



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 6, 2021 – 02:31 PM EST

PDB ID : 7M2T
Title : Crystallographic Structure of the Monoclinic Form of Satellite Tobacco Mosaic Virus
Authors : McPherson, A.
Deposited on : 2021-03-17
Resolution : 2.71 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.24

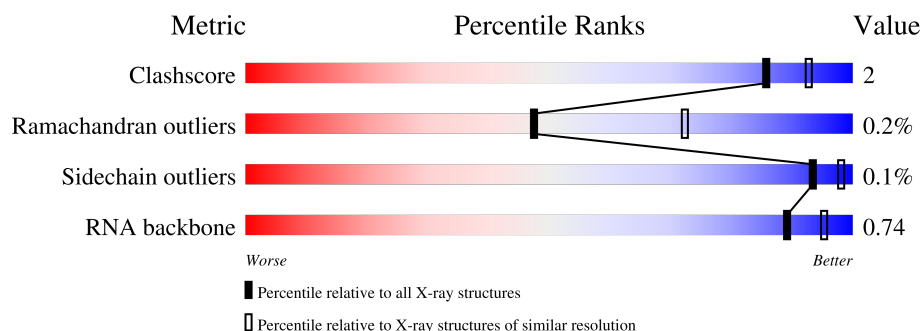
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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))
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RNA backbone	3102	1067 (3.00-2.44)











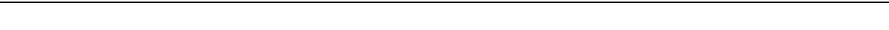

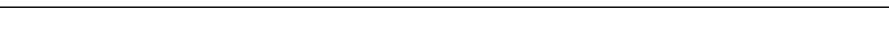
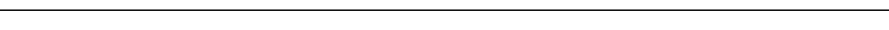











The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	159	
1	B	159	
1	BB	159	
1	C	159	
1	CC	159	
1	D	159	


























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Mol	Chain	Length	Quality of chain
1	DD	159	 87% 0% 9%
1	E	159	 86% 0% 9%
1	EE	159	 89% 0% 9%
1	F	159	 85% 6% 9%
1	FF	159	 85% 6% 9%
1	G	159	 87% 0% 9%
1	GG	159	 88% 0% 9%
1	H	159	 87% 0% 9%
1	HH	159	 86% 5% 9%
1	I	159	 87% 0% 9%
1	II	159	 87% 0% 9%
1	J	159	 87% 0% 9%
1	JJ	159	 84% 7% 9%
1	K	159	 87% 0% 9%
1	KK	159	 87% 0% 9%
1	L	159	 86% 0% 9%
1	LL	159	 87% 0% 9%
1	M	159	 89% 0% 9%
1	MM	159	 86% 0% 9%
1	N	159	 87% 0% 9%
1	NN	159	 89% 0% 9%
1	O	159	 86% 5% 9%
1	OO	159	 86% 5% 9%
1	PP	159	 89% 0% 9%
2	P	12	 75% 8% 17%














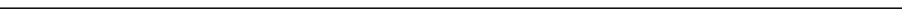











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Mol	Chain	Length	Quality of chain
2	Q	12	
2	QQ	12	
2	R	12	
2	RR	12	
2	S	12	
2	SS	12	
2	T	12	
2	TT	12	
2	U	12	
2	UU	12	
2	V	12	
2	VV	12	
2	W	12	
2	WW	12	
2	X	12	
2	Y	12	
2	YY	12	
2	Z	12	
2	ZZ	12	
2	a	12	
2	b	12	
2	bb	12	
2	c	12	
2	cc	12	
2	d	12	











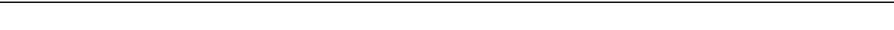

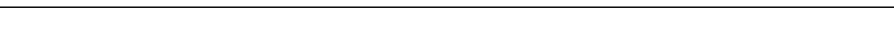
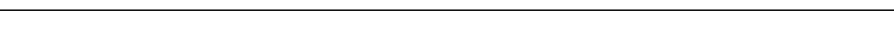











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Mol	Chain	Length	Quality of chain
2	dd	12	 67% 17% 17%
2	ee	12	 67% 17% 17%
2	ff	12	 75% 8% 17%
2	gg	12	 75% 8% 17%
3	1	27	 93%
3	2	27	 93%
3	3	27	 93%
3	4	27	 93%
3	5	27	 93%
3	6	27	 93%
3	7	27	 67% 15% 19%
3	8	27	 93%
3	e	27	 30% 7% 63%
3	f	27	 30% 7% 63%
3	g	27	 30% 7% 63%
3	h	27	 30% 7% 63%
3	hh	27	 30% 7% 63%
3	i	27	 30% 7% 63%
3	ii	27	 30% 7% 63%
3	j	27	 30% 7% 63%
3	jj	27	 30% 7% 63%
3	k	27	 30% 7% 63%
3	kk	27	 30% 7% 63%
3	l	27	 30% 7% 63%
3	ll	27	 30% 7% 63%




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Mol	Chain	Length	Quality of chain
3	m	27	 30% 7% 63%
3	mm	27	 30% 7% 63%
3	n	27	 30% 7% 63%
3	nn	27	 30% 7% 63%
3	o	27	 30% 7% 63%
3	oo	27	 30% 7% 63%
3	p	27	 30% 7% 63%
3	pp	27	 30% 7% 63%
3	q	27	 30% 7% 63%
3	qq	27	 30% 7% 63%
3	r	27	 30% 7% 63%
3	rr	27	 30% 7% 63%
3	s	27	 30% 7% 63%
3	ss	27	 26% 74%
3	t	27	 93%
3	tt	27	 30% 7% 63%
3	u	27	 93%
3	uu	27	 30% 7% 63%
3	v	27	 93%
3	vv	27	 30% 7% 63%
3	w	27	 93%
3	ww	27	 93%
3	x	27	 93%
3	xx	27	 93%
3	y	27	 93%

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Mol	Chain	Length	Quality of chain
3	yy	27	 93%
3	z	27	 93%
3	zz	27	 93%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 49909 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Coat protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	144	Total	C	N	O	S	0	12	0
			1118	703	199	210	6			
1	B	144	Total	C	N	O	S	0	10	0
			1118	703	199	210	6			
1	C	144	Total	C	N	O	S	0	13	0
			1118	703	199	210	6			
1	D	144	Total	C	N	O	S	0	14	0
			1118	703	199	210	6			
1	E	144	Total	C	N	O	S	0	11	0
			1118	703	199	210	6			
1	F	144	Total	C	N	O	S	0	11	0
			1118	703	199	210	6			
1	G	144	Total	C	N	O	S	0	11	0
			1126	708	202	210	6			
1	H	144	Total	C	N	O	S	0	12	0
			1118	703	199	210	6			
1	I	144	Total	C	N	O	S	0	10	0
			1118	703	199	210	6			
1	J	144	Total	C	N	O	S	0	11	0
			1118	703	199	210	6			
1	K	144	Total	C	N	O	S	0	12	0
			1126	708	202	210	6			
1	L	144	Total	C	N	O	S	0	11	0
			1126	708	202	210	6			
1	M	144	Total	C	N	O	S	0	10	0
			1126	708	202	210	6			
1	N	144	Total	C	N	O	S	0	11	0
			1118	703	199	210	6			
1	O	144	Total	C	N	O	S	0	12	0
			1126	708	202	210	6			
1	BB	144	Total	C	N	O	S	0	19	0
			1118	703	199	210	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	CC	144	Total	C	N	O	S	0	17	0
			1118	703	199	210	6			
1	DD	144	Total	C	N	O	S	0	19	0
			1126	708	202	210	6			
1	EE	144	Total	C	N	O	S	0	22	0
			1118	703	199	210	6			
1	FF	144	Total	C	N	O	S	0	19	0
			1118	703	199	210	6			
1	GG	144	Total	C	N	O	S	0	11	0
			1118	703	199	210	6			
1	HH	144	Total	C	N	O	S	0	11	0
			1118	703	199	210	6			
1	II	144	Total	C	N	O	S	0	12	0
			1118	703	199	210	6			
1	JJ	144	Total	C	N	O	S	0	11	0
			1118	703	199	210	6			
1	KK	144	Total	C	N	O	S	0	11	0
			1118	703	199	210	6			
1	LL	144	Total	C	N	O	S	0	12	0
			1126	708	202	210	6			
1	MM	144	Total	C	N	O	S	0	11	0
			1126	708	202	210	6			
1	NN	144	Total	C	N	O	S	0	10	0
			1126	708	202	210	6			
1	OO	144	Total	C	N	O	S	0	11	0
			1118	703	199	210	6			
1	PP	144	Total	C	N	O	S	0	12	0
			1118	703	199	210	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	10	Total	C	N	O	P	0	10	0
			221	100	50	61	10			
2	Q	10	Total	C	N	O	P	0	10	0
			221	100	50	61	10			
2	R	10	Total	C	N	O	P	0	10	0
			221	100	50	61	10			
2	S	10	Total	C	N	O	P	0	10	0
			221	100	50	61	10			
2	T	10	Total	C	N	O	P	0	10	0
			221	100	50	61	10			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	U	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
2	V	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
2	W	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
2	X	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
2	Y	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
2	Z	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
2	a	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
2	b	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
2	c	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
2	d	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
2	QQ	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
2	RR	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
2	SS	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
2	TT	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
2	UU	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
2	VV	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
2	WW	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
2	YY	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
2	ZZ	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
2	bb	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
2	cc	10	Total 221	C 100	N 50	O 61	P 10	0	10	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	dd	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
2	ee	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
2	ff	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
2	gg	10	Total 221	C 100	N 50	O 61	P 10	0	10	0

