



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 16, 2017 – 01:47 pm GMT

PDB ID : 4V99
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	FAILED
Xtriage (Phenix)	:	1.9-1692
EDS	:	recalc28986
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28986

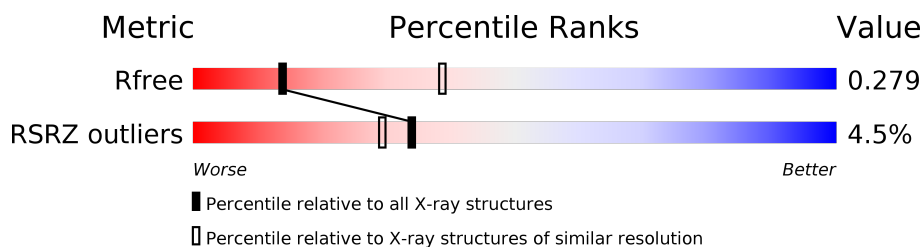
1 Overall quality at a glance

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}	100719	1586 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CA	E4	301	-	-	-	X
3	CA	JP	301	-	-	-	X

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	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	G1	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	G4	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	G5	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	G6	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	HA	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	HB	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	HC	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	HF	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	HG	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	HH	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	HK	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	HL	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	HM	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	HP	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	HQ	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	HR	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	HU	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	HV	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	HW	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	HZ	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	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 349	C 157	N 46	O 129	P 17	0	0	0
2	Jw	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	J2	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	J7	17	Total 349	C 157	N 46	O 129	P 17	0	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	Jt	1	Total 1	Ca 1	0	0
3	FU	1	Total 1	Ca 1	0	0
3	CA	1	Total 1	Ca 1	0	0
3	IZ	1	Total 1	Ca 1	0	0
3	Eo	1	Total 1	Ca 1	0	0
3	FK	1	Total 1	Ca 1	0	0
3	DZ	1	Total 1	Ca 1	0	0
3	Ce	1	Total 1	Ca 1	0	0
3	Af	1	Total 1	Ca 1	0	0
3	EF	1	Total 1	Ca 1	0	0
3	JL	1	Total 1	Ca 1	0	0
3	C4	1	Total 1	Ca 1	0	0
3	Gt	1	Total 1	Ca 1	0	0
3	Df	1	Total 1	Ca 1	0	0
3	HF	1	Total 1	Ca 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	Be	1	Total 1	Ca 1	0	0
3	AA	1	Total 1	Ca 1	0	0
3	Hj	1	Total 1	Ca 1	0	0
3	JA	1	Total 1	Ca 1	0	0
3	A4	1	Total 1	Ca 1	0	0
3	D4	1	Total 1	Ca 1	0	0
3	AL	1	Total 1	Ca 1	0	0
3	JZ	1	Total 1	Ca 1	0	0
3	DP	1	Total 1	Ca 1	0	0
3	Hg	1	Total 1	Ca 1	0	0
3	GK	1	Total 1	Ca 1	0	0
3	HZ	1	Total 1	Ca 1	0	0
3	JF	1	Total 1	Ca 1	0	0
3	EU	1	Total 1	Ca 1	0	0
3	AF	1	Total 1	Ca 1	0	0
3	CZ	1	Total 1	Ca 1	0	0
3	Ek	1	Total 1	Ca 1	0	0
3	Bo	1	Total 1	Ca 1	0	0
3	DK	1	Total 1	Ca 1	0	0
3	DF	1	Total 1	Ca 1	0	0
3	GA	1	Total 1	Ca 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	DU	1	Total 1	Ca 1	0	0
3	Ao	1	Total 1	Ca 1	0	0
3	Jy	1	Total 1	Ca 1	0	0
3	CU	1	Total 1	Ca 1	0	0
3	Co	1	Total 1	Ca 1	0	0
3	Gj	1	Total 1	Ca 1	0	0
3	Et	1	Total 1	Ca 1	0	0
3	Cy	1	Total 1	Ca 1	0	0
3	BU	1	Total 1	Ca 1	0	0
3	Aj	1	Total 1	Ca 1	0	0
3	HP	1	Total 1	Ca 1	0	0
3	FF	1	Total 1	Ca 1	0	0
3	CP	1	Total 1	Ca 1	0	0
3	DA	1	Total 1	Ca 1	0	0
3	AU	1	Total 1	Ca 1	0	0
3	Ht	1	Total 1	Ca 1	0	0
3	GZ	1	Total 1	Ca 1	0	0
3	EK	1	Total 1	Ca 1	0	0
3	Fo	1	Total 1	Ca 1	0	0
3	Ct	1	Total 1	Ca 1	0	0
3	BZ	1	Total 1	Ca 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	FP	1	Total 1	Ca 1	0	0
3	Bk	1	Total 1	Ca 1	0	0
3	GP	1	Total 1	Ca 1	0	0
3	AP	1	Total 1	Ca 1	0	0
3	I1	1	Total 1	Ca 1	0	0
3	Ft	1	Total 1	Ca 1	0	0
3	At	1	Total 1	Ca 1	0	0
3	B5	1	Total 1	Ca 1	0	0
3	IR	1	Total 1	Ca 1	0	0
3	BF	1	Total 1	Ca 1	0	0
3	BQ	1	Total 1	Ca 1	0	0
3	I4	1	Total 1	Ca 1	0	0
3	CG	1	Total 1	Ca 1	0	0
3	HK	1	Total 1	Ca 1	0	0
3	G1	1	Total 1	Ca 1	0	0
3	A1	1	Total 1	Ca 1	0	0
3	FZ	1	Total 1	Ca 1	0	0
3	AZ	1	Total 1	Ca 1	0	0
3	Ho	1	Total 1	Ca 1	0	0
3	BK	1	Total 1	Ca 1	0	0
3	If	1	Total 1	Ca 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G4	1	Total 1	Ca 1	0	0
3	J4	1	Total 1	Ca 1	0	0
3	Jj	1	Total 1	Ca 1	0	0
3	Ey	1	Total 1	Ca 1	0	0
3	Je	1	Total 1	Ca 1	0	0
3	IA	1	Total 1	Ca 1	0	0
3	JP	1	Total 1	Ca 1	0	0
3	GF	1	Total 1	Ca 1	0	0
3	Dj	1	Total 1	Ca 1	0	0
3	EP	1	Total 1	Ca 1	0	0
3	Dy	1	Total 1	Ca 1	0	0
3	HA	1	Total 1	Ca 1	0	0
3	Dt	1	Total 1	Ca 1	0	0
3	H4	1	Total 1	Ca 1	0	0
3	Jo	1	Total 1	Ca 1	0	0
3	Go	1	Total 1	Ca 1	0	0
3	IK	1	Total 1	Ca 1	0	0
3	BB	1	Total 1	Ca 1	0	0
3	JU	1	Total 1	Ca 1	0	0
3	EZ	1	Total 1	Ca 1	0	0
3	Do	1	Total 1	Ca 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	Io	1	Total 1	Ca 1	0	0
3	Fk	1	Total 1	Ca 1	0	0
3	CK	1	Total 1	Ca 1	0	0
3	Ge	1	Total 1	Ca 1	0	0
3	IU	1	Total 1	Ca 1	0	0
3	FA	1	Total 1	Ca 1	0	0
3	Bt	1	Total 1	Ca 1	0	0
3	IF	1	Total 1	Ca 1	0	0
3	F4	1	Total 1	Ca 1	0	0
3	Fe	1	Total 1	Ca 1	0	0
3	HU	1	Total 1	Ca 1	0	0
