



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 26, 2026 – 05:00 AM EDT

PDB ID : 7M2T / pdb_00007m2t
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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

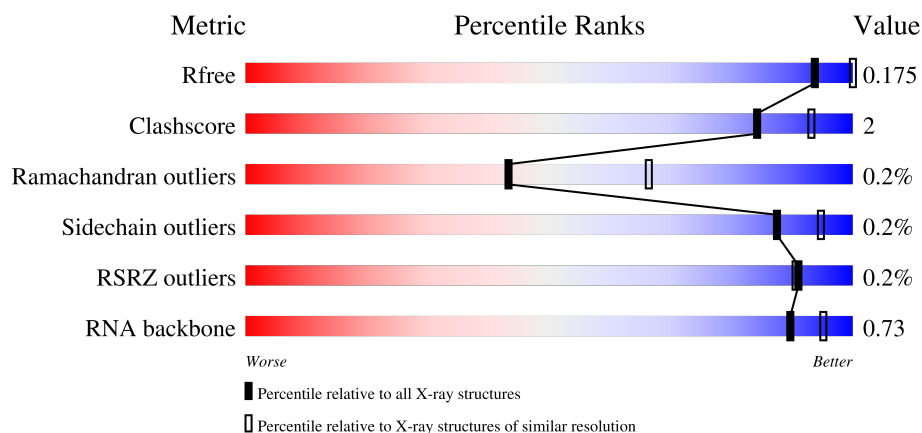
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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))
R_{free}	180053	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)
RNA backbone	3983	1073 (2.94-2.50)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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

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Mol	Chain	Length	Quality of chain
1	E	159	 86% • 9%
1	F	159	 85% 6% 9%
1	G	159	 86% • 9%
1	H	159	 87% • 9%

2 Entry composition [i](#)

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

- 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 221	C 100	N 50	O 61	P 10	0	10	0
2	Q	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
2	R	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
2	S	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
2	T	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	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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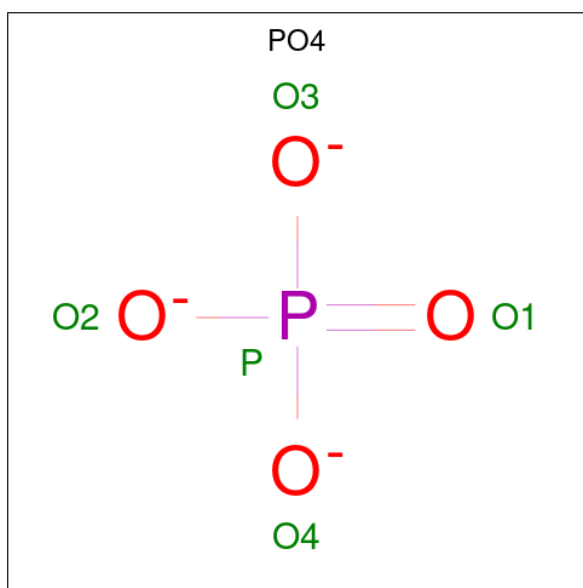
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	nn	10	Total	C	N	O	P	0	10	0
			201	90	20	81	10			
3	oo	10	Total	C	N	O	P	0	10	0
			201	90	20	81	10			
3	pp	10	Total	C	N	O	P	0	10	0
			201	90	20	81	10			
3	qq	10	Total	C	N	O	P	0	10	0
			201	90	20	81	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 (CCD ID: MG) (formula: Mg).