- Molecule 3 is a RNA chain called RNA (27-mer).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	e	10	Total 201	C 90	N 20	O 81	P 10	0	10	0
3	f	10	Total 201	C 90	N 20	O 81	P 10	0	10	0
3	g	10	Total 201	C 90	N 20	O 81	P 10	0	10	0
3	h	10	Total 201	C 90	N 20	O 81	P 10	0	10	0
3	i	10	Total 201	C 90	N 20	O 81	P 10	0	10	0
3	j	10	Total 201	C 90	N 20	O 81	P 10	0	10	0
3	k	10	Total 201	C 90	N 20	O 81	P 10	0	10	0
3	l	10	Total 201	C 90	N 20	O 81	P 10	0	10	0
3	m	10	Total 201	C 90	N 20	O 81	P 10	0	10	0
3	n	10	Total 201	C 90	N 20	O 81	P 10	0	10	0
3	o	10	Total 201	C 90	N 20	O 81	P 10	0	10	0
3	p	10	Total 201	C 90	N 20	O 81	P 10	0	10	0
3	q	10	Total 201	C 90	N 20	O 81	P 10	0	10	0
3	r	10	Total 201	C 90	N 20	O 81	P 10	0	10	0
3	s	10	Total 201	C 90	N 20	O 81	P 10	0	10	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	t	2	Total 26	C 10	N 2	O 12	P 2	0	2	0
3	u	2	Total 26	C 10	N 2	O 12	P 2	0	2	0
3	v	2	Total 26	C 10	N 2	O 12	P 2	0	2	0
3	w	2	Total 26	C 10	N 2	O 12	P 2	0	2	0
3	x	2	Total 26	C 10	N 2	O 12	P 2	0	2	0
3	y	2	Total 26	C 10	N 2	O 12	P 2	0	2	0
3	z	2	Total 26	C 10	N 2	O 12	P 2	0	2	0
3	1	2	Total 26	C 10	N 2	O 12	P 2	0	2	0
3	2	2	Total 26	C 10	N 2	O 12	P 2	0	2	0
3	3	2	Total 26	C 10	N 2	O 12	P 2	0	2	0
3	4	2	Total 26	C 10	N 2	O 12	P 2	0	2	0
3	5	2	Total 26	C 10	N 2	O 12	P 2	0	2	0
3	6	2	Total 26	C 10	N 2	O 12	P 2	0	2	0
3	7	22	Total 276	C 110	N 22	O 122	P 22	0	22	0
3	8	2	Total 26	C 10	N 2	O 12	P 2	0	2	0
3	hh	10	Total 201	C 90	N 20	O 81	P 10	0	10	0
3	ii	10	Total 201	C 90	N 20	O 81	P 10	0	10	0
3	jj	10	Total 201	C 90	N 20	O 81	P 10	0	10	0
3	kk	10	Total 201	C 90	N 20	O 81	P 10	0	10	0
3	ll	10	Total 201	C 90	N 20	O 81	P 10	0	10	0
3	mm	10	Total 201	C 90	N 20	O 81	P 10	0	10	0

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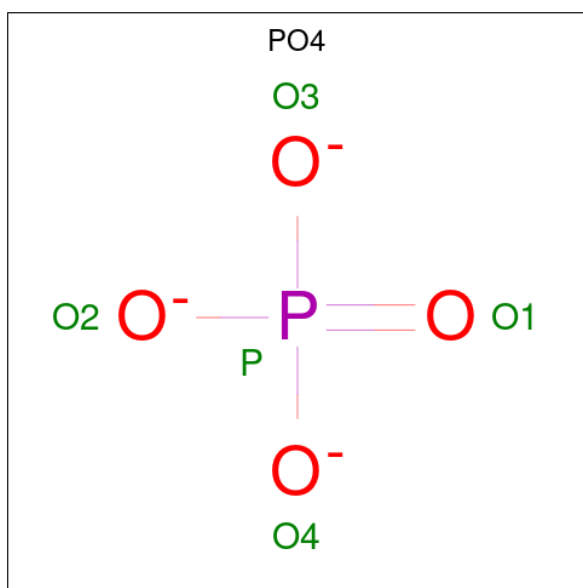
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	nn	10	Total	C	N	O	P	0	10	0
			201	90	20	81	10			
3	oo	10	Total	C	N	O	P	0	10	0
			201	90	20	81	10			
3	pp	10	Total	C	N	O	P	0	10	0
			201	90	20	81	10			
3	qq	10	Total	C	N	O	P	0	10	0
			201	90	20	81	10			
3	rr	10	Total	C	N	O	P	0	10	0
			201	90	20	81	10			
3	ss	7	Total	C	N	O	P	0	7	0
			140	63	14	56	7			
3	tt	10	Total	C	N	O	P	0	10	0
			201	90	20	81	10			
3	uu	10	Total	C	N	O	P	0	10	0
			201	90	20	81	10			
3	vv	10	Total	C	N	O	P	0	10	0
			201	90	20	81	10			
3	ww	2	Total	C	N	O	P	0	2	0
			26	10	2	12	2			
3	xx	2	Total	C	N	O	P	0	2	0
			26	10	2	12	2			
3	yy	2	Total	C	N	O	P	0	2	0
			26	10	2	12	2			
3	zz	2	Total	C	N	O	P	0	2	0
			26	10	2	12	2			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	G	1	Total	Mg	0	0
			1	1		
4	L	1	Total	Mg	0	0
			1	1		
4	EE	1	Total	Mg	0	0
			1	1		
4	JJ	1	Total	Mg	0	0
			1	1		
4	LL	1	Total	Mg	0	0
			1	1		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	1
			21	20	1		
5	G	1	Total	O	P	0	1
			21	20	1		
5	N	1	Total	O	P	0	1
			21	20	1		
5	DD	1	Total	O	P	0	1
			21	20	1		
5	GG	1	Total	O	P	0	1
			21	20	1		
5	LL	1	Total	O	P	0	1
			21	20	1		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	E	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	I	1	Total	O	S	0	0
			5	4	1		
6	FF	1	Total	O	S	0	0
			5	4	1		
6	GG	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	96	Total	O	0	5
			96	96		
7	B	95	Total	O	0	4
			95	95		
7	C	87	Total	O	0	0
			87	87		
7	D	91	Total	O	0	7
			91	91		
7	E	89	Total	O	0	3
			89	89		
7	F	97	Total	O	0	4
			97	97		
7	G	82	Total	O	0	4
			82	82		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	H	93	Total O 93 93	0	4
7	I	85	Total O 85 85	0	4
7	J	89	Total O 89 89	0	2
7	K	82	Total O 82 82	0	4
7	L	83	Total O 83 83	0	6
7	M	93	Total O 93 93	0	5
7	N	91	Total O 91 91	0	0
7	O	93	Total O 93 93	0	8
7	Q	7	Total O 7 7	0	0
7	R	2	Total O 2 2	0	0
7	S	2	Total O 2 2	0	0
7	T	3	Total O 3 3	0	0
7	U	1	Total O 1 1	0	0
7	V	4	Total O 4 4	0	0
7	W	1	Total O 1 1	0	0
7	X	4	Total O 4 4	0	0
7	Y	4	Total O 4 4	0	0
7	Z	3	Total O 3 3	0	0
7	a	5	Total O 5 5	0	0
7	b	4	Total O 4 4	0	0
7	c	3	Total O 3 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	d	2	Total 2	O 2	0	0
7	e	3	Total 3	O 3	0	0
7	f	1	Total 1	O 1	0	0
7	g	1	Total 1	O 1	0	1
7	h	2	Total 2	O 2	0	0
7	i	5	Total 5	O 5	0	0
7	j	3	Total 3	O 3	0	0
7	k	2	Total 2	O 2	0	0
7	l	2	Total 2	O 2	0	0
7	n	4	Total 4	O 4	0	0
7	o	4	Total 4	O 4	0	0
7	p	1	Total 1	O 1	0	0
7	q	1	Total 1	O 1	0	0
7	r	1	Total 1	O 1	0	0
7	s	3	Total 3	O 3	0	0
7	w	1	Total 1	O 1	0	0
7	x	1	Total 1	O 1	0	0
7	7	2	Total 2	O 2	0	0
7	BB	88	Total 88	O 88	0	2
7	CC	102	Total 102	O 102	0	5
7	DD	90	Total 90	O 90	0	2

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	EE	88	Total 88	O 88	0	6
7	FF	87	Total 87	O 87	0	6
7	GG	96	Total 96	O 96	0	6
7	HH	90	Total 90	O 90	0	9
7	II	93	Total 93	O 93	0	6
7	JJ	72	Total 72	O 72	0	3
7	KK	83	Total 83	O 83	0	4
7	LL	83	Total 83	O 83	0	5
7	MM	84	Total 84	O 84	0	6
7	NN	88	Total 88	O 88	0	7
7	OO	92	Total 92	O 92	0	9
7	PP	87	Total 87	O 87	0	8
7	QQ	2	Total 2	O 2	0	0
7	RR	6	Total 6	O 6	0	0
7	SS	4	Total 4	O 4	0	0
7	TT	2	Total 2	O 2	0	0
7	UU	1	Total 1	O 1	0	0
7	WW	1	Total 1	O 1	0	0
7	YY	1	Total 1	O 1	0	0
7	ZZ	4	Total 4	O 4	0	0
7	cc	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	dd	2	Total 2	O 2	0	0
7	ee	1	Total 1	O 1	0	0
7	jj	2	Total 2	O 2	0	1
7	kk	4	Total 4	O 4	0	0
7	ll	3	Total 3	O 3	0	0
7	mm	2	Total 2	O 2	0	0
7	oo	2	Total 2	O 2	0	0
7	pp	2	Total 2	O 2	0	0
7	qq	3	Total 3	O 3	0	0
7	vv	2	Total 2	O 2	0	0

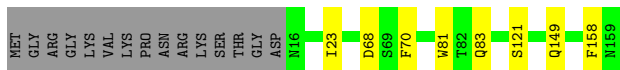
3 Residue-property plots [i](#)

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


Note EDS failed to run properly.