3	Ij	1	Total 1	Ca 1	0	0
3	Cj	1	Total 1	Ca 1	0	0
3	Hy	1	Total 1	Ca 1	0	0
3	Ee	1	Total 1	Ca 1	0	0
3	By	1	Total 1	Ca 1	0	0
3	GU	1	Total 1	Ca 1	0	0
3	F1	1	Total 1	Ca 1	0	0
3	E4	1	Total 1	Ca 1	0	0
3	EC	1	Total 1	Ca 1	0	0
3	It	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 0.248 , 0.279	Depositor DCC
R_{free} test set	221945 reflections (11.12%)	DCC
Wilson B-factor (Å ²)	45.5	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 51.3	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	0.87	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](#)

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

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 carbohydrates 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 [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

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%)	-0.14	5 (2%) 61 57	26, 56, 111, 194	0
1	A4	185/242 (76%)	-0.23	1 (0%) 90 90	23, 52, 88, 132	0
1	A5	189/242 (78%)	-0.31	2 (1%) 80 79	18, 52, 92, 153	0
1	A6	217/242 (89%)	-0.15	8 (3%) 42 37	20, 53, 107, 200	0
1	AA	185/242 (76%)	-0.38	0 100 100	29, 54, 87, 113	0
1	AB	189/242 (78%)	-0.38	2 (1%) 80 79	25, 49, 90, 154	0
1	AC	217/242 (89%)	-0.16	7 (3%) 48 42	21, 50, 108, 201	0
1	AF	185/242 (76%)	-0.43	0 100 100	22, 48, 85, 115	0
1	AG	189/242 (78%)	-0.50	1 (0%) 90 90	17, 42, 85, 140	0
1	AH	217/242 (89%)	-0.23	7 (3%) 48 42	21, 50, 114, 203	0
1	AK	185/242 (76%)	-0.34	1 (0%) 90 90	17, 51, 88, 123	0
1	AL	189/242 (78%)	-0.39	2 (1%) 80 79	24, 47, 91, 137	0
1	AM	217/242 (89%)	-0.24	6 (2%) 53 48	19, 48, 106, 200	0
1	AP	185/242 (76%)	-0.40	0 100 100	21, 47, 87, 124	0
1	AQ	189/242 (78%)	-0.45	2 (1%) 80 79	17, 47, 87, 127	0
1	AR	217/242 (89%)	-0.24	6 (2%) 53 48	17, 49, 103, 199	0
1	AU	185/242 (76%)	-0.29	0 100 100	36, 61, 96, 124	0
1	AV	189/242 (78%)	-0.36	3 (1%) 72 70	35, 58, 91, 153	0
1	AW	217/242 (89%)	-0.07	8 (3%) 42 37	27, 58, 108, 201	0
1	AZ	185/242 (76%)	-0.54	0 100 100	14, 38, 69, 107	0
1	Aa	189/242 (78%)	-0.46	0 100 100	14, 37, 79, 138	0
1	Ab	217/242 (89%)	-0.17	6 (2%) 53 48	16, 43, 107, 197	0
1	Ae	185/242 (76%)	-0.47	0 100 100	17, 48, 92, 113	0
1	Af	189/242 (78%)	-0.38	2 (1%) 80 79	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%)	-0.26	6 (2%) 53 48	18, 48, 95, 199	0
1	Aj	185/242 (76%)	-0.44	0 100 100	15, 48, 82, 114	0
1	Ak	189/242 (78%)	-0.39	0 100 100	21, 47, 85, 136	0
1	Al	217/242 (89%)	-0.18	6 (2%) 53 48	19, 44, 104, 191	0
1	Ao	185/242 (76%)	-0.28	3 (1%) 72 70	20, 46, 79, 105	0
1	Ap	189/242 (78%)	-0.50	1 (0%) 90 90	19, 44, 80, 137	0
1	Aq	217/242 (89%)	-0.19	6 (2%) 53 48	16, 46, 100, 197	0
1	At	185/242 (76%)	-0.49	0 100 100	19, 45, 81, 112	0
1	Au	189/242 (78%)	-0.47	0 100 100	9, 41, 85, 128	0
1	Av	217/242 (89%)	-0.10	6 (2%) 53 48	10, 45, 106, 196	0
1	Ay	185/242 (76%)	-0.30	0 100 100	26, 57, 89, 119	0
1	Az	189/242 (78%)	-0.40	0 100 100	27, 54, 96, 132	0
1	B1	217/242 (89%)	-0.31	6 (2%) 53 48	18, 44, 101, 188	0
1	B4	185/242 (76%)	-0.30	0 100 100	36, 61, 85, 117	0
1	B5	189/242 (78%)	-0.30	2 (1%) 80 79	29, 55, 93, 145	0
1	B6	217/242 (89%)	-0.13	7 (3%) 48 42	26, 54, 116, 209	0
1	BA	185/242 (76%)	-0.32	1 (0%) 90 90	17, 56, 91, 116	0
1	BB	189/242 (78%)	-0.36	1 (0%) 90 90	22, 50, 92, 146	0
1	BC	217/242 (89%)	-0.18	7 (3%) 48 42	8, 50, 108, 193	0
1	BF	185/242 (76%)	-0.42	0 100 100	18, 45, 81, 116	0
1	BG	189/242 (78%)	-0.55	2 (1%) 80 79	10, 38, 85, 127	0
1	BH	217/242 (89%)	-0.18	6 (2%) 53 48	13, 40, 95, 200	0
1	BK	185/242 (76%)	-0.33	0 100 100	12, 48, 87, 133	0
1	BL	189/242 (78%)	-0.40	0 100 100	17, 47, 86, 130	0
1	BM	217/242 (89%)	-0.18	7 (3%) 48 42	21, 48, 107, 209	0
1	BP	185/242 (76%)	-0.44	0 100 100	22, 48, 84, 109	0
1	BQ	189/242 (78%)	-0.44	0 100 100	27, 48, 84, 139	0
1	BR	217/242 (89%)	-0.30	6 (2%) 53 48	15, 46, 101, 202	0
1	BU	185/242 (76%)	-0.27	2 (1%) 80 79	29, 59, 97, 130	0
1	BV	189/242 (78%)	-0.42	0 100 100	26, 54, 93, 137	0
1	BW	217/242 (89%)	-0.12	7 (3%) 48 42	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%)	-0.46	0 100 100	15, 43, 81, 120	0
1	Ba	189/242 (78%)	-0.48	0 100 100	22, 46, 88, 121	0
1	Bb	217/242 (89%)	-0.27	6 (2%) 53 48	19, 45, 111, 192	0
1	Be	185/242 (76%)	-0.44	0 100 100	17, 44, 83, 112	0
1	Bf	189/242 (78%)	-0.46	0 100 100	14, 41, 86, 119	0
1	Bg	217/242 (89%)	-0.29	7 (3%) 48 42	18, 45, 105, 176	0
1	Bj	185/242 (76%)	-0.42	0 100 100	19, 46, 79, 117	0
1	Bk	189/242 (78%)	-0.46	0 100 100	18, 47, 88, 127	0
1	Bl	217/242 (89%)	-0.22	7 (3%) 48 42	16, 48, 101, 206	0
1	Bo	185/242 (76%)	-0.36	0 100 100	20, 50, 77, 121	0
1	Bp	189/242 (78%)	-0.40	0 100 100	21, 46, 92, 129	0
1	Bq	217/242 (89%)	-0.22	6 (2%) 53 48	26, 48, 106, 189	0
1	Bt	185/242 (76%)	-0.19	2 (1%) 80 79	33, 60, 94, 120	0
1	Bu	189/242 (78%)	-0.33	0 100 100	20, 51, 94, 133	0
1	Bv	217/242 (89%)	-0.09	8 (3%) 42 37	25, 56, 111, 187	0
1	By	185/242 (76%)	-0.41	0 100 100	14, 46, 84, 123	0
1	Bz	189/242 (78%)	-0.54	1 (0%) 90 90	14, 40, 81, 139	0
1	C1	217/242 (89%)	-0.12	6 (2%) 53 48	12, 39, 104, 212	0