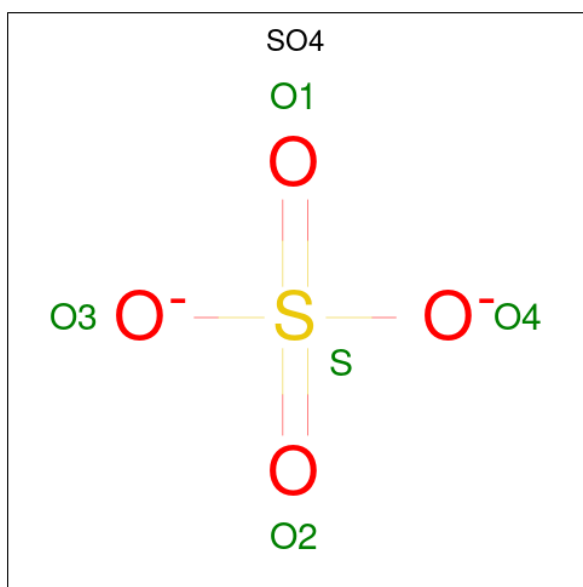
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	G	1	Total	Mg	0	0
			1	1		
4	L	1	Total	Mg	0	0
			1	1		
4	EE	1	Total	Mg	0	0
			1	1		
4	JJ	1	Total	Mg	0	0
			1	1		
4	LL	1	Total	Mg	0	0
			1	1		

- Molecule 5 is PHOSPHATE ION (CCD ID: 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 (CCD ID: 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 93	O 93	0	4
7	I	85	Total 85	O 85	0	4
7	J	89	Total 89	O 89	0	2
7	K	82	Total 82	O 82	0	4
7	L	83	Total 83	O 83	0	6
7	M	93	Total 93	O 93	0	5
7	N	91	Total 91	O 91	0	0
7	O	93	Total 93	O 93	0	8
7	Q	7	Total 7	O 7	0	0
7	R	2	Total 2	O 2	0	0
7	S	2	Total 2	O 2	0	0
7	T	3	Total 3	O 3	0	0
7	U	1	Total 1	O 1	0	0
7	V	4	Total 4	O 4	0	0
7	W	1	Total 1	O 1	0	0
7	X	4	Total 4	O 4	0	0
7	Y	4	Total 4	O 4	0	0
7	Z	3	Total 3	O 3	0	0
7	a	5	Total 5	O 5	0	0
7	b	4	Total 4	O 4	0	0
7	c	3	Total 3	O 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	O	0	0
			2	2		
7	ee	1	Total	O	0	0
			1	1		
7	jj	2	Total	O	0	1
			2	2		
7	kk	4	Total	O	0	0
			4	4		
7	ll	3	Total	O	0	0
			3	3		
7	mm	2	Total	O	0	0
			2	2		
7	oo	2	Total	O	0	0
			2	2		
7	pp	2	Total	O	0	0
			2	2		
7	qq	3	Total	O	0	0
			3	3		
7	vv	2	Total	O	0	0
			2	2		

SEQUENCE-PLOTS INFOmissingINFO

3 Data and refinement statistics

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 49.95 – 2.71	Depositor EDS
% Data completeness (in resolution range)	91.8 (49.95-2.71) 92.2 (49.95-2.71)	Depositor EDS
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 0.129 , 0.175	Depositor DCC
R_{free} test set	8870 reflections (4.54%)	wwPDB-VP
Wilson B-factor (Å ²)	20.1	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 35.7	EDS
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
F_o, F_c correlation	0.96	EDS
Total number of atoms	49909	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

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.

Xtrriage'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.*

4 Model quality

4.1 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	0.14	0/1142	0.33	0/1556
1	B	0.14	0/1142	0.34	0/1556
1	BB	0.14	0/1142	0.33	0/1556
1	C	0.14	0/1142	0.34	0/1556
1	CC	0.14	0/1142	0.34	0/1556
1	D	0.14	0/1142	0.35	0/1556
1	DD	0.14	0/1153	0.35	0/1570
1	E	0.14	0/1142	0.35	0/1556
1	EE	0.14	0/1142	0.35	0/1556
1	F	0.14	0/1142	0.34	0/1556
1	FF	0.14	0/1142	0.34	0/1556
1	G	0.14	0/1153	0.35	0/1570
1	GG	0.13	0/1142	0.34	0/1556
1	H	0.14	0/1142	0.36	0/1556
1	HH	0.14	0/1142	0.33	0/1556
1	I	0.14	0/1142	0.34	0/1556
1	II	0.14	0/1142	0.34	0/1556
1	J	0.14	0/1142	0.33	0/1556
1	JJ	0.13	0/1142	0.35	0/1556
1	K	0.14	0/1153	0.33	0/1570
1	KK	0.14	0/1142	0.33	0/1556
1	L	0.13	0/1153	0.34	0/1570
1	LL	0.14	0/1153	0.35	0/1570
1	M	0.13	0/1153	0.33	0/1570
1	MM	0.14	0/1153	0.33	0/1570
1	N	0.14	0/1142	0.34	0/1556
1	NN	0.14	0/1153	0.34	0/1570
1	O	0.14	0/1153	0.35	0/1570
1	OO	0.15	0/1142	0.36	0/1556
1	PP	0.14	0/1142	0.33	0/1556
2	P	0.09	0/250	0.23	0/386
2	Q	0.12	0/250	0.23	0/386