- Molecule 1: Coat protein

Chain A:  86% 5% 9%




- Molecule 1: Coat protein

Chain B:  87% 0% 9%




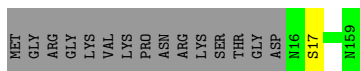
- Molecule 1: Coat protein

Chain C:  86% 0% 9%




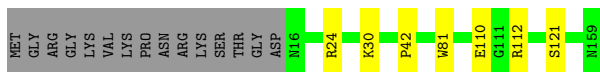
- Molecule 1: Coat protein

Chain D:  90% 0% 9%




- Molecule 1: Coat protein

Chain E:  86% 0% 9%




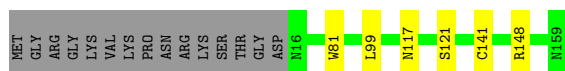
- Molecule 1: Coat protein

Chain F:  85% 6% 9%



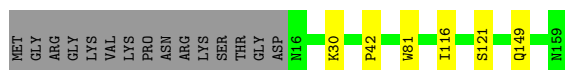
- Molecule 1: Coat protein

Chain G:  87% 0% 9%




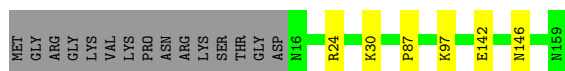
- Molecule 1: Coat protein

Chain H:  87% 0% 9%




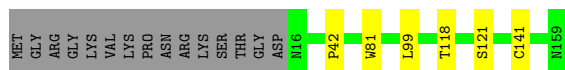
- Molecule 1: Coat protein

Chain I:  87% 0% 9%




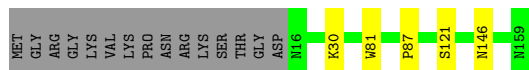
- Molecule 1: Coat protein

Chain J:  87% 0% 9%




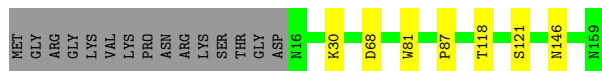
- Molecule 1: Coat protein

Chain K:  87% 0% 9%




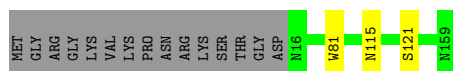
- Molecule 1: Coat protein

Chain L:  86% 0% 9%




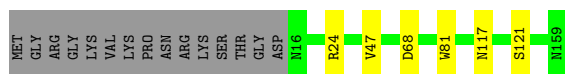
- Molecule 1: Coat protein

Chain M:  89% 9%



- Molecule 1: Coat protein

Chain N:  87% 9%




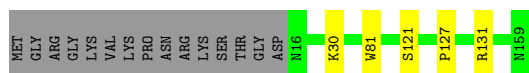
- Molecule 1: Coat protein

Chain O:  86% 5% 9%




- Molecule 1: Coat protein

Chain BB:  87% 9%



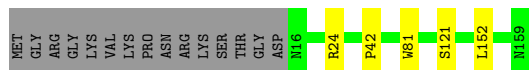
- Molecule 1: Coat protein

Chain CC:  87% 9%



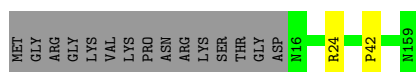
- Molecule 1: Coat protein

Chain DD:  87% 9%




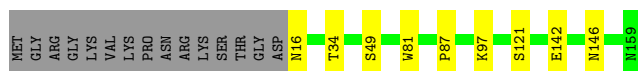
- Molecule 1: Coat protein

Chain EE:  89% 9%



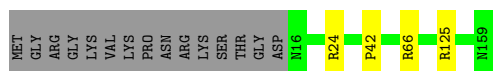
- Molecule 1: Coat protein

Chain FF:  85% 6% 9%




- Molecule 1: Coat protein

Chain GG:  88% 0% 9%




- Molecule 1: Coat protein

Chain HH:  86% 5% 9%




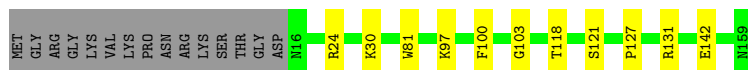
- Molecule 1: Coat protein

Chain II:  87% 0% 9%



- Molecule 1: Coat protein

Chain JJ:  84% 7% 9%




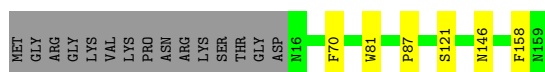
- Molecule 1: Coat protein

Chain KK:  87% 0% 9%



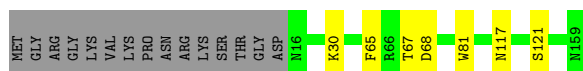
- Molecule 1: Coat protein

Chain LL:  87% 0% 9%



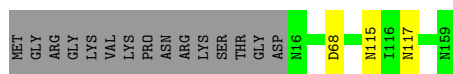
- Molecule 1: Coat protein

Chain MM:  86% 9%



- Molecule 1: Coat protein

Chain NN:  89% 9%



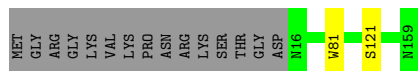
- Molecule 1: Coat protein

Chain OO:  86% 5% 9%



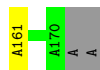
- Molecule 1: Coat protein

Chain PP:  89% 9%



- Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

Chain P:  75% 8% 17%



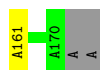
- Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

Chain Q:  42% 42% 17%



- Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

Chain R:  75% 8% 17%




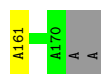
- Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

Chain S:  58% 25% 17%



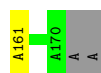
- Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

Chain T:  75% 8% 17%



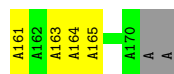
- Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

Chain U:  75% 8% 17%



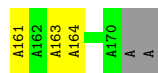
- Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

Chain V:  50% 33% 17%



- Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

Chain W:  58% 25% 17%



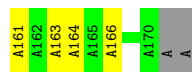
- Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

Chain X:  58% 25% 17%



- Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

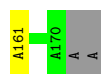
Chain Y:  50% 33% 17%



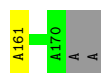
- Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')



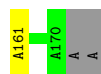
- Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')



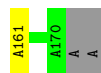
- Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')



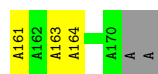
- Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')



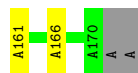
- Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')



- Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')



- Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')



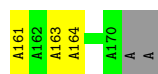
- Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

Chain SS: 



- Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

Chain TT: 



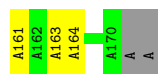
- Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

Chain UU: 



- Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

Chain VV: 



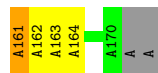
- Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

Chain WW: 



- Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

Chain YY: 




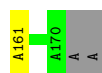
- Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

Chain ZZ: 




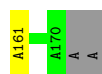
- Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

Chain bb:  75% 8% 17%



- Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

Chain cc:  75% 8% 17%



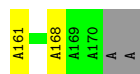
- Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

Chain dd:  67% 17% 17%




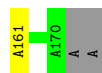
- Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

Chain ee:  67% 17% 17%




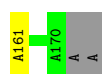
- Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

Chain ff:  75% 8% 17%



- Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

Chain gg:  75% 8% 17%



- Molecule 3: RNA (27-mer)

Chain e:  30% 7% 63%



- Molecule 3: RNA (27-mer)

Chain f:  30% 7% 63%



● Molecule 3: RNA (27-mer)

Chain g:  30% 7% 63%



● Molecule 3: RNA (27-mer)

Chain h:  30% 7% 63%



● Molecule 3: RNA (27-mer)

Chain i:  30% 7% 63%



● Molecule 3: RNA (27-mer)

Chain j:  30% 7% 63%



● Molecule 3: RNA (27-mer)

Chain k:  30% 7% 63%



● Molecule 3: RNA (27-mer)

Chain l:  30% 7% 63%



● Molecule 3: RNA (27-mer)

Chain m:  30% 7% 63%



● Molecule 3: RNA (27-mer)

Chain n:  30% 7% 63%



● Molecule 3: RNA (27-mer)

Chain o:  30% 7% 63%



● Molecule 3: RNA (27-mer)

Chain p:  30% 7% 63%



● Molecule 3: RNA (27-mer)

Chain q:  30% 7% 63%



● Molecule 3: RNA (27-mer)

Chain r:  30% 7% 63%



● Molecule 3: RNA (27-mer)

Chain s:  30% 7% 63%



● Molecule 3: RNA (27-mer)

Chain t:  93%



- Molecule 3: RNA (27-mer)

Chain u:  93%



- Molecule 3: RNA (27-mer)

Chain v:  93%



- Molecule 3: RNA (27-mer)

Chain w:  93%



- Molecule 3: RNA (27-mer)

Chain x:  93%



- Molecule 3: RNA (27-mer)

Chain y:  93%



- Molecule 3: RNA (27-mer)

Chain z:  93%



- Molecule 3: RNA (27-mer)

Chain 1:  93%



- Molecule 3: RNA (27-mer)

Chain 2: . . 93%



- Molecule 3: RNA (27-mer)

Chain 3: . . 93%



- Molecule 3: RNA (27-mer)

Chain 4: . . 93%



- Molecule 3: RNA (27-mer)

Chain 5: . . 93%



- Molecule 3: RNA (27-mer)

Chain 6: . . 93%



- Molecule 3: RNA (27-mer)

Chain 7: 67% 15% 19%



- Molecule 3: RNA (27-mer)