1	C4	185/242 (76%)	-0.36	0 100 100	19, 55, 92, 112	0
1	C5	189/242 (78%)	-0.42	1 (0%) 90 90	23, 51, 89, 164	0
1	C6	217/242 (89%)	-0.16	6 (2%) 53 48	24, 52, 109, 189	0
1	CA	185/242 (76%)	-0.28	1 (0%) 90 90	28, 52, 94, 114	0
1	CB	189/242 (78%)	-0.38	1 (0%) 90 90	18, 50, 81, 123	0
1	CC	217/242 (89%)	-0.12	7 (3%) 48 42	22, 51, 107, 181	0
1	CF	185/242 (76%)	-0.52	1 (0%) 90 90	15, 37, 79, 119	0
1	CG	189/242 (78%)	-0.53	1 (0%) 90 90	9, 36, 82, 131	0
1	CH	217/242 (89%)	-0.27	6 (2%) 53 48	15, 35, 90, 195	0
1	CK	185/242 (76%)	-0.27	2 (1%) 80 79	23, 53, 82, 125	0
1	CL	189/242 (78%)	-0.37	1 (0%) 90 90	13, 47, 84, 149	0
1	CM	217/242 (89%)	-0.12	6 (2%) 53 48	16, 50, 108, 206	0
1	CP	185/242 (76%)	-0.36	1 (0%) 90 90	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%)	-0.42	1 (0%) 90 90	16, 44, 92, 126	0
1	CR	217/242 (89%)	-0.20	6 (2%) 53 48	24, 50, 106, 195	0
1	CU	185/242 (76%)	-0.31	0 100 100	28, 56, 91, 117	0
1	CV	189/242 (78%)	-0.36	3 (1%) 72 70	21, 52, 92, 145	0
1	CW	217/242 (89%)	-0.22	6 (2%) 53 48	21, 51, 107, 194	0
1	CZ	185/242 (76%)	-0.37	0 100 100	26, 55, 91, 108	0
1	Ca	189/242 (78%)	-0.44	2 (1%) 80 79	22, 53, 93, 141	0
1	Cb	217/242 (89%)	-0.23	7 (3%) 48 42	15, 50, 106, 197	0
1	Ce	185/242 (76%)	-0.45	0 100 100	17, 49, 82, 117	0
1	Cf	189/242 (78%)	-0.40	1 (0%) 90 90	20, 46, 96, 130	0
1	Cg	217/242 (89%)	-0.09	6 (2%) 53 48	16, 50, 104, 215	0
1	Cj	185/242 (76%)	-0.43	0 100 100	20, 48, 84, 109	0
1	Ck	189/242 (78%)	-0.43	1 (0%) 90 90	20, 49, 98, 146	0
1	Cl	217/242 (89%)	-0.18	6 (2%) 53 48	20, 46, 105, 204	0
1	Co	185/242 (76%)	-0.43	0 100 100	24, 49, 77, 110	0
1	Cp	189/242 (78%)	-0.45	2 (1%) 80 79	16, 47, 90, 145	0
1	Cq	217/242 (89%)	-0.14	5 (2%) 61 57	27, 52, 109, 204	0
1	Ct	185/242 (76%)	-0.44	1 (0%) 90 90	21, 45, 78, 116	0
1	Cu	189/242 (78%)	-0.55	0 100 100	11, 39, 89, 136	0
1	Cv	217/242 (89%)	-0.24	9 (4%) 38 32	19, 42, 99, 199	0
1	Cy	185/242 (76%)	-0.53	0 100 100	13, 38, 78, 107	0
1	Cz	189/242 (78%)	-0.55	4 (2%) 64 60	12, 34, 82, 123	0
1	D1	217/242 (89%)	-0.18	6 (2%) 53 48	14, 42, 106, 203	0
1	D4	185/242 (76%)	-0.44	0 100 100	19, 41, 85, 110	0
1	D5	189/242 (78%)	-0.56	1 (0%) 90 90	12, 35, 78, 121	0
1	D6	217/242 (89%)	-0.24	7 (3%) 48 42	15, 38, 95, 205	0
1	DA	185/242 (76%)	-0.32	1 (0%) 90 90	20, 49, 83, 111	0
1	DB	189/242 (78%)	-0.34	1 (0%) 90 90	16, 47, 85, 130	0
1	DC	217/242 (89%)	-0.19	6 (2%) 53 48	17, 48, 103, 188	0
1	DF	185/242 (76%)	-0.30	1 (0%) 90 90	25, 54, 85, 123	0
1	DG	189/242 (78%)	-0.45	0 100 100	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%)	-0.19	6 (2%)	53	48	22, 53, 106, 186	0
1	DK	185/242 (76%)	-0.40	1 (0%)	90	90	18, 45, 78, 105	0
1	DL	189/242 (78%)	-0.45	1 (0%)	90	90	13, 40, 84, 129	0
1	DM	217/242 (89%)	-0.27	7 (3%)	48	42	15, 43, 105, 207	0
1	DP	185/242 (76%)	-0.35	0	100	100	26, 52, 91, 123	0
1	DQ	189/242 (78%)	-0.40	0	100	100	19, 47, 86, 137	0
1	DR	217/242 (89%)	-0.22	6 (2%)	53	48	17, 46, 102, 190	0
1	DU	185/242 (76%)	-0.24	3 (1%)	72	70	26, 63, 95, 128	0
1	DV	189/242 (78%)	-0.40	2 (1%)	80	79	27, 57, 94, 149	0
1	DW	217/242 (89%)	-0.08	9 (4%)	38	32	32, 60, 111, 195	0
1	DZ	185/242 (76%)	-0.40	0	100	100	22, 50, 94, 123	0
1	Da	189/242 (78%)	-0.47	0	100	100	18, 46, 89, 134	0
1	Db	217/242 (89%)	-0.01	8 (3%)	42	37	19, 49, 102, 207	0
1	De	185/242 (76%)	-0.31	0	100	100	31, 62, 93, 116	0
1	Df	189/242 (78%)	-0.43	0	100	100	22, 54, 92, 139	0
1	Dg	217/242 (89%)	-0.14	6 (2%)	53	48	24, 56, 108, 184	0
1	Dj	185/242 (76%)	-0.40	0	100	100	22, 48, 84, 115	0
1	Dk	189/242 (78%)	-0.49	3 (1%)	72	70	14, 41, 88, 147	0
1	DI	217/242 (89%)	-0.21	6 (2%)	53	48	21, 47, 102, 192	0
1	Do	185/242 (76%)	-0.27	1 (0%)	90	90	32, 59, 96, 120	0
1	Dp	189/242 (78%)	-0.33	2 (1%)	80	79	26, 57, 97, 164	0
1	Dq	217/242 (89%)	-0.12	7 (3%)	48	42	24, 56, 111, 193	0
1	Dt	185/242 (76%)	-0.31	2 (1%)	80	79	16, 48, 80, 132	0
1	Du	189/242 (78%)	-0.38	2 (1%)	80	79	23, 47, 90, 143	0
1	Dv	217/242 (89%)	-0.22	6 (2%)	53	48	18, 50, 101, 190	0
1	Dy	185/242 (76%)	-0.46	0	100	100	7, 38, 76, 98	0
1	Dz	189/242 (78%)	-0.48	2 (1%)	80	79	16, 38, 75, 130	0
1	E1	217/242 (89%)	-0.28	6 (2%)	53	48	14, 43, 102, 207	0
1	E4	185/242 (76%)	-0.46	0	100	100	18, 46, 87, 114	0
1	E5	189/242 (78%)	-0.45	1 (0%)	90	90	15, 43, 84, 124	0
1	E6	217/242 (89%)	-0.32	6 (2%)	53	48	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%)	-0.35	1 (0%) 90 90	12, 43, 74, 108	0
1	EB	189/242 (78%)	-0.46	1 (0%) 90 90	12, 41, 81, 122	0
1	EC	217/242 (89%)	-0.22	6 (2%) 53 48	18, 43, 98, 186	0
1	EF	185/242 (76%)	-0.35	1 (0%) 90 90	22, 52, 90, 126	0
1	EG	189/242 (78%)	-0.42	1 (0%) 90 90	21, 51, 92, 151	0
1	EH	217/242 (89%)	-0.17	7 (3%) 48 42	24, 55, 114, 189	0
1	EK	185/242 (76%)	-0.34	0 100 100	25, 54, 89, 122	0
1	EL	189/242 (78%)	-0.32	1 (0%) 90 90	27, 53, 95, 126	0
1	EM	217/242 (89%)	-0.21	7 (3%) 48 42	21, 52, 108, 195	0
1	EP	185/242 (76%)	-0.41	0 100 100	17, 45, 86, 118	0
1	EQ	189/242 (78%)	-0.50	0 100 100	15, 43, 78, 131	0
1	ER	217/242 (89%)	-0.22	6 (2%) 53 48	15, 46, 105, 192	0
1	EU	185/242 (76%)	-0.40	1 (0%) 90 90	22, 52, 83, 128	0