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	QQ	0.08	0/250	0.23	0/386
2	R	0.09	0/250	0.21	0/386
2	RR	0.10	0/250	0.21	0/386
2	S	0.08	0/250	0.23	0/386
2	SS	0.08	0/250	0.24	0/386
2	T	0.08	0/250	0.22	0/386
2	TT	0.08	0/250	0.22	0/386
2	U	0.08	0/250	0.25	0/386
2	UU	0.08	0/250	0.23	0/386
2	V	0.13	0/250	0.24	0/386
2	VV	0.09	0/250	0.26	0/386
2	W	0.08	0/250	0.23	0/386
2	WW	0.12	0/250	0.23	0/386
2	X	0.08	0/250	0.22	0/386
2	Y	0.08	0/250	0.24	0/386
2	YY	0.08	0/250	0.23	0/386
2	Z	0.09	0/250	0.24	0/386
2	ZZ	0.08	0/250	0.23	0/386
2	a	0.12	0/250	0.22	0/386
2	b	0.09	0/250	0.24	0/386
2	bb	0.08	0/250	0.24	0/386
2	c	0.08	0/250	0.21	0/386
2	cc	0.09	0/250	0.23	0/386
2	d	0.09	0/250	0.26	0/386
2	dd	0.12	0/250	0.22	0/386
2	ee	0.09	0/250	0.27	0/386
2	ff	0.08	0/250	0.23	0/386
2	gg	0.09	0/250	0.24	0/386
3	1	0.10	0/27	0.34	0/38
3	2	0.11	0/27	0.30	0/38
3	3	0.12	0/27	0.35	0/38
3	4	0.11	0/27	0.35	0/38
3	5	0.09	0/27	0.26	0/38
3	6	0.11	0/27	0.33	0/38
3	7	0.11	0/287	0.32	0/418
3	8	0.12	0/27	0.38	0/38
3	e	0.09	0/220	0.19	0/336
3	f	0.08	0/220	0.19	0/336
3	g	0.08	0/220	0.18	0/336
3	h	0.09	0/220	0.20	0/336
3	hh	0.09	0/220	0.19	0/336
3	i	0.09	0/220	0.20	0/336
3	ii	0.09	0/220	0.20	0/336

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	j	0.08	0/220	0.15	0/336
3	jj	0.09	0/220	0.18	0/336
3	k	0.08	0/220	0.17	0/336
3	kk	0.09	0/220	0.20	0/336
3	l	0.08	0/220	0.17	0/336
3	ll	0.09	0/220	0.19	0/336
3	m	0.09	0/220	0.18	0/336
3	mm	0.09	0/220	0.18	0/336
3	n	0.08	0/220	0.17	0/336
3	nn	0.09	0/220	0.19	0/336
3	o	0.09	0/220	0.20	0/336
3	oo	0.08	0/220	0.18	0/336
3	p	0.09	0/220	0.20	0/336
3	pp	0.09	0/220	0.20	0/336
3	q	0.09	0/220	0.18	0/336
3	qq	0.09	0/220	0.19	0/336
3	r	0.08	0/220	0.15	0/336
3	rr	0.09	0/220	0.20	0/336
3	s	0.09	0/220	0.19	0/336
3	ss	0.09	0/153	0.21	0/234
3	t	0.11	0/27	0.37	0/38
3	tt	0.09	0/220	0.17	0/336
3	u	0.12	0/27	0.39	0/38
3	uu	0.09	0/220	0.19	0/336
3	v	0.09	0/27	0.28	0/38
3	vv	0.09	0/220	0.21	0/336
3	w	0.12	0/27	0.31	0/38
3	ww	0.11	0/27	0.38	0/38
3	x	0.10	0/27	0.30	0/38
3	xx	0.11	0/27	0.35	0/38
3	y	0.09	0/27	0.28	0/38
3	yy	0.10	0/27	0.37	0/38
3	z	0.10	0/27	0.34	0/38
3	zz	0.09	0/27	0.30	0/38
All	All	0.13	0/49165	0.31	0/69466