Chain 8: . . 93%



● Molecule 3: RNA (27-mer)

Chain hh:  30% 7% 63%

● Molecule 3: RNA (27-mer)

Chain ii:  30% 7% 63%

● Molecule 3: RNA (27-mer)

Chain jj:  30% 7% 63%

● Molecule 3: RNA (27-mer)

Chain kk:  30% 7% 63%

● Molecule 3: RNA (27-mer)

Chain ll:  30% 7% 63%

● Molecule 3: RNA (27-mer)

Chain mm:  30% 7% 63%

● Molecule 3: RNA (27-mer)

Chain nn:  30% 7% 63%

● Molecule 3: RNA (27-mer)

Chain oo:  30% 7% 63%

● Molecule 3: RNA (27-mer)

Chain pp:  30% 7% 63%

● Molecule 3: RNA (27-mer)

Chain qq:  30% 7% 63%

● Molecule 3: RNA (27-mer)

Chain rr:  30% 7% 63%

● Molecule 3: RNA (27-mer)

Chain ss:  26% 74%

● Molecule 3: RNA (27-mer)

Chain tt:  30% 7% 63%

● Molecule 3: RNA (27-mer)

Chain uu:  30% 7% 63%

• Molecule 3: RNA (27-mer)

Chain vv:  30% 7% 63%

• Molecule 3: RNA (27-mer)

Chain ww:  93%

• Molecule 3: RNA (27-mer)

Chain xx:  93%

• Molecule 3: RNA (27-mer)

Chain yy:  93%

• Molecule 3: RNA (27-mer)

Chain zz:  93%

4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	175.76Å 169.86Å 244.56Å 90.00° 92.69° 90.00°	Depositor
Resolution (Å)	49.95 – 2.71	Depositor
% Data completeness (in resolution range)	91.8 (49.95-2.71)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.129 , 0.177	Depositor
Wilson B-factor (Å ²)	20.1	Xtriage
Anisotropy	0.057	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.001 for $-1/2^*h+1/2^*k-1/2^*l, -1/2^*h+1/2^*k+1/2^*l, h+k$ 0.001 for $-1/2^*h+1/2^*k+1/2^*l, -1/2^*h+1/2^*k-1/2^*l, -h-k$ 0.001 for $-1/2^*h-1/2^*k+1/2^*l, 1/2^*h+1/2^*k+1/2^*l, -h+k$ 0.001 for $-1/2^*h-1/2^*k-1/2^*l, 1/2^*h+1/2^*k-1/2^*l, h-k$ 0.000 for $k, h, -l$ 0.000 for $-k, -h, -l$ 0.000 for $-1/2^*h-1/2^*k-1/2^*l, -1/2^*h-1/2^*k+1/2^*l, -h+k$ 0.000 for $-1/2^*h+1/2^*k-1/2^*l, 1/2^*h-1/2^*k-1/2^*l, -h-k$ 0.467 for $-1/2^*h+1/2^*k+1/2^*l, 1/2^*h-1/2^*k+1/2^*l, h+k$ 0.468 for $-1/2^*h-1/2^*k+1/2^*l, -1/2^*h-1/2^*k-1/2^*l, h-k$ 0.002 for $h, -k, -l$	Xtriage
Total number of atoms	49909	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, MG, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.27	0/1142	0.55	0/1556
1	B	0.27	0/1142	0.55	0/1556
1	BB	0.27	0/1142	0.55	0/1556
1	C	0.27	0/1142	0.55	0/1556
1	CC	0.27	0/1142	0.55	0/1556
1	D	0.27	0/1142	0.55	0/1556
1	DD	0.27	0/1153	0.56	0/1570
1	E	0.27	0/1142	0.55	0/1556
1	EE	0.27	0/1142	0.55	0/1556
1	F	0.27	0/1142	0.55	0/1556
1	FF	0.27	0/1142	0.55	0/1556
1	G	0.27	0/1153	0.56	0/1570
1	GG	0.27	0/1142	0.55	0/1556
1	H	0.27	0/1142	0.56	0/1556
1	HH	0.27	0/1142	0.55	0/1556
1	I	0.27	0/1142	0.55	0/1556
1	II	0.28	0/1142	0.55	0/1556
1	J	0.27	0/1142	0.55	0/1556
1	JJ	0.27	0/1142	0.55	0/1556
1	K	0.28	0/1153	0.55	0/1570
1	KK	0.27	0/1142	0.55	0/1556
1	L	0.27	0/1153	0.56	0/1570
1	LL	0.27	0/1153	0.55	0/1570
1	M	0.28	0/1153	0.56	0/1570
1	MM	0.28	0/1153	0.55	0/1570
1	N	0.27	0/1142	0.55	0/1556
1	NN	0.28	0/1153	0.56	0/1570
1	O	0.27	0/1153	0.56	0/1570
1	OO	0.27	0/1142	0.55	0/1556
1	PP	0.27	0/1142	0.55	0/1556
2	P	0.69	1/250 (0.4%)	0.68	0/386
2	Q	0.72	1/250 (0.4%)	0.82	0/386

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	QQ	0.69	1/250 (0.4%)	0.67	0/386
2	R	0.69	1/250 (0.4%)	0.65	0/386
2	RR	0.71	1/250 (0.4%)	0.74	0/386
2	S	0.68	1/250 (0.4%)	0.67	0/386
2	SS	0.69	1/250 (0.4%)	0.68	0/386
2	T	0.68	1/250 (0.4%)	0.65	0/386
2	TT	0.69	1/250 (0.4%)	0.68	0/386
2	U	0.69	1/250 (0.4%)	0.67	0/386
2	UU	0.68	1/250 (0.4%)	0.67	0/386
2	V	0.74	1/250 (0.4%)	0.85	0/386
2	VV	0.69	1/250 (0.4%)	0.68	0/386
2	W	0.69	1/250 (0.4%)	0.66	0/386
2	WW	0.72	1/250 (0.4%)	0.82	0/386
2	X	0.69	1/250 (0.4%)	0.67	0/386
2	Y	0.68	1/250 (0.4%)	0.67	0/386
2	YY	0.69	1/250 (0.4%)	0.68	0/386
2	Z	0.69	1/250 (0.4%)	0.68	0/386
2	ZZ	0.69	1/250 (0.4%)	0.67	0/386
2	a	0.72	1/250 (0.4%)	0.81	0/386
2	b	0.69	1/250 (0.4%)	0.66	0/386
2	bb	0.69	1/250 (0.4%)	0.67	0/386
2	c	0.69	1/250 (0.4%)	0.65	0/386
2	cc	0.69	1/250 (0.4%)	0.66	0/386
2	d	0.69	1/250 (0.4%)	0.69	0/386
2	dd	0.72	1/250 (0.4%)	0.78	0/386
2	ee	0.68	1/250 (0.4%)	0.68	0/386
2	ff	0.69	1/250 (0.4%)	0.67	0/386
2	gg	0.69	1/250 (0.4%)	0.67	0/386
3	1	2.08	1/27 (3.7%)	0.71	0/38
3	2	2.09	1/27 (3.7%)	0.68	0/38
3	3	2.10	1/27 (3.7%)	0.80	0/38
3	4	2.09	1/27 (3.7%)	0.72	0/38
3	5	2.08	1/27 (3.7%)	0.70	0/38
3	6	2.10	1/27 (3.7%)	0.68	0/38
3	7	0.65	1/287 (0.3%)	0.73	0/418
3	8	2.08	1/27 (3.7%)	0.81	0/38
3	e	0.73	1/220 (0.5%)	0.72	0/336
3	f	0.72	1/220 (0.5%)	0.69	0/336
3	g	0.72	1/220 (0.5%)	0.70	0/336
3	h	0.72	1/220 (0.5%)	0.72	0/336
3	hh	0.73	1/220 (0.5%)	0.70	0/336
3	i	0.72	1/220 (0.5%)	0.71	0/336
3	ii	0.73	1/220 (0.5%)	0.70	0/336

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	j	0.72	1/220 (0.5%)	0.70	0/336
3	jj	0.73	1/220 (0.5%)	0.71	0/336
3	k	0.73	1/220 (0.5%)	0.70	0/336
3	kk	0.72	1/220 (0.5%)	0.72	0/336
3	l	0.72	1/220 (0.5%)	0.71	0/336
3	ll	0.72	1/220 (0.5%)	0.71	0/336
3	m	0.73	1/220 (0.5%)	0.70	0/336
3	mm	0.72	1/220 (0.5%)	0.71	0/336
3	n	0.72	1/220 (0.5%)	0.71	0/336
3	nn	0.72	1/220 (0.5%)	0.72	0/336
3	o	0.72	1/220 (0.5%)	0.71	0/336
3	oo	0.73	1/220 (0.5%)	0.71	0/336
3	p	0.72	1/220 (0.5%)	0.69	0/336
3	pp	0.72	1/220 (0.5%)	0.70	0/336
3	q	0.72	1/220 (0.5%)	0.70	0/336
3	qq	0.72	1/220 (0.5%)	0.72	0/336
3	r	0.72	1/220 (0.5%)	0.71	0/336
3	rr	0.72	1/220 (0.5%)	0.70	0/336
3	s	0.72	1/220 (0.5%)	0.73	0/336
3	ss	0.13	0/153	0.72	0/234
3	t	2.09	1/27 (3.7%)	0.75	0/38
3	tt	0.72	1/220 (0.5%)	0.70	0/336
3	u	2.09	1/27 (3.7%)	0.82	0/38
3	uu	0.72	1/220 (0.5%)	0.72	0/336
3	v	2.10	1/27 (3.7%)	0.63	0/38
3	vv	0.72	1/220 (0.5%)	0.72	0/336
3	w	2.09	1/27 (3.7%)	0.75	0/38
3	ww	2.09	1/27 (3.7%)	0.82	0/38
3	x	2.07	1/27 (3.7%)	0.70	0/38
3	xx	2.08	1/27 (3.7%)	0.77	0/38
3	y	2.08	1/27 (3.7%)	0.70	0/38
3	yy	2.09	1/27 (3.7%)	0.71	0/38
3	z	2.08	1/27 (3.7%)	0.76	0/38
3	zz	2.11	1/27 (3.7%)	0.68	0/38
All	All	0.49	78/49165 (0.2%)	0.61	0/69466