1	EV	189/242 (78%)	-0.47	1 (0%) 90 90	16, 46, 89, 135	0
1	EW	217/242 (89%)	-0.17	6 (2%) 53 48	21, 50, 103, 200	0
1	EZ	185/242 (76%)	-0.31	2 (1%) 80 79	30, 53, 85, 118	0
1	Ea	189/242 (78%)	-0.37	0 100 100	20, 48, 90, 143	0
1	Eb	217/242 (89%)	-0.16	7 (3%) 48 42	16, 50, 105, 190	0
1	Ee	185/242 (76%)	-0.36	0 100 100	33, 59, 88, 116	0
1	Ef	189/242 (78%)	-0.39	0 100 100	21, 54, 93, 136	0
1	Eg	217/242 (89%)	0.01	8 (3%) 42 37	24, 60, 113, 203	0
1	Ej	185/242 (76%)	-0.17	2 (1%) 80 79	22, 58, 90, 113	0
1	Ek	189/242 (78%)	-0.38	4 (2%) 64 60	29, 57, 94, 139	0
1	El	217/242 (89%)	-0.06	5 (2%) 61 57	30, 56, 107, 191	0
1	Eo	185/242 (76%)	-0.36	0 100 100	25, 54, 84, 113	0
1	Ep	189/242 (78%)	-0.38	4 (2%) 64 60	20, 46, 89, 162	0
1	Eq	217/242 (89%)	-0.27	5 (2%) 61 57	23, 52, 112, 190	0
1	Et	185/242 (76%)	-0.46	0 100 100	17, 38, 77, 114	0
1	Eu	189/242 (78%)	-0.50	1 (0%) 90 90	13, 37, 80, 134	0
1	Ev	217/242 (89%)	-0.22	8 (3%) 42 37	12, 38, 97, 197	0
1	Ey	185/242 (76%)	-0.47	0 100 100	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%)	-0.55	0 100 100	19, 43, 84, 139	0
1	F1	217/242 (89%)	0.25	10 (4%) 33 28	49, 80, 119, 186	0
1	F4	185/242 (76%)	-0.34	0 100 100	26, 57, 86, 112	0
1	F5	189/242 (78%)	-0.32	3 (1%) 72 70	28, 57, 94, 140	0
1	F6	217/242 (89%)	-0.06	9 (4%) 38 32	31, 64, 117, 195	0
1	FA	185/242 (76%)	-0.27	1 (0%) 90 90	22, 59, 95, 134	0
1	FB	189/242 (78%)	-0.46	1 (0%) 90 90	20, 47, 90, 148	0
1	FC	217/242 (89%)	0.15	10 (4%) 33 28	29, 62, 110, 205	0
1	FF	185/242 (76%)	-0.29	0 100 100	30, 55, 92, 114	0
1	FG	189/242 (78%)	-0.36	1 (0%) 90 90	20, 51, 92, 133	0
1	FH	217/242 (89%)	-0.11	6 (2%) 53 48	24, 60, 106, 197	0
1	FK	185/242 (76%)	-0.24	0 100 100	28, 59, 90, 131	0
1	FL	189/242 (78%)	-0.19	4 (2%) 64 60	24, 59, 100, 150	0
1	FM	217/242 (89%)	-0.11	6 (2%) 53 48	22, 54, 101, 200	0
1	FP	185/242 (76%)	-0.11	2 (1%) 80 79	24, 62, 101, 112	0
1	FQ	189/242 (78%)	-0.11	3 (1%) 72 70	23, 61, 94, 134	0
1	FR	217/242 (89%)	0.03	9 (4%) 38 32	26, 55, 118, 222	0
1	FU	185/242 (76%)	-0.37	0 100 100	32, 55, 86, 119	0
1	FV	189/242 (78%)	-0.41	1 (0%) 90 90	21, 48, 87, 130	0
1	FW	217/242 (89%)	-0.08	7 (3%) 48 42	19, 52, 105, 190	0
1	FZ	185/242 (76%)	-0.05	3 (1%) 72 70	42, 78, 106, 129	0
1	Fa	189/242 (78%)	-0.17	5 (2%) 56 51	34, 70, 104, 157	0
1	Fb	217/242 (89%)	0.09	7 (3%) 48 42	41, 70, 117, 212	0
1	Fe	185/242 (76%)	0.41	13 (7%) 17 12	63, 97, 124, 151	0
1	Ff	189/242 (78%)	0.25	14 (7%) 15 11	52, 93, 121, 163	0
1	Fg	217/242 (89%)	0.61	19 (8%) 11 7	58, 92, 134, 190	0
1	Fj	185/242 (76%)	0.06	3 (1%) 72 70	38, 74, 107, 128	0
1	Fk	189/242 (78%)	0.07	8 (4%) 37 32	35, 75, 111, 141	0
1	Fl	217/242 (89%)	0.30	8 (3%) 42 37	41, 79, 127, 203	0
1	Fo	185/242 (76%)	-0.23	5 (2%) 55 50	26, 54, 92, 120	0
1	Fp	189/242 (78%)	-0.28	0 100 100	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%)	-0.19	6 (2%) 53 48	11, 50, 103, 203	0
1	Ft	185/242 (76%)	-0.30	0 100 100	27, 55, 92, 127	0
1	Fu	189/242 (78%)	-0.40	1 (0%) 90 90	24, 51, 88, 140	0
1	Fv	217/242 (89%)	-0.18	6 (2%) 53 48	20, 53, 102, 187	0
1	Fy	185/242 (76%)	0.10	0 100 100	59, 90, 117, 135	0
1	Fz	189/242 (78%)	-0.16	5 (2%) 56 51	40, 76, 113, 150	0
1	G1	217/242 (89%)	0.08	10 (4%) 33 28	34, 66, 116, 201	0
1	G4	185/242 (76%)	0.12	6 (3%) 48 42	57, 89, 114, 148	0
1	G5	189/242 (78%)	0.16	10 (5%) 27 23	45, 83, 114, 159	0
1	G6	217/242 (89%)	0.22	12 (5%) 26 21	38, 73, 126, 187	0
1	GA	185/242 (76%)	-0.21	1 (0%) 90 90	20, 57, 92, 118	0
1	GB	189/242 (78%)	-0.29	0 100 100	28, 59, 96, 125	0
1	GC	217/242 (89%)	-0.02	10 (4%) 33 28	23, 58, 113, 202	0
1	GF	185/242 (76%)	-0.28	0 100 100	20, 56, 83, 116	0
1	GG	189/242 (78%)	-0.31	2 (1%) 80 79	22, 53, 94, 132	0
1	GH	217/242 (89%)	-0.14	6 (2%) 53 48	25, 54, 105, 188	0
1	GK	185/242 (76%)	0.27	7 (3%) 41 35	61, 90, 117, 142	0
1	GL	189/242 (78%)	0.13	10 (5%) 27 23	52, 84, 119, 165	0
1	GM	217/242 (89%)	0.22	8 (3%) 42 37	42, 77, 118, 205	0
1	GP	185/242 (76%)	-0.31	0 100 100	20, 55, 91, 125	0
1	GQ	189/242 (78%)	-0.21	2 (1%) 80 79	26, 58, 93, 117	0
1	GR	217/242 (89%)	-0.07	6 (2%) 53 48	25, 55, 106, 199	0
1	GU	185/242 (76%)	-0.34	2 (1%) 80 79	26, 55, 87, 128	0
1	GV	189/242 (78%)	-0.44	2 (1%) 80 79	15, 46, 88, 131	0
1	GW	217/242 (89%)	-0.09	6 (2%) 53 48	23, 48, 103, 194	0
1	GZ	185/242 (76%)	0.02	0 100 100	26, 67, 96, 131	0
1	Ga	189/242 (78%)	-0.27	2 (1%) 80 79	20, 55, 99, 172	0
1	Gb	217/242 (89%)	0.08	10 (4%) 33 28	32, 61, 109, 200	0
1	Ge	185/242 (76%)	0.10	6 (3%) 48 42	33, 67, 100, 126	0
1	Gf	189/242 (78%)	-0.03	3 (1%) 72 70	28, 70, 108, 147	0
1	Gg	217/242 (89%)	0.22	9 (4%) 38 32	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%)	0.26	7 (3%) 41 35	51, 89, 118, 144	0
1	Gk	189/242 (78%)	0.08	5 (2%) 56 51	53, 82, 114, 143	0
1	Gl	217/242 (89%)	0.27	15 (6%) 18 13	38, 75, 119, 194	0
1	Go	185/242 (76%)	0.48	15 (8%) 13 9	62, 92, 120, 144	0
1	Gp	189/242 (78%)	0.32	12 (6%) 21 16	56, 95, 124, 162	0
1	Gq	217/242 (89%)	0.23	10 (4%) 33 28	57, 91, 129, 191	0
1	Gt	185/242 (76%)	-0.24	2 (1%) 80 79	25, 56, 90, 118	0
