	0
3	CA	GK	301	1/1	0.95	0.08	97,97,97,97	0
3	CA	Ey	301	1/1	0.95	0.23	95,95,95,95	0
3	CA	E4	301	1/1	0.95	0.26	98,98,98,98	0
3	CA	BQ	301	1/1	0.95	0.13	93,93,93,93	0
3	CA	FF	301	1/1	0.95	0.15	100,100,100,100	0
3	CA	FK	301	1/1	0.95	0.11	91,91,91,91	0
3	CA	Jj	301	1/1	0.95	0.10	74,74,74,74	0
3	CA	FU	301	1/1	0.95	0.12	91,91,91,91	0
3	CA	Cy	301	1/1	0.95	0.12	78,78,78,78	0
3	CA	At	301	1/1	0.95	0.16	99,99,99,99	0
3	CA	Fo	301	1/1	0.95	0.07	96,96,96,96	0
3	CA	IU	301	1/1	0.96	0.13	88,88,88,88	0
3	CA	A1	301	1/1	0.96	0.14	106,106,106,106	0
3	CA	EP	301	1/1	0.96	0.19	84,84,84,84	0
3	CA	AZ	301	1/1	0.96	0.20	82,82,82,82	0
3	CA	EZ	301	1/1	0.96	0.15	88,88,88,88	0
3	CA	Ct	301	1/1	0.96	0.14	79,79,79,79	0
3	CA	Ek	301	1/1	0.96	0.09	74,74,74,74	0
3	CA	HU	301	1/1	0.96	0.13	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CA	CA	301	1/1	0.96	0.10	93,93,93,93	0
3	CA	Go	301	1/1	0.96	0.12	102,102,102,102	0
3	CA	FZ	301	1/1	0.97	0.10	106,106,106,106	0
3	CA	Aj	301	1/1	0.97	0.12	70,70,70,70	0
3	CA	DA	301	1/1	0.97	0.08	67,67,67,67	0
3	CA	Dj	301	1/1	0.97	0.10	86,86,86,86	0
3	CA	FP	301	1/1	0.97	0.10	80,80,80,80	0
3	CA	D4	301	1/1	0.97	0.14	77,77,77,77	0
3	CA	HP	301	1/1	0.98	0.15	81,81,81,81	0

5.5 Other polymers [i](#)

There are no such residues in this entry.