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	zz	195[B]	U	OP3-P	-10.93	1.48	1.61
3	v	195[B]	U	OP3-P	-10.87	1.48	1.61
3	6	195[A]	U	OP3-P	-10.86	1.48	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2	195[B]	U	OP3-P	-10.84	1.48	1.61
3	4	195[A]	U	OP3-P	-10.84	1.48	1.61
3	3	195[B]	U	OP3-P	-10.84	1.48	1.61
3	w	195[B]	U	OP3-P	-10.82	1.48	1.61
3	yy	195[A]	U	OP3-P	-10.82	1.48	1.61
3	u	195[A]	U	OP3-P	-10.82	1.48	1.61
3	t	195[B]	U	OP3-P	-10.81	1.48	1.61
3	ww	195[B]	U	OP3-P	-10.81	1.48	1.61
3	5	195[A]	U	OP3-P	-10.80	1.48	1.61
3	xx	195[B]	U	OP3-P	-10.79	1.48	1.61
3	y	195[A]	U	OP3-P	-10.78	1.48	1.61
3	z	195[A]	U	OP3-P	-10.78	1.48	1.61
3	1	195[A]	U	OP3-P	-10.77	1.48	1.61
3	8	195[A]	U	OP3-P	-10.77	1.48	1.61
3	x	195[B]	U	OP3-P	-10.72	1.48	1.61
3	7	195[A]	U	OP3-P	-10.67	1.48	1.61
3	oo	181[B]	U	OP3-P	-10.63	1.48	1.61
3	hh	181[A]	U	OP3-P	-10.62	1.48	1.61
3	m	181[A]	U	OP3-P	-10.61	1.48	1.61
3	k	181[B]	U	OP3-P	-10.60	1.48	1.61
3	e	181[A]	U	OP3-P	-10.59	1.48	1.61
3	ii	181[B]	U	OP3-P	-10.59	1.48	1.61
3	mm	181[B]	U	OP3-P	-10.58	1.48	1.61
3	jj	181[A]	U	OP3-P	-10.57	1.48	1.61
3	r	181[B]	U	OP3-P	-10.57	1.48	1.61
3	g	181[A]	U	OP3-P	-10.56	1.48	1.61
3	l	181[B]	U	OP3-P	-10.56	1.48	1.61
3	q	181[B]	U	OP3-P	-10.55	1.48	1.61
2	gg	161[B]	A	OP3-P	-10.55	1.48	1.61
2	c	161[B]	A	OP3-P	-10.55	1.48	1.61
3	qq	181[A]	U	OP3-P	-10.55	1.48	1.61
3	h	181[A]	U	OP3-P	-10.55	1.48	1.61
2	QQ	161[A]	A	OP3-P	-10.55	1.48	1.61
3	i	181[A]	U	OP3-P	-10.54	1.48	1.61
3	ll	181[A]	U	OP3-P	-10.54	1.48	1.61
3	p	181[B]	U	OP3-P	-10.54	1.48	1.61
3	tt	181[B]	U	OP3-P	-10.54	1.48	1.61
2	X	161[A]	A	OP3-P	-10.54	1.48	1.61
3	uu	181[B]	U	OP3-P	-10.53	1.48	1.61
3	vv	181[B]	U	OP3-P	-10.53	1.48	1.61
2	W	161[B]	A	OP3-P	-10.52	1.48	1.61
2	WW	161[A]	A	OP3-P	-10.52	1.48	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	ZZ	161[A]	A	OP3-P	-10.52	1.48	1.61
2	P	161[A]	A	OP3-P	-10.52	1.48	1.61
3	f	181[B]	U	OP3-P	-10.52	1.48	1.61
3	o	181[B]	U	OP3-P	-10.52	1.48	1.61
2	V	161[A]	A	OP3-P	-10.52	1.48	1.61
2	SS	161[A]	A	OP3-P	-10.52	1.48	1.61
2	YY	161[B]	A	OP3-P	-10.52	1.48	1.61
2	b	161[B]	A	OP3-P	-10.51	1.48	1.61
3	s	181[B]	U	OP3-P	-10.51	1.48	1.61
2	cc	161[B]	A	OP3-P	-10.51	1.48	1.61
3	j	181[B]	U	OP3-P	-10.51	1.48	1.61
2	Z	161[B]	A	OP3-P	-10.51	1.48	1.61
2	U	161[B]	A	OP3-P	-10.50	1.48	1.61
2	Q	161[A]	A	OP3-P	-10.50	1.48	1.61
2	R	161[A]	A	OP3-P	-10.50	1.48	1.61
2	RR	161[A]	A	OP3-P	-10.50	1.48	1.61
2	a	161[A]	A	OP3-P	-10.50	1.48	1.61
2	VV	161[B]	A	OP3-P	-10.50	1.48	1.61
2	ff	161[B]	A	OP3-P	-10.50	1.48	1.61
3	n	181[A]	U	OP3-P	-10.49	1.48	1.61
3	nn	181[B]	U	OP3-P	-10.49	1.48	1.61
2	d	161[B]	A	OP3-P	-10.48	1.48	1.61
2	dd	161[A]	A	OP3-P	-10.48	1.48	1.61
3	rr	181[B]	U	OP3-P	-10.48	1.48	1.61
3	pp	181[A]	U	OP3-P	-10.48	1.48	1.61
2	TT	161[A]	A	OP3-P	-10.47	1.48	1.61
2	bb	161[A]	A	OP3-P	-10.47	1.48	1.61
2	Y	161[A]	A	OP3-P	-10.47	1.48	1.61
2	UU	161[A]	A	OP3-P	-10.47	1.48	1.61
2	S	161[A]	A	OP3-P	-10.47	1.48	1.61
2	T	161[A]	A	OP3-P	-10.46	1.48	1.61
3	kk	181[A]	U	OP3-P	-10.46	1.48	1.61
2	ee	161[B]	A	OP3-P	-10.43	1.48	1.61