1	Gu	189/242 (78%)	-0.32	0 100 100	24, 51, 89, 145	0
1	Gv	217/242 (89%)	-0.13	6 (2%) 53 48	24, 53, 105, 199	0
1	Gy	185/242 (76%)	-0.07	2 (1%) 80 79	35, 64, 98, 129	0
1	Gz	189/242 (78%)	-0.30	2 (1%) 80 79	34, 63, 97, 153	0
1	H1	217/242 (89%)	0.10	8 (3%) 42 37	32, 69, 116, 189	0
1	H4	185/242 (76%)	0.32	12 (6%) 20 15	56, 91, 125, 144	0
1	H5	189/242 (78%)	0.32	8 (4%) 37 32	57, 93, 122, 143	0
1	H6	217/242 (89%)	0.41	15 (6%) 18 13	55, 92, 133, 193	0
1	HA	185/242 (76%)	-0.22	2 (1%) 80 79	41, 71, 100, 130	0
1	HB	189/242 (78%)	-0.23	2 (1%) 80 79	34, 67, 106, 131	0
1	HC	217/242 (89%)	0.19	10 (4%) 33 28	46, 78, 133, 205	0
1	HF	185/242 (76%)	-0.03	1 (0%) 90 90	40, 70, 98, 130	0
1	HG	189/242 (78%)	-0.25	2 (1%) 80 79	32, 58, 99, 136	0
1	HH	217/242 (89%)	-0.04	7 (3%) 48 42	26, 60, 105, 206	0
1	HK	185/242 (76%)	-0.26	1 (0%) 90 90	30, 62, 97, 119	0
1	HL	189/242 (78%)	-0.24	1 (0%) 90 90	24, 52, 93, 141	0
1	HM	217/242 (89%)	0.02	6 (2%) 53 48	25, 64, 112, 190	0
1	HP	185/242 (76%)	-0.18	0 100 100	23, 66, 103, 127	0
1	HQ	189/242 (78%)	-0.35	0 100 100	21, 54, 99, 137	0
1	HR	217/242 (89%)	0.09	10 (4%) 33 28	24, 62, 118, 186	0
1	HU	185/242 (76%)	-0.21	2 (1%) 80 79	27, 60, 89, 126	0
1	HV	189/242 (78%)	-0.30	1 (0%) 90 90	31, 60, 104, 142	0
1	HW	217/242 (89%)	0.09	11 (5%) 29 24	38, 67, 112, 183	0
1	HZ	185/242 (76%)	-0.11	2 (1%) 80 79	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%)	-0.29	3 (1%) 72 70	26, 57, 95, 154	0
1	Hb	217/242 (89%)	0.14	7 (3%) 48 42	33, 65, 107, 199	0
1	He	185/242 (76%)	0.30	8 (4%) 36 31	55, 96, 127, 153	0
1	Hf	189/242 (78%)	0.34	11 (5%) 24 19	50, 88, 122, 171	0
1	Hg	217/242 (89%)	0.50	18 (8%) 12 9	54, 94, 131, 203	0
1	Hj	185/242 (76%)	0.12	7 (3%) 41 35	51, 88, 110, 134	0
1	Hk	189/242 (78%)	-0.18	1 (0%) 90 90	35, 73, 112, 169	0
1	Hi	217/242 (89%)	0.16	9 (4%) 38 32	39, 71, 121, 178	0
1	Ho	185/242 (76%)	-0.24	1 (0%) 90 90	37, 65, 100, 127	0
1	Hp	189/242 (78%)	-0.28	1 (0%) 90 90	32, 61, 96, 139	0
1	Hq	217/242 (89%)	-0.07	7 (3%) 48 42	31, 62, 106, 201	0
1	Ht	185/242 (76%)	-0.02	4 (2%) 62 59	27, 67, 98, 131	0
1	Hu	189/242 (78%)	-0.10	5 (2%) 56 51	23, 62, 106, 162	0
1	Hv	217/242 (89%)	-0.06	8 (3%) 42 37	25, 57, 111, 205	0
1	Hy	185/242 (76%)	-0.16	0 100 100	37, 68, 108, 132	0
1	Hx	189/242 (78%)	-0.19	4 (2%) 64 60	25, 62, 101, 141	0
1	I1	217/242 (89%)	0.10	11 (5%) 29 24	23, 63, 112, 193	0
1	I4	185/242 (76%)	-0.05	4 (2%) 62 59	29, 67, 97, 116	0
1	I5	189/242 (78%)	-0.26	4 (2%) 64 60	31, 58, 97, 146	0
1	I6	217/242 (89%)	0.10	6 (2%) 53 48	30, 69, 117, 212	0
1	IA	185/242 (76%)	0.40	14 (7%) 15 10	67, 98, 122, 151	0
1	IB	189/242 (78%)	0.23	9 (4%) 31 27	53, 89, 127, 196	0
1	IC	217/242 (89%)	0.63	23 (10%) 7 5	56, 98, 138, 201	0
1	IF	185/242 (76%)	-0.06	5 (2%) 55 50	34, 68, 102, 130	0
1	IG	189/242 (78%)	-0.02	3 (1%) 72 70	46, 73, 104, 142	0
1	IH	217/242 (89%)	0.11	9 (4%) 38 32	42, 71, 118, 184	0
1	IK	185/242 (76%)	-0.28	0 100 100	35, 60, 90, 127	0
1	IL	189/242 (78%)	-0.38	1 (0%) 90 90	22, 50, 90, 138	0
1	IM	217/242 (89%)	-0.13	6 (2%) 53 48	27, 58, 112, 188	0
1	IP	185/242 (76%)	-0.11	3 (1%) 72 70	36, 68, 101, 128	0
1	IQ	189/242 (78%)	-0.22	3 (1%) 72 70	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%)	-0.03	7 (3%) 48 42	40, 69, 111, 186	0
1	IU	185/242 (76%)	-0.27	0 100 100	21, 55, 88, 116	0
1	IV	189/242 (78%)	-0.47	0 100 100	18, 48, 81, 134	0
1	IW	217/242 (89%)	-0.03	6 (2%) 53 48	21, 52, 107, 195	0
1	IZ	185/242 (76%)	-0.29	1 (0%) 90 90	21, 58, 87, 123	0
1	Ia	189/242 (78%)	-0.42	0 100 100	17, 46, 86, 144	0
1	Ib	217/242 (89%)	-0.15	7 (3%) 48 42	23, 50, 105, 194	0
1	Ie	185/242 (76%)	0.10	4 (2%) 62 59	53, 85, 115, 136	0
1	If	189/242 (78%)	-0.03	3 (1%) 72 70	37, 71, 116, 154	0
1	Ig	217/242 (89%)	0.09	9 (4%) 38 32	34, 70, 116, 193	0
1	Ij	185/242 (76%)	0.44	15 (8%) 13 9	56, 89, 121, 143	0
1	Ik	189/242 (78%)	0.12	4 (2%) 64 60	34, 76, 114, 152	0
1	Il	217/242 (89%)	0.44	13 (5%) 23 17	40, 85, 123, 212	0
1	Io	185/242 (76%)	-0.29	2 (1%) 80 79	26, 56, 94, 123	0
1	Ip	189/242 (78%)	-0.42	0 100 100	21, 51, 90, 140	0
1	Iq	217/242 (89%)	-0.06	7 (3%) 48 42	26, 58, 112, 189	0
1	It	185/242 (76%)	-0.22	1 (0%) 90 90	29, 59, 94, 132	0
1	Iu	189/242 (78%)	-0.32	2 (1%) 80 79	21, 53, 102, 135	0
1	Iv	217/242 (89%)	-0.14	5 (2%) 61 57	26, 54, 103, 186	0
1	Iy	185/242 (76%)	-0.10	3 (1%) 72 70	44, 73, 104, 132	0
1	Iz	189/242 (78%)	-0.26	3 (1%) 72 70	37, 67, 105, 162	0
1	J1	217/242 (89%)	0.14	6 (2%) 53 48	23, 66, 107, 195	0
1	J4	185/242 (76%)	0.33	11 (5%) 23 18	43, 83, 113, 139	0
1	J5	189/242 (78%)	0.06	6 (3%) 48 42	27, 73, 118, 145	0
1	J6	217/242 (89%)	0.32	9 (4%) 38 32	34, 74, 126, 198	0
1	JA	185/242 (76%)	0.09	4 (2%) 62 59	35, 70, 105, 127	0
1	JB	189/242 (78%)	-0.04	1 (0%) 90 90	32, 65, 110, 139	0
1	JC	217/242 (89%)	0.28	10 (4%) 33 28	31, 74, 118, 188	0
1	JF	185/242 (76%)	-0.03	3 (1%) 72 70	39, 73, 109, 134	0
1	JG	189/242 (78%)	-0.09	2 (1%) 80 79	24, 70, 109, 153	0
1	JH	217/242 (89%)	0.31	8 (3%) 42 37	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%)	0.49	19 (10%) 7 5	63, 97, 126, 150	0
1	JL	189/242 (78%)	0.03	4 (2%) 64 60	52, 87, 125, 168	0
1	JM	217/242 (89%)	0.53	14 (6%) 20 15	62, 98, 136, 192	0
1	JP	185/242 (76%)	0.25	9 (4%) 30 26	58, 90, 114, 148	0
1	JQ	189/242 (78%)	-0.09	2 (1%) 80 79	44, 77, 116, 137	0
1	JR	217/242 (89%)	0.34	13 (5%) 23 17	47, 85, 125, 215	0
1	JU	185/242 (76%)	-0.03	6 (3%) 48 42	38, 69, 105, 133	0
1	JV	189/242 (78%)	-0.18	1 (0%) 90 90	35, 67, 102, 152	0
1	JW	217/242 (89%)	0.18	13 (5%) 23 17	42, 79, 121, 215	0
1	JZ	185/242 (76%)	-0.13	4 (2%) 62 59	38, 68, 101, 131	0
1	Ja	189/242 (78%)	-0.06	4 (2%) 64 60	41, 76, 108, 163	0
1	Jb	217/242 (89%)	0.00	7 (3%) 48 42	36, 69, 115, 195	0
1	Je	185/242 (76%)	-0.27	0 100 100	29, 57, 92, 124	0
1	Jf	189/242 (78%)	-0.31	0 100 100	28, 58, 98, 135	0
1	Jg	217/242 (89%)	-0.14	6 (2%) 53 48	19, 51, 99, 197	0
1	Jj	185/242 (76%)	-0.40	0 100 100	22, 49, 80, 117	0
1	Jk	189/242 (78%)	-0.46	1 (0%) 90 90	14, 44, 91, 123	0
1	Jl	217/242 (89%)	-0.17	6 (2%) 53 48	17, 44, 92, 208	0
1	Jo	185/242 (76%)	-0.27	0 100 100	31, 59, 91, 124	0
1	Jp	189/242 (78%)	-0.20	1 (0%) 90 90	31, 62, 101, 130	0
1	Jq	217/242 (89%)	-0.12	8 (3%) 42 37	24, 54, 108, 199	0
1	Jt	185/242 (76%)	-0.07	1 (0%) 90 90	36, 73, 106, 129	0
1	Ju	189/242 (78%)	-0.04	5 (2%) 56 51	34, 69, 102, 152	0
1	Jv	217/242 (89%)	0.11	6 (2%) 53 48	34, 68, 121, 185	0
1	Jy	185/242 (76%)	0.07	3 (1%) 72 70	36, 71, 108, 126	0
1	Jz	189/242 (78%)	0.05	5 (2%) 56 51	34, 73, 110, 141	0
2	A2	17/17 (100%)	4.78	14 (82%) 0 0	159, 199, 279, 304	0
2	A7	17/17 (100%)	4.92	17 (100%) 0 0	154, 204, 269, 286	0
2	AD	17/17 (100%)	5.47	15 (88%) 0 0	157, 204, 281, 286	0
2	AI	17/17 (100%)	4.65	16 (94%) 0 0	164, 188, 256, 267	0
2	AN	17/17 (100%)	4.27	16 (94%) 0 0	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%)	3.85	12 (70%)	0	0	154, 202, 274, 275	0
2	AX	17/17 (100%)	4.06	13 (76%)	0	0	164, 193, 269, 273	0
2	Ac	17/17 (100%)	4.28	15 (88%)	0	0	141, 188, 262, 275	0
2	Ah	17/17 (100%)	5.01	16 (94%)	0	0	154, 193, 271, 272	0
2	Am	17/17 (100%)	4.48	16 (94%)	0	0	137, 213, 264, 277	0
2	Ar	17/17 (100%)	5.10	15 (88%)	0	0	149, 198, 271, 283	0
2	Aw	17/17 (100%)	4.75	17 (100%)	0	0	163, 197, 284, 286	0
2	B2	17/17 (100%)	5.11	16 (94%)	0	0	162, 190, 261, 267	0
2	B7	17/17 (100%)	4.42	15 (88%)	0	0	177, 200, 254, 265	0
2	BD	17/17 (100%)	5.57	17 (100%)	0	0	160, 209, 274, 279	0
2	BI	17/17 (100%)	4.84	16 (94%)	0	0	156, 207, 280, 280	0
2	BN	17/17 (100%)	4.37	11 (64%)	0	0	156, 200, 262, 264	0
2	BS	17/17 (100%)	4.93	15 (88%)	0	0	159, 208, 260, 270	0
2	BX	17/17 (100%)	4.79	16 (94%)	0	0	174, 199, 274, 277	0
2	Bc	17/17 (100%)	4.65	14 (82%)	0	0	165, 199, 272, 280	0
2	Bh	17/17 (100%)	4.40	16 (94%)	0	0	163, 199, 271, 273	0
2	Bm	17/17 (100%)	4.58	16 (94%)	0	0	154, 202, 276, 289	0
2	Br	17/17 (100%)	4.89	16 (94%)	0	0	144, 200, 289, 290	0
2	Bw	17/17 (100%)	4.25	16 (94%)	0	0	154, 195, 277, 282	0
2	C2	17/17 (100%)	3.52	13 (76%)	0	0	144, 205, 267, 273	0
2	C7	17/17 (100%)	4.53	14 (82%)	0	0	164, 209, 267, 273	0
2	CD	17/17 (100%)	5.33	16 (94%)	0	0	158, 202, 277, 281	0
2	CI	17/17 (100%)	5.98	16 (94%)	0	0	159, 206, 278, 289	0
2	CN	17/17 (100%)	5.03	16 (94%)	0	0	168, 187, 268, 276	0
2	CS	17/17 (100%)	4.28	13 (76%)	0	0	157, 199, 273, 276	0
2	CX	17/17 (100%)	5.13	16 (94%)	0	0	162, 189, 274, 293	0
2	Cc	17/17 (100%)	5.33	16 (94%)	0	0	161, 205, 260, 270	0
2	Ch	17/17 (100%)	4.24	11 (64%)	0	0	151, 201, 273, 279	0
2	Cm	17/17 (100%)	5.38	17 (100%)	0	0	152, 201, 267, 268	0
2	Cr	17/17 (100%)	4.72	14 (82%)	0	0	152, 206, 261, 272	0
2	Cw	17/17 (100%)	4.92	15 (88%)	0	0	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%)	4.30	17 (100%)	0	0	152, 201, 267, 269	0
2	D7	17/17 (100%)	4.95	15 (88%)	0	0	152, 194, 266, 269	0
2	DD	17/17 (100%)	4.80	16 (94%)	0	0	161, 204, 270, 283	0
2	DI	17/17 (100%)	4.52	13 (76%)	0	0	164, 212, 272, 278	0
2	DN	17/17 (100%)	5.20	17 (100%)	0	0	162, 207, 268, 275	0
2	DS	17/17 (100%)	4.48	14 (82%)	0	0	168, 199, 259, 264	0
2	DX	17/17 (100%)	5.42	17 (100%)	0	0	176, 203, 267, 271	0
2	Dc	17/17 (100%)	4.15	14 (82%)	0	0	159, 209, 267, 279	0
2	Dh	17/17 (100%)	5.72	17 (100%)	0	0	164, 208, 269, 280	0
2	Dm	17/17 (100%)	4.69	13 (76%)	0	0	148, 199, 269, 272	0
2	Dr	17/17 (100%)	5.89	17 (100%)	0	0	157, 207, 277, 281	0
2	Dw	17/17 (100%)	4.90	15 (88%)	0	0	152, 191, 275, 293	0
2	E2	17/17 (100%)	5.19	16 (94%)	0	0	156, 193, 283, 293	0
2	E7	17/17 (100%)	4.75	15 (88%)	0	0	156, 195, 271, 287	0
2	ED	17/17 (100%)	4.48	15 (88%)	0	0	152, 188, 275, 277	0
2	EI	17/17 (100%)	4.57	14 (82%)	0	0	160, 206, 260, 264	0
2	EN	17/17 (100%)	4.45	15 (88%)	0	0	156, 192, 258, 286	0
2	ES	17/17 (100%)	4.90	15 (88%)	0	0	162, 204, 265, 279	0
2	EX	17/17 (100%)	4.61	15 (88%)	0	0	158, 195, 272, 273	0
2	Ec	17/17 (100%)	4.08	14 (82%)	0	0	157, 196, 258, 270	0
2	Eh	17/17 (100%)	4.04	16 (94%)	0	0	172, 198, 263, 268	0
2	Em	17/17 (100%)	4.18	13 (76%)	0	0	147, 194, 261, 261	0
2	Er	17/17 (100%)	5.02	17 (100%)	0	0	159, 202, 272, 280	0
2	Ew	17/17 (100%)	5.14	17 (100%)	0	0	150, 183, 263, 264	0