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1118	0	1110	5	0
1	B	1118	0	1109	3	0
1	BB	1118	0	1106	3	0
1	C	1118	0	1106	4	0
1	CC	1118	0	1105	4	0
1	D	1118	0	1106	1	0
1	DD	1126	0	1116	2	0
1	E	1118	0	1108	4	0
1	EE	1118	0	1099	1	0
1	F	1118	0	1107	6	0
1	FF	1118	0	1100	6	0
1	G	1126	0	1120	5	0
1	GG	1118	0	1107	3	0
1	H	1118	0	1106	4	0
1	HH	1118	0	1107	7	0
1	I	1118	0	1107	4	0
1	II	1118	0	1106	4	0
1	J	1118	0	1108	3	0
1	JJ	1118	0	1106	7	0
1	K	1126	0	1116	3	0
1	KK	1118	0	1108	4	0
1	L	1126	0	1120	5	0
1	LL	1126	0	1116	3	0
1	M	1126	0	1121	2	0
1	MM	1126	0	1120	5	0
1	N	1118	0	1106	4	0
1	NN	1126	0	1121	3	0
1	O	1126	0	1119	7	0
1	OO	1118	0	1106	7	0
1	PP	1118	0	1106	1	0
2	P	221	0	97	0	0
2	Q	221	0	111	3	0
2	QQ	221	0	96	1	0
2	R	221	0	111	0	0
2	RR	221	0	111	1	0
2	S	221	0	95	1	0
2	SS	221	0	111	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	T	221	0	97	0	0
2	TT	221	0	97	1	0
2	U	221	0	97	0	0
2	UU	221	0	94	2	0
2	V	221	0	97	6	0
2	VV	221	0	96	2	0
2	W	221	0	98	2	0
2	WW	221	0	95	6	0
2	X	221	0	111	1	0
2	Y	221	0	98	1	1
2	YY	221	0	101	2	0
2	Z	221	0	96	1	0
2	ZZ	221	0	111	2	0
2	a	221	0	111	0	0
2	b	221	0	111	0	0
2	bb	221	0	96	0	0
2	c	221	0	111	0	0
2	cc	221	0	97	0	0
2	d	221	0	97	0	0
2	dd	221	0	111	0	1
2	ee	221	0	111	0	1
2	ff	221	0	111	0	0
2	gg	221	0	95	0	0
3	1	26	0	10	0	0
3	2	26	0	10	0	0
3	3	26	0	10	0	0
3	4	26	0	10	0	0
3	5	26	0	10	0	0
3	6	26	0	10	0	0
3	7	276	0	110	5	0
3	8	26	0	10	2	0
3	e	201	0	83	0	0
3	f	201	0	101	0	0
3	g	201	0	101	0	0
3	h	201	0	82	0	0
3	hh	201	0	84	0	0
3	i	201	0	85	0	0
3	ii	201	0	101	0	0
3	j	201	0	86	0	0
3	jj	201	0	101	0	0
3	k	201	0	85	0	0
3	kk	201	0	82	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	l	201	0	85	0	0
3	ll	201	0	83	0	0
3	m	201	0	101	0	0
3	mm	201	0	82	0	0
3	n	201	0	82	0	0
3	nn	201	0	82	0	0
3	o	201	0	82	0	0
3	oo	201	0	83	0	0
3	p	201	0	101	0	0
3	pp	201	0	101	0	0
3	q	201	0	101	0	0
3	qq	201	0	82	0	0
3	r	201	0	101	0	0
3	rr	201	0	82	0	0
3	s	201	0	82	0	0
3	ss	140	0	71	0	0
3	t	26	0	10	0	0
3	tt	201	0	101	0	0
3	u	26	0	10	0	0
3	uu	201	0	101	0	0
3	v	26	0	10	0	0
3	vv	201	0	83	0	0
3	w	26	0	10	0	0
3	ww	26	0	10	0	0
3	x	26	0	10	0	0
3	xx	26	0	10	0	0
3	y	26	0	10	0	0
3	yy	26	0	10	0	0
3	z	26	0	10	0	0
3	zz	26	0	10	0	0
4	A	1	0	0	0	0
4	EE	1	0	0	0	0
4	G	1	0	0	0	0
4	JJ	1	0	0	0	0
4	L	1	0	0	0	0
4	LL	1	0	0	0	0
5	A	21	0	0	0	0
5	DD	21	0	0	0	0
5	G	21	0	0	1	0
5	GG	21	0	0	0	0
5	LL	21	0	0	1	0
5	N	21	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	10	0	0	1	0
6	FF	5	0	0	0	0
6	GG	5	0	0	0	0
6	I	5	0	0	0	1
7	7	2	0	0	0	0
7	A	96	0	0	0	0
7	B	95	0	0	0	0
7	BB	88	0	0	0	0
7	C	87	0	0	0	0
7	CC	102	0	0	1	1
7	D	91	0	0	0	0
7	DD	90	0	0	0	1
7	E	89	0	0	0	0
7	EE	88	0	0	0	0
7	F	97	0	0	0	0
7	FF	87	0	0	2	0
7	G	82	0	0	1	0
7	GG	96	0	0	0	0
7	H	93	0	0	1	0
7	HH	90	0	0	0	0
7	I	85	0	0	0	1
7	II	93	0	0	1	0
7	J	89	0	0	0	0
7	JJ	72	0	0	0	0
7	K	82	0	0	0	0
7	KK	83	0	0	0	0
7	L	83	0	0	0	0
7	LL	83	0	0	0	0
7	M	93	0	0	1	0
7	MM	84	0	0	0	1
7	N	91	0	0	0	0
7	NN	88	0	0	0	1
7	O	93	0	0	0	0
7	OO	92	0	0	2	0
7	PP	87	0	0	0	0
7	Q	7	0	0	0	0
7	QQ	2	0	0	0	0
7	R	2	0	0	0	0
7	RR	6	0	0	1	0
7	S	2	0	0	0	0
7	SS	4	0	0	0	0
7	T	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	TT	2	0	0	0	0
7	U	1	0	0	0	0
7	UU	1	0	0	0	0
7	V	4	0	0	0	0
7	W	1	0	0	0	0
7	WW	1	0	0	0	0
7	X	4	0	0	0	0
7	Y	4	0	0	0	0
7	YY	1	0	0	0	0
7	Z	3	0	0	0	0
7	ZZ	4	0	0	0	0
7	a	5	0	0	0	0
7	b	4	0	0	0	0
7	c	3	0	0	0	0
7	cc	2	0	0	0	0
7	d	2	0	0	0	0
7	dd	2	0	0	0	0
7	e	3	0	0	0	0
7	ee	1	0	0	0	0
7	f	1	0	0	0	0
7	g	1	0	0	0	0
7	h	2	0	0	0	0
7	i	5	0	0	0	0
7	j	3	0	0	0	0
7	jj	2	0	0	0	0
7	k	2	0	0	0	0
7	kk	4	0	0	0	0
7	l	2	0	0	0	0
7	ll	3	0	0	0	0
7	mm	2	0	0	0	0
7	n	4	0	0	0	0
7	o	4	0	0	0	0
7	oo	2	0	0	0	0
7	p	1	0	0	0	1
7	pp	2	0	0	0	0
7	q	1	0	0	0	0
7	qq	3	0	0	0	0
7	r	1	0	0	0	0
7	s	3	0	0	0	0
7	vv	2	0	0	0	0
7	w	1	0	0	0	0
7	x	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	49909	0	39336	130	5