2	F2	17/17 (100%)	5.40	17 (100%)	0	0	194, 214, 267, 274	0
2	F7	17/17 (100%)	4.10	15 (88%)	0	0	159, 205, 277, 289	0
2	FD	17/17 (100%)	3.83	13 (76%)	0	0	167, 208, 268, 288	0
2	FI	17/17 (100%)	3.92	15 (88%)	0	0	170, 198, 262, 266	0
2	FN	17/17 (100%)	5.26	17 (100%)	0	0	163, 208, 292, 304	0
2	FS	17/17 (100%)	4.05	13 (76%)	0	0	174, 204, 274, 289	0
2	FX	17/17 (100%)	5.25	16 (94%)	0	0	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%)	5.03	17 (100%) 0 0	179, 218, 269, 281	0
2	Fh	17/17 (100%)	4.01	13 (76%) 0 0	180, 240, 287, 293	0
2	Fm	17/17 (100%)	5.37	17 (100%) 0 0	181, 216, 278, 291	0
2	Fr	17/17 (100%)	5.65	16 (94%) 0 0	167, 200, 274, 280	0
2	Fw	17/17 (100%)	4.22	15 (88%) 0 0	165, 214, 287, 290	0
2	G2	17/17 (100%)	4.50	16 (94%) 0 0	170, 212, 259, 261	0
2	G7	17/17 (100%)	4.27	14 (82%) 0 0	189, 209, 259, 271	0
2	GD	17/17 (100%)	5.44	17 (100%) 0 0	168, 211, 281, 286	0
2	GI	17/17 (100%)	5.36	17 (100%) 0 0	163, 209, 263, 277	0
2	GN	17/17 (100%)	5.80	17 (100%) 0 0	185, 217, 288, 291	0
2	GS	17/17 (100%)	4.82	17 (100%) 0 0	184, 209, 263, 275	0
2	GX	17/17 (100%)	4.11	12 (70%) 0 0	166, 203, 273, 303	0
2	Gc	17/17 (100%)	4.21	13 (76%) 0 0	165, 211, 270, 276	0
2	Gh	17/17 (100%)	5.72	17 (100%) 0 0	162, 216, 260, 260	0
2	Gm	17/17 (100%)	6.01	17 (100%) 0 0	191, 213, 278, 289	0
2	Gr	17/17 (100%)	3.97	14 (82%) 0 0	192, 219, 275, 295	0
2	Gw	17/17 (100%)	5.79	16 (94%) 0 0	165, 218, 280, 284	0
2	H2	17/17 (100%)	5.56	17 (100%) 0 0	173, 207, 289, 293	0
2	H7	17/17 (100%)	5.46	17 (100%) 0 0	195, 214, 276, 279	0
2	HD	17/17 (100%)	4.91	15 (88%) 0 0	177, 229, 281, 286	0
2	HI	17/17 (100%)	4.61	16 (94%) 0 0	173, 194, 258, 289	0
2	HN	17/17 (100%)	5.18	17 (100%) 0 0	167, 214, 281, 292	0
2	HS	17/17 (100%)	4.14	15 (88%) 0 0	174, 213, 281, 294	0
2	HX	17/17 (100%)	3.92	11 (64%) 0 0	158, 206, 276, 283	0
2	Hc	17/17 (100%)	4.47	11 (64%) 0 0	173, 208, 274, 293	0
2	Hh	17/17 (100%)	5.59	16 (94%) 0 0	196, 227, 270, 292	0
2	Hm	17/17 (100%)	5.11	15 (88%) 0 0	191, 215, 278, 297	0
2	Hr	17/17 (100%)	4.63	16 (94%) 0 0	170, 214, 284, 291	0
2	Hw	17/17 (100%)	5.61	16 (94%) 0 0	170, 214, 272, 286	0
2	I2	17/17 (100%)	4.54	14 (82%) 0 0	173, 227, 265, 269	0
2	I7	17/17 (100%)	5.34	15 (88%) 0 0	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%)	5.49	17 (100%) 0 0	197, 230, 270, 282	0
2	II	17/17 (100%)	5.36	17 (100%) 0 0	181, 209, 283, 298	0
2	IN	17/17 (100%)	4.78	14 (82%) 0 0	170, 195, 279, 286	0
2	IS	17/17 (100%)	5.81	17 (100%) 0 0	180, 207, 271, 276	0
2	IX	17/17 (100%)	4.48	16 (94%) 0 0	168, 215, 279, 286	0
2	Ic	17/17 (100%)	4.14	14 (82%) 0 0	165, 214, 265, 278	0
2	Ih	17/17 (100%)	5.40	17 (100%) 0 0	176, 208, 264, 275	0
2	Im	17/17 (100%)	4.52	14 (82%) 0 0	193, 215, 278, 294	0
2	Ir	17/17 (100%)	5.09	16 (94%) 0 0	175, 206, 269, 274	0
2	Iw	17/17 (100%)	4.68	16 (94%) 0 0	167, 208, 273, 276	0
2	J2	17/17 (100%)	5.61	17 (100%) 0 0	187, 220, 287, 302	0
2	J7	17/17 (100%)	4.60	17 (100%) 0 0	181, 227, 279, 294	0
2	JD	17/17 (100%)	3.84	12 (70%) 0 0	169, 211, 260, 265	0
2	JI	17/17 (100%)	5.85	16 (94%) 0 0	179, 213, 269, 274	0
2	JN	17/17 (100%)	4.87	15 (88%) 0 0	193, 227, 264, 264	0
2	JS	17/17 (100%)	5.35	16 (94%) 0 0	203, 222, 276, 276	0
2	JX	17/17 (100%)	5.35	17 (100%) 0 0	175, 221, 275, 281	0
2	Jc	17/17 (100%)	4.92	17 (100%) 0 0	177, 215, 290, 291	0
2	Jh	17/17 (100%)	4.52	13 (76%) 0 0	156, 200, 280, 285	0
2	Jm	17/17 (100%)	5.02	15 (88%) 0 0	165, 207, 294, 298	0
2	Jr	17/17 (100%)	4.48	17 (100%) 0 0	165, 208, 270, 278	0
2	Jw	17/17 (100%)	4.01	13 (76%) 0 0	180, 215, 280, 291	0
All	All	72960/89160 (81%)	-0.04	3292 (4%) 34 29	7, 58, 123, 304	0

The worst 5 of 3292 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	IW	25	ALA	25.8
1	DC	25	ALA	20.7
1	AC	25	ALA	20.2
1	Cg	25	ALA	19.7
1	Ab	25	ALA	19.2

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

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

5.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.4 Ligands [i](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	CA	JP	301	1/1	0.87	0.32	2.52	143,143,143,143	0
3	CA	E4	301	1/1	0.91	0.19	2.17	98,98,98,98	0
3	CA	Ey	301	1/1	0.95	0.24	1.99	95,95,95,95	0
3	CA	DU	301	1/1	0.91	0.20	1.52	113,113,113,113	0
3	CA	Dy	301	1/1	0.96	0.18	1.10	65,65,65,65	0
3	CA	Hy	301	1/1	0.65	0.21	1.07	138,138,138,138	0
3	CA	GF	301	1/1	0.92	0.20	0.89	105,105,105,105	0
3	CA	Ce	301	1/1	0.78	0.16	0.77	113,113,113,113	0
3	CA	EP	301	1/1	0.94	0.17	0.61	84,84,84,84	0
3	CA	I4	301	1/1	0.69	0.22	0.57	147,147,147,147	0
3	CA	Ge	301	1/1	0.86	0.18	0.28	121,121,121,121	0
3	CA	BZ	301	1/1	0.94	0.14	0.17	97,97,97,97	0
3	CA	EC	301	1/1	0.95	0.16	0.05	90,90,90,90	0
3	CA	BK	301	1/1	0.94	0.15	-0.20	96,96,96,96	0
3	CA	AL	301	1/1	0.97	0.13	-0.31	85,85,85,85	0
3	CA	Ho	301	1/1	0.95	0.17	-0.33	95,95,95,95	0
3	CA	FA	301	1/1	0.78	0.14	-0.56	94,94,94,94	0
3	CA	BB	301	1/1	0.95	0.15	-0.59	114,114,114,114	0
3	CA	D4	301	1/1	0.94	0.15	-0.62	77,77,77,77	0
3	CA	G1	301	1/1	0.89	0.12	-0.68	103,103,103,103	0
3	CA	C4	301	1/1	0.77	0.12	-0.70	127,127,127,127	0
3	CA	Ij	301	1/1	0.63	0.17	-0.72	130,130,130,130	0
3	CA	AZ	301	1/1	0.97	0.12	-0.74	82,82,82,82	0
3	CA	Eo	301	1/1	0.82	0.13	-0.88	105,105,105,105	0
3	CA	FK	301	1/1	0.97	0.11	-0.92	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	CA	If	301	1/1	0.82	0.11	-0.96	124,124,124,124	0
3	CA	IZ	301	1/1	0.96	0.14	-1.00	94,94,94,94	0
3	CA	Ct	301	1/1	0.97	0.11	-1.03	79,79,79,79	0
3	CA	EU	301	1/1	0.96	0.11	-1.05	109,109,109,109	0
3	CA	Je	301	1/1	0.91	0.12	-1.06	112,112,112,112	0
3	CA	IK	301	1/1	0.92	0.11	-1.09	105,105,105,105	0
3	CA	JA	301	1/1	0.90	0.14	-1.12	109,109,109,109	0
3	CA	Jj	301	1/1	0.97	0.13	-1.20	74,74,74,74	0
3	CA	Ee	301	1/1	0.86	0.11	-1.22	102,102,102,102	0
3	CA	IA	301	1/1	0.82	0.09	-1.22	115,115,115,115	0
3	CA	EK	301	1/1	0.94	0.10	-1.28	89,89,89,89	0
3	CA	A4	301	1/1	0.90	0.13	-1.28	81,81,81,81	0
3	CA	Af	301	1/1	0.92	0.13	-1.31	105,105,105,105	0
3	CA	HP	301	1/1	0.98	0.12	-1.32	81,81,81,81	0
3	CA	Bo	301	1/1	0.97	0.11	-1.33	74,74,74,74	0
3	CA	CP	301	1/1	0.94	0.12	-1.38	71,71,71,71	0
3	CA	Do	301	1/1	0.90	0.10	-1.39	87,87,87,87	0
3	CA	B5	301	1/1	0.95	0.10	-1.39	95,95,95,95	0
3	CA	Cy	301	1/1	0.94	0.08	-1.45	78,78,78,78	0
3	CA	HZ	301	1/1	0.92	0.11	-1.46	88,88,88,88	0
3	CA	Jt	301	1/1	0.81	0.11	-1.46	154,154,154,154	0
3	CA	Hg	301	1/1	0.94	0.07	-1.46	102,102,102,102	0
3	CA	Ht	301	1/1	0.78	0.11	-1.46	88,88,88,88	0
3	CA	GZ	301	1/1	0.94	0.12	-1.46	104,104,104,104	0
3	CA	DK	301	1/1	0.95	0.10	-1.49	101,101,101,101	0
3	CA	G4	301	1/1	0.90	0.07	-1.51	109,109,109,109	0
3	CA	At	301	1/1	0.87	0.09	-1.51	99,99,99,99	0
3	CA	IR	301	1/1	0.80	0.10	-1.54	119,119,119,119	0
3	CA	FP	301	1/1	0.98	0.13	-1.54	80,80,80,80	0
3	CA	Co	301	1/1	0.96	0.09	-1.55	86,86,86,86	0
3	CA	FU	301	1/1	0.96	0.11	-1.56	91,91,91,91	0
3	CA	DZ	301	1/1	0.92	0.12	-1.57	68,68,68,68	0
3	CA	HF	301	1/1	0.92	0.11	-1.59	101,101,101,101	0
3	CA	GA	301	1/1	0.96	0.07	-1.59	90,90,90,90	0
3	CA	AU	301	1/1	0.96	0.11	-1.60	102,102,102,102	0
3	CA	AA	301	1/1	0.96	0.12	-1.61	75,75,75,75	0
3	CA	Hj	301	1/1	0.95	0.12	-1.61	104,104,104,104	0
3	CA	By	301	1/1	0.92	0.11	-1.67	90,90,90,90	0
3	CA	Dj	301	1/1	0.94	0.11	-1.72	86,86,86,86	0
3	CA	IF	301	1/1	0.91	0.12	-1.74	111,111,111,111	0
3	CA	Jy	301	1/1	0.89	0.08	-1.75	123,123,123,123	0
3	CA	I1	301	1/1	0.93	0.07	-1.76	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	CA	JL	301	1/1	0.73	0.11	-1.80	141,141,141,141	0
3	CA	F1	301	1/1	0.83	0.10	-1.84	102,102,102,102	0
3	CA	Ek	301	1/1	0.97	0.10	-1.85	74,74,74,74	0
3	CA	JZ	301	1/1	0.95	0.10	-1.88	109,109,109,109	0
3	CA	AF	301	1/1	0.88	0.11	-1.90	92,92,92,92	0
3	CA	H4	301	1/1	0.89	0.11	-1.97	115,115,115,115	0
3	CA	BQ	301	1/1	0.93	0.10	-1.97	93,93,93,93	0
3	CA	Bt	301	1/1	0.83	0.08	-1.99	90,90,90,90	0
3	CA	CZ	301	1/1	0.96	0.07	-2.00	84,84,84,84	0
3	CA	FZ	301	1/1	0.90	0.07	-2.00	106,106,106,106	0
3	CA	A1	301	1/1	0.90	0.09	-2.08	106,106,106,106	0
3	CA	EF	301	1/1	0.97	0.10	-2.12	112,112,112,112	0
3	CA	Fe	301	1/1	0.90	0.09	-2.13	123,123,123,123	0
3	CA	AP	301	1/1	0.90	0.09	-2.14	81,81,81,81	0
3	CA	FF	301	1/1	0.95	0.09	-2.16	100,100,100,100	0
3	CA	Et	301	1/1	0.96	0.07	-2.22	71,71,71,71	0
3	CA	Jo	301	1/1	0.88	0.11	-2.22	105,105,105,105	0
3	CA	It	301	1/1	0.93	0.07	-2.24	102,102,102,102	0
3	CA	EZ	301	1/1	0.92	0.08	-2.26	88,88,88,88	0
3	CA	IU	301	1/1	0.91	0.09	-2.47	88,88,88,88	0
3	CA	Fk	301	1/1	0.91	0.09	-2.49	96,96,96,96	0
3	CA	HK	301	1/1	0.94	0.08	-2.49	88,88,88,88	0
3	CA	JF	301	1/1	0.74	0.09	-2.55	103,103,103,103	0
3	CA	Gt	301	1/1	0.91	0.09	-2.55	92,92,92,92	0
3	CA	GU	301	1/1	0.94	0.09	-2.55	84,84,84,84	0
3	CA	Ao	301	1/1	0.95	0.05	-2.58	93,93,93,93	0
3	CA	Ft	301	1/1	0.93	0.05	-2.59	88,88,88,88	0
3	CA	GP	301	1/1	0.94	0.04	-2.60	91,91,91,91	0
3	CA	Bk	301	1/1	0.97	0.07	-2.60	90,90,90,90	0
3	CA	BU	301	1/1	0.92	0.07	-2.65	110,110,110,110	0
3	CA	HU	301	1/1	0.96	0.09	-2.67	78,78,78,78	0
3	CA	Gj	301	1/1	0.94	0.09	-2.74	126,126,126,126	0
3	CA	F4	301	1/1	0.94	0.06	-2.76	95,95,95,95	0
3	CA	Be	301	1/1	0.94	0.09	-2.80	53,53,53,53	0
3	CA	DP	301	1/1	0.94	0.08	-2.84	67,67,67,67	0
3	CA	Dt	301	1/1	0.94	0.08	-2.87	76,76,76,76	0
3	CA	Go	301	1/1	0.94	0.07	-2.93	102,102,102,102	0
3	CA	Aj	301	1/1	0.96	0.09	-3.02	70,70,70,70	0
3	CA	J4	301	1/1	0.88	0.07	-3.07	110,110,110,110	0
3	CA	DA	301	1/1	0.98	0.09	-3.08	67,67,67,67	0
3	CA	BF	301	1/1	0.98	0.05	-3.22	88,88,88,88	0
3	CA	CU	301	1/1	0.87	0.07	-3.25	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	CA	DF	301	1/1	0.96	0.05	-3.28	94,94,94,94	0
3	CA	Cj	301	1/1	0.96	0.07	-3.33	87,87,87,87	0
3	CA	Df	301	1/1	0.96	0.05	-3.43	74,74,74,74	0
3	CA	GK	301	1/1	0.97	0.04	-3.65	97,97,97,97	0
3	CA	HA	301	1/1	0.94	0.07	-3.65	93,93,93,93	0
3	CA	CA	301	1/1	0.95	0.04	-3.79	93,93,93,93	0
3	CA	Fo	301	1/1	0.96	0.07	-3.83	96,96,96,96	0
3	CA	CG	301	1/1	0.95	0.07	-4.83	79,79,79,79	0
3	CA	Io	301	1/1	0.81	0.09	-4.95	85,85,85,85	0
3	CA	CK	301	1/1	0.95	0.09	-5.00	105,105,105,105	0
3	CA	JU	301	1/1	0.89	0.10	-5.12	100,100,100,100	0

5.5 Other polymers ⓘ

There are no such residues in this entry.