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (130) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CC:16:ASN:OD1	7:CC:201:HOH:O	2.07	0.71
1:G:148:ARG:NH2	7:G:301:HOH:O	2.30	0.64
1:F:24:ARG:HG2	1:II:30:LYS:HG3	1.80	0.62
2:Q:163[A]:A:H2'	2:Q:164[A]:A:H8	1.65	0.62
1:E:24:ARG:HG2	1:K:30:LYS:HG3	1.82	0.60
1:B:30:LYS:HG3	1:N:24:ARG:HG2	1.84	0.59
1:F:81:TRP:CD1	1:F:121:SER:HB3	2.39	0.58
2:W:163[B]:A:H2'	2:W:164[B]:A:H8	1.70	0.57
2:V:165[A]:A:H61	2:WW:165[A]:A:H61	1.51	0.56
1:OO:105[A]:SER:HB2	7:OO:202:HOH:O	2.05	0.56
2:Q:163[A]:A:H2'	2:Q:164[A]:A:C8	2.40	0.55
2:VV:163[B]:A:H2'	2:VV:164[B]:A:H8	1.72	0.54
1:C:24:ARG:HG2	1:JJ:30:LYS:HG3	1.88	0.54
2:UU:163[A]:A:H2'	2:UU:164[A]:A:H8	1.71	0.54
2:RR:166[A]:A:OP1	7:RR:201:HOH:O	2.19	0.53
6:E:202:SO4:O1	1:F:23:ILE:HD13	2.09	0.53
2:YY:163[B]:A:H2'	2:YY:164[B]:A:H8	1.75	0.52
1:NN:68:ASP:OD1	1:NN:68:ASP:N	2.43	0.52
2:ZZ:163[A]:A:H2'	2:ZZ:164[A]:A:H8	1.75	0.52
1:JJ:81:TRP:CD1	1:JJ:121:SER:HB3	2.45	0.51
1:H:30:LYS:HG3	1:GG:24:ARG:HG2	1.91	0.51
1:B:81:TRP:CD1	1:B:121:SER:HB3	2.46	0.51
1:E:30:LYS:HG3	1:HH:24:ARG:HG2	1.91	0.51
1:I:30:LYS:HG3	1:DD:24:ARG:HG2	1.93	0.50
3:7:215[A]:U:H3'	1:OO:125:ARG:HE	1.75	0.50
1:II:83:GLN:HB3	1:II:149:GLN:HB3	1.93	0.50
1:E:81:TRP:CD1	1:E:121:SER:HB3	2.46	0.50
1:O:125:ARG:HE	3:8:195[A]:U:H3'	1.76	0.49
2:Z:163[B]:A:H2'	2:Z:164[B]:A:H8	1.77	0.49
2:WW:163[A]:A:H2'	2:WW:164[A]:A:H8	1.78	0.49
2:V:165[A]:A:N1	2:WW:165[A]:A:N1	2.60	0.49
2:V:163[A]:A:H2'	2:V:164[A]:A:H8	1.77	0.49
1:M:81:TRP:CD1	1:M:121:SER:HB3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:165[A]:A:H61	2:WW:165[A]:A:N6	2.11	0.49
1:LL:81:TRP:CD1	1:LL:121:SER:HB3	2.47	0.48
1:K:81:TRP:CD1	1:K:121:SER:HB3	2.49	0.48
1:FF:81:TRP:CD1	1:FF:121:SER:HB3	2.48	0.48
2:V:165[A]:A:N6	2:WW:165[A]:A:H61	2.11	0.48
1:L:81:TRP:CD1	1:L:121:SER:HB3	2.49	0.48
1:O:81:TRP:CD1	1:O:121:SER:HB3	2.49	0.48
1:C:81:TRP:CD1	1:C:121:SER:HB3	2.49	0.47
1:HH:81:TRP:CD1	1:HH:121:SER:HB3	2.49	0.47
1:MM:81:TRP:CD1	1:MM:121:SER:HB3	2.49	0.47
1:II:24:ARG:NH2	7:II:304:HOH:O	2.47	0.47
2:Q:165[A]:A:H2'	2:Q:166[A]:A:C8	2.50	0.47
1:FF:16:ASN:ND2	7:FF:303:HOH:O	2.46	0.47
2:X:163[A]:A:H2'	2:X:164[A]:A:H8	1.80	0.47
1:N:68:ASP:OD1	1:N:68:ASP:N	2.48	0.47
1:I:87:PRO:HD3	1:I:146:ASN:O	2.15	0.47
1:FF:49[A]:SER:HB3	7:FF:359:HOH:O	2.14	0.47
1:OO:68:ASP:OD1	1:OO:68:ASP:N	2.48	0.46
1:JJ:118:THR:HG22	1:KK:115:ASN:HB2	1.97	0.46
2:W:163[B]:A:H2'	2:W:164[B]:A:C8	2.49	0.46
1:BB:30:LYS:HG3	1:KK:24:ARG:HG2	1.97	0.46
1:HH:95:ARG:HG2	1:HH:110:GLU:HG3	1.98	0.46
1:HH:68:ASP:OD1	1:HH:68:ASP:N	2.49	0.46
2:UU:163[A]:A:H2'	2:UU:164[A]:A:C8	2.50	0.46
2:VV:163[B]:A:H2'	2:VV:164[B]:A:C8	2.50	0.46
1:EE:24:ARG:HG2	1:HH:30:LYS:HG3	1.98	0.46
2:Y:163[A]:A:H2'	2:Y:164[A]:A:H8	1.80	0.45
1:FF:34:THR:HB	1:GG:66:ARG:NH2	2.31	0.45
1:MM:65:PHE:O	1:MM:67:THR:HG23	2.16	0.45
1:II:81:TRP:CD1	1:II:121:SER:HB3	2.51	0.45
1:A:23:ILE:HG21	1:O:79[B]:ARG:HE	1.81	0.45
1:JJ:100:PHE:HB2	1:JJ:103:GLY:O	2.16	0.45
5:LL:201[D]:PO4:O3	1:NN:117:ASN:ND2	2.45	0.45
1:CC:30:LYS:HG3	1:OO:24:ARG:HG2	1.98	0.45
1:A:70:PHE:CD1	1:A:158:PHE:HB3	2.52	0.44
1:PP:81:TRP:CD1	1:PP:121:SER:HB3	2.52	0.44
1:I:24:ARG:HG2	1:L:30:LYS:HG3	1.99	0.44
1:BB:81:TRP:CD1	1:BB:121:SER:HB3	2.52	0.44
1:FF:87:PRO:HD3	1:FF:146:ASN:O	2.17	0.44
1:DD:81:TRP:CD1	1:DD:121:SER:HB3	2.53	0.44
1:OO:81:TRP:CD1	1:OO:121:SER:HB3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:81:TRP:CD1	1:G:121:SER:HB3	2.51	0.43
1:H:81:TRP:CD1	1:H:121:SER:HB3	2.53	0.43
1:N:117:ASN:ND2	5:N:201[E]:PO4:O3	2.45	0.43
1:O:125:ARG:NE	3:8:195[A]:U:H3'	2.32	0.43
2:S:163[A]:A:H2'	2:S:164[A]:A:H8	1.83	0.43
1:J:81:TRP:CD1	1:J:121:SER:HB3	2.53	0.43
1:L:87:PRO:HD3	1:L:146:ASN:O	2.19	0.43
1:O:68:ASP:OD1	1:O:68:ASP:N	2.51	0.43
2:QQ:163[A]:A:H2'	2:QQ:164[A]:A:H8	1.83	0.43
2:YY:161[B]:A:H2'	2:YY:162[B]:A:H8	1.83	0.43
3:7:203[A]:U:H3'	1:GG:125:ARG:HE	1.84	0.43
1:F:30:LYS:HG3	1:O:24:ARG:HG2	2.01	0.43
1:G:117:ASN:ND2	5:G:202[B]:PO4:O3	2.49	0.43
1:I:97:LYS:HB3	1:I:142:GLU:HB2	1.99	0.43
1:KK:68:ASP:N	1:KK:68:ASP:OD1	2.51	0.43
2:ZZ:161[A]:A:H2'	2:ZZ:162[A]:A:H8	1.84	0.43
1:MM:68:ASP:N	1:MM:68:ASP:OD1	2.52	0.42
1:JJ:24:ARG:HG2	1:MM:30:LYS:HG3	2.01	0.42
1:CC:81:TRP:CD1	1:CC:121:SER:HB3	2.54	0.42
2:SS:163[A]:A:H2'	2:SS:164[A]:A:H8	1.83	0.42
1:D:17:SER:HA	2:V:164[A]:A:O2'	2.20	0.42
1:G:99:LEU:HG	1:G:141:CYS:HA	2.00	0.42
3:7:205[A]:U:H3'	1:HH:125:ARG:NE	2.35	0.42
1:JJ:97:LYS:HB3	1:JJ:142:GLU:HB2	2.02	0.42
1:KK:81:TRP:CD1	1:KK:121:SER:HB3	2.55	0.42
2:SS:161[A]:A:H2'	2:SS:162[A]:A:H8	1.84	0.42
1:C:16:ASN:OD1	1:C:17:SER:N	2.50	0.41
1:LL:87:PRO:HD3	1:LL:146:ASN:O	2.20	0.41
1:A:83:GLN:HB3	1:A:149:GLN:HB3	2.01	0.41
1:F:60:LEU:HD21	1:F:154:ILE:HD12	2.02	0.41
1:L:118:THR:HG22	1:M:115:ASN:HB2	2.03	0.41
1:J:99:LEU:HG	1:J:141:CYS:HA	2.03	0.41
1:E:110:GLU:OE2	1:E:112:ARG:NE	2.43	0.41
1:O:99:LEU:HG	1:O:141:CYS:HA	2.03	0.41
1:BB:127:PRO:O	1:BB:131:ARG:HG3	2.20	0.41
1:JJ:127:PRO:O	1:JJ:131:ARG:HG3	2.21	0.41
1:K:87:PRO:HD3	1:K:146:ASN:O	2.21	0.41
1:OO:23:ILE:HG22	7:OO:248:HOH:O	2.20	0.41
1:CC:68:ASP:OD1	1:CC:68:ASP:N	2.50	0.41
2:TT:163[A]:A:H2'	2:TT:164[A]:A:H8	1.86	0.41
2:WW:163[A]:A:H2'	2:WW:164[A]:A:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ASP:OD1	1:A:68:ASP:N	2.53	0.40
1:C:87:PRO:HD3	1:C:146:ASN:O	2.21	0.40
1:F:114:SER:O	1:J:118:THR:HA	2.21	0.40
3:7:205[A]:U:H3'	1:HH:125:ARG:HE	1.87	0.40
3:7:215[A]:U:H3'	1:OO:125:ARG:NE	2.35	0.40
1:FF:97[A]:LYS:HB3	1:FF:142:GLU:HB2	2.03	0.40
1:LL:70:PHE:CD1	1:LL:158:PHE:HB3	2.56	0.40
1:G:117:ASN:HB3	1:H:116:ILE:HG12	2.01	0.40
1:N:81:TRP:CD1	1:N:121:SER:HB3	2.57	0.40
1:B:99:LEU:HG	1:B:141:CYS:HA	2.03	0.40
1:A:81:TRP:CD1	1:A:121:SER:HB3	2.56	0.40
1:H:149:GLN:OE1	7:H:201:HOH:O	2.22	0.40
1:L:68:ASP:OD1	1:L:68:ASP:N	2.54	0.40
1:MM:117:ASN:O	1:NN:115:ASN:HA	2.21	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:201:SO4:O4	7:NN:208:HOH:O[2_555]	2.08	0.12
2:dd:166[A]:A:OP1	7:p:301:HOH:O[2_555]	2.09	0.11
2:Y:166[A]:A:OP1	7:MM:250:HOH:O[2_555]	2.17	0.03
2:ee:168[B]:A:OP1	7:I:301:HOH:O[2_555]	2.18	0.02
7:CC:260:HOH:O	7:DD:356:HOH:O[2_555]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	142/159 (89%)	136 (96%)	6 (4%)	0	100	100
1	B	142/159 (89%)	136 (96%)	5 (4%)	1 (1%)	22	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BB	142/159 (89%)	137 (96%)	5 (4%)	0	100	100
1	C	142/159 (89%)	136 (96%)	6 (4%)	0	100	100
1	CC	142/159 (89%)	136 (96%)	5 (4%)	1 (1%)	22	45
1	D	142/159 (89%)	137 (96%)	5 (4%)	0	100	100
1	DD	143/159 (90%)	139 (97%)	3 (2%)	1 (1%)	22	45
1	E	142/159 (89%)	137 (96%)	4 (3%)	1 (1%)	22	45
1	EE	142/159 (89%)	137 (96%)	4 (3%)	1 (1%)	22	45
1	F	142/159 (89%)	137 (96%)	4 (3%)	1 (1%)	22	45
1	FF	142/159 (89%)	136 (96%)	6 (4%)	0	100	100
1	G	143/159 (90%)	137 (96%)	6 (4%)	0	100	100
1	GG	142/159 (89%)	136 (96%)	5 (4%)	1 (1%)	22	45
1	H	142/159 (89%)	137 (96%)	4 (3%)	1 (1%)	22	45
1	HH	142/159 (89%)	138 (97%)	4 (3%)	0	100	100
1	I	142/159 (89%)	136 (96%)	6 (4%)	0	100	100
1	II	142/159 (89%)	136 (96%)	6 (4%)	0	100	100
1	J	142/159 (89%)	137 (96%)	4 (3%)	1 (1%)	22	45
1	JJ	142/159 (89%)	137 (96%)	5 (4%)	0	100	100
1	K	143/159 (90%)	138 (96%)	5 (4%)	0	100	100
1	KK	142/159 (89%)	137 (96%)	5 (4%)	0	100	100
1	L	143/159 (90%)	138 (96%)	5 (4%)	0	100	100
1	LL	143/159 (90%)	139 (97%)	4 (3%)	0	100	100
1	M	143/159 (90%)	138 (96%)	5 (4%)	0	100	100
1	MM	143/159 (90%)	136 (95%)	7 (5%)	0	100	100
1	N	142/159 (89%)	138 (97%)	4 (3%)	0	100	100
1	NN	143/159 (90%)	139 (97%)	4 (3%)	0	100	100
1	O	143/159 (90%)	138 (96%)	5 (4%)	0	100	100
1	OO	142/159 (89%)	137 (96%)	4 (3%)	1 (1%)	22	45
1	PP	142/159 (89%)	137 (96%)	5 (4%)	0	100	100
All	All	4269/4770 (90%)	4113 (96%)	146 (3%)	10 (0%)	47	72

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	42	PRO
1	E	42	PRO
1	EE	42	PRO
1	F	42	PRO
1	GG	42	PRO
1	H	42	PRO
1	J	42	PRO
1	CC	42	PRO
1	DD	42	PRO
1	OO	42	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	128/140 (91%)	128 (100%)	0	100	100
1	B	128/140 (91%)	128 (100%)	0	100	100
1	BB	128/140 (91%)	128 (100%)	0	100	100
1	C	128/140 (91%)	128 (100%)	0	100	100
1	CC	128/140 (91%)	128 (100%)	0	100	100
1	D	128/140 (91%)	128 (100%)	0	100	100
1	DD	129/140 (92%)	128 (99%)	1 (1%)	81	92
1	E	128/140 (91%)	128 (100%)	0	100	100
1	EE	128/140 (91%)	128 (100%)	0	100	100
1	F	128/140 (91%)	128 (100%)	0	100	100
1	FF	128/140 (91%)	128 (100%)	0	100	100
1	G	129/140 (92%)	129 (100%)	0	100	100
1	GG	128/140 (91%)	128 (100%)	0	100	100
1	H	128/140 (91%)	128 (100%)	0	100	100
1	HH	128/140 (91%)	128 (100%)	0	100	100
1	I	128/140 (91%)	128 (100%)	0	100	100
1	II	128/140 (91%)	128 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	128/140 (91%)	128 (100%)	0	100	100
1	JJ	128/140 (91%)	128 (100%)	0	100	100
1	K	129/140 (92%)	129 (100%)	0	100	100
1	KK	128/140 (91%)	127 (99%)	1 (1%)	81	92
1	L	129/140 (92%)	129 (100%)	0	100	100
1	LL	129/140 (92%)	129 (100%)	0	100	100
1	M	129/140 (92%)	129 (100%)	0	100	100
1	MM	129/140 (92%)	129 (100%)	0	100	100
1	N	128/140 (91%)	127 (99%)	1 (1%)	81	92
1	NN	129/140 (92%)	129 (100%)	0	100	100
1	O	129/140 (92%)	129 (100%)	0	100	100
1	OO	128/140 (91%)	128 (100%)	0	100	100
1	PP	128/140 (91%)	128 (100%)	0	100	100
All	All	3849/4200 (92%)	3846 (100%)	3 (0%)	93	98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	47	VAL
1	DD	152[A]	LEU
1	KK	47	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	P	9/12 (75%)	0	0
2	Q	9/12 (75%)	0	0
2	QQ	9/12 (75%)	0	0
2	R	9/12 (75%)	0	0
2	RR	9/12 (75%)	0	0
2	S	9/12 (75%)	0	0
2	SS	9/12 (75%)	0	0
2	T	9/12 (75%)	0	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	TT	9/12 (75%)	0	0
2	U	9/12 (75%)	0	0
2	UU	9/12 (75%)	0	0
2	V	9/12 (75%)	0	0
2	VV	9/12 (75%)	0	0
2	W	9/12 (75%)	0	0
2	WW	9/12 (75%)	0	0
2	X	9/12 (75%)	0	0
2	Y	9/12 (75%)	0	0
2	YY	9/12 (75%)	0	0
2	Z	9/12 (75%)	0	0
2	ZZ	9/12 (75%)	0	0
2	a	9/12 (75%)	0	0
2	b	9/12 (75%)	0	0
2	bb	9/12 (75%)	0	0
2	c	9/12 (75%)	0	0
2	cc	9/12 (75%)	0	0
2	d	9/12 (75%)	0	0
2	dd	9/12 (75%)	0	0
2	ee	9/12 (75%)	0	0
2	ff	9/12 (75%)	0	0
2	gg	9/12 (75%)	0	0
3	1	0/27	-	-
3	2	0/27	-	-
3	3	0/27	-	-
3	4	0/27	-	-
3	5	0/27	-	-
3	6	0/27	-	-
3	7	0/27	-	-
3	8	0/27	-	-
3	e	9/27 (33%)	1 (11%)	0
3	f	9/27 (33%)	1 (11%)	0
3	g	9/27 (33%)	1 (11%)	0
3	h	9/27 (33%)	1 (11%)	0
3	hh	9/27 (33%)	1 (11%)	0
3	i	9/27 (33%)	1 (11%)	0
3	ii	9/27 (33%)	1 (11%)	0
3	j	9/27 (33%)	1 (11%)	0
3	jj	9/27 (33%)	1 (11%)	0
3	k	9/27 (33%)	1 (11%)	0
3	kk	9/27 (33%)	1 (11%)	0
3	l	9/27 (33%)	1 (11%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	ll	9/27 (33%)	1 (11%)	0
3	m	9/27 (33%)	1 (11%)	0
3	mm	9/27 (33%)	1 (11%)	0
3	n	9/27 (33%)	1 (11%)	0
3	nn	9/27 (33%)	1 (11%)	0
3	o	9/27 (33%)	1 (11%)	0
3	oo	9/27 (33%)	1 (11%)	0
3	p	9/27 (33%)	1 (11%)	0
3	pp	9/27 (33%)	1 (11%)	0
3	q	9/27 (33%)	1 (11%)	0
3	qq	9/27 (33%)	1 (11%)	0
3	r	9/27 (33%)	1 (11%)	0
3	rr	9/27 (33%)	1 (11%)	0
3	s	9/27 (33%)	1 (11%)	0
3	ss	6/27 (22%)	0	0
3	t	0/27	-	-
3	tt	9/27 (33%)	1 (11%)	0
3	u	0/27	-	-
3	uu	9/27 (33%)	1 (11%)	0
3	v	0/27	-	-
3	vv	9/27 (33%)	1 (11%)	0
3	w	0/27	-	-
3	ww	0/27	-	-
3	x	0/27	-	-
3	xx	0/27	-	-
3	y	0/27	-	-
3	yy	0/27	-	-
3	z	0/27	-	-
3	zz	0/27	-	-
All	All	537/1683 (31%)	29 (5%)	0

All (29) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	e	183[A]	U
3	f	183[B]	U
3	g	183[A]	U
3	h	183[A]	U
3	i	183[A]	U
3	j	183[B]	U
3	k	183[B]	U
3	l	183[B]	U

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Mol	Chain	Res	Type
3	m	183[A]	U
3	n	183[A]	U
3	o	183[B]	U
3	p	183[B]	U
3	q	183[B]	U
3	r	183[B]	U
3	s	183[B]	U
3	hh	183[A]	U
3	ii	183[B]	U
3	jj	183[A]	U
3	kk	183[A]	U
3	ll	183[A]	U
3	mm	183[B]	U
3	nn	183[B]	U
3	oo	183[B]	U
3	pp	183[A]	U
3	qq	183[A]	U
3	rr	183[B]	U
3	tt	183[B]	U
3	uu	183[B]	U
3	vv	183[B]	U

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 41 ligands modelled in this entry, 6 are monoatomic - leaving 35 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	PO4	G	202[C]	4	4,4,4	0.98	0	6,6,6	0.42	0
5	PO4	N	201[A]	-	4,4,4	0.98	0	6,6,6	0.44	0
5	PO4	N	201[C]	4	4,4,4	0.97	0	6,6,6	0.44	0
5	PO4	A	202[D]	4	4,4,4	0.99	0	6,6,6	0.43	0
5	PO4	LL	201[B]	4	4,4,4	0.97	0	6,6,6	0.43	0
5	PO4	DD	201[B]	-	4,4,4	0.98	0	6,6,6	0.43	0
6	SO4	FF	201	-	4,4,4	0.15	0	6,6,6	0.05	0
5	PO4	GG	202[B]	-	4,4,4	0.97	0	6,6,6	0.43	0
5	PO4	A	202[A]	4	4,4,4	0.99	0	6,6,6	0.44	0
6	SO4	E	201	-	4,4,4	0.13	0	6,6,6	0.06	0
6	SO4	E	202	-	4,4,4	0.20	0	6,6,6	0.20	0
5	PO4	A	202[C]	4	4,4,4	0.98	0	6,6,6	0.42	0
5	PO4	G	202[E]	-	4,4,4	0.98	0	6,6,6	0.42	0
5	PO4	DD	201[D]	-	4,4,4	0.98	0	6,6,6	0.44	0
5	PO4	LL	201[D]	4	4,4,4	0.97	0	6,6,6	0.42	0
5	PO4	GG	202[D]	-	4,4,4	0.97	0	6,6,6	0.42	0
5	PO4	N	201[E]	-	4,4,4	0.98	0	6,6,6	0.43	0
5	PO4	DD	201[A]	-	4,4,4	0.98	0	6,6,6	0.43	0
5	PO4	N	201[D]	4	4,4,4	0.98	0	6,6,6	0.43	0
5	PO4	LL	201[A]	4	4,4,4	0.98	0	6,6,6	0.43	0
5	PO4	GG	202[A]	-	4,4,4	0.98	0	6,6,6	0.43	0
5	PO4	LL	201[C]	4	4,4,4	0.97	0	6,6,6	0.44	0
5	PO4	DD	201[C]	-	4,4,4	0.97	0	6,6,6	0.41	0
5	PO4	GG	202[C]	-	4,4,4	0.97	0	6,6,6	0.42	0
5	PO4	A	202[E]	4	4,4,4	0.98	0	6,6,6	0.43	0
5	PO4	G	202[B]	-	4,4,4	0.98	0	6,6,6	0.42	0
6	SO4	GG	201	-	4,4,4	0.14	0	6,6,6	0.14	0
5	PO4	N	201[B]	4	4,4,4	0.97	0	6,6,6	0.44	0
5	PO4	LL	201[E]	4	4,4,4	0.98	0	6,6,6	0.42	0
5	PO4	G	202[D]	-	4,4,4	0.98	0	6,6,6	0.43	0
6	SO4	I	201	-	4,4,4	0.13	0	6,6,6	0.17	0
5	PO4	DD	201[E]	-	4,4,4	0.98	0	6,6,6	0.43	0
5	PO4	GG	202[E]	4	4,4,4	0.97	0	6,6,6	0.42	0
5	PO4	A	202[B]	4	4,4,4	0.98	0	6,6,6	0.42	0
5	PO4	G	202[A]	-	4,4,4	0.98	0	6,6,6	0.44	0

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.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	202	SO4	1	0
5	LL	201[D]	PO4	1	0
5	N	201[E]	PO4	1	0
5	G	202[B]	PO4	1	0
6	I	201	SO4	0	1

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

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

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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