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

4.2 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	4	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	6	0
1	GG	1118	0	1107	4	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	5	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	6	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	2	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	3	0
2	a	221	0	111	3	0
2	b	221	0	111	2	0
2	bb	221	0	96	1	0
2	c	221	0	111	1	0
2	cc	221	0	97	1	0
2	d	221	0	97	1	0
2	dd	221	0	111	0	1
2	ee	221	0	111	2	1
2	ff	221	0	111	1	0
2	gg	221	0	95	1	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	1	0
3	hh	201	0	84	1	0
3	i	201	0	85	0	0
3	ii	201	0	101	0	0
3	j	201	0	86	2	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	1	0
3	mm	201	0	82	0	0
3	n	201	0	82	1	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	3	0
3	q	201	0	101	2	0
3	qq	201	0	82	1	0
3	r	201	0	101	1	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	1	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	2	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	1	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	157	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.

The worst 5 of 157 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
2:a:166[A]:A:OP1	7:a:201:HOH:O	2.11	0.67
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

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

4.3 Torsion angles

4.3.1 Protein backbone

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%)	18	39

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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%)	18	39
1	D	142/159 (89%)	137 (96%)	5 (4%)	0	100	100
1	DD	143/159 (90%)	139 (97%)	3 (2%)	1 (1%)	18	39
1	E	142/159 (89%)	137 (96%)	4 (3%)	1 (1%)	18	39
1	EE	142/159 (89%)	137 (96%)	4 (3%)	1 (1%)	18	39
1	F	142/159 (89%)	137 (96%)	4 (3%)	1 (1%)	18	39
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%)	18	39
1	H	142/159 (89%)	137 (96%)	4 (3%)	1 (1%)	18	39
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%)	18	39
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%)	18	39
1	PP	142/159 (89%)	137 (96%)	5 (4%)	0	100	100
All	All	4269/4770 (90%)	4113 (96%)	146 (3%)	10 (0%)	43	66

5 of 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

4.3.2 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%)	129 (100%)	0	100	100
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%)	127 (99%)	1 (1%)	73	87
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%)	127 (99%)	1 (1%)	73	87
1	J	128/140 (91%)	127 (99%)	1 (1%)	73	87
1	JJ	128/140 (91%)	128 (100%)	0	100	100
1	K	129/140 (92%)	129 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	KK	128/140 (91%)	127 (99%)	1 (1%)	73	87
1	L	129/140 (92%)	129 (100%)	0	100	100
1	LL	129/140 (92%)	128 (99%)	1 (1%)	73	87
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%)	126 (98%)	2 (2%)	55	78
1	NN	129/140 (92%)	129 (100%)	0	100	100
1	O	129/140 (92%)	128 (99%)	1 (1%)	73	87
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%)	3841 (100%)	8 (0%)	87	95

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	LL	128[A]	THR
1	KK	47	VAL
1	FF	128[A]	THR
1	O	134	THR
1	II	47	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	O	18[A]	ASN
1	PP	18[A]	ASN
1	EE	48	GLN
1	LL	132	GLN
1	DD	132	GLN

4.3.3 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

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
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
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

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
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
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

5 of 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

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Mol	Chain	Res	Type
3	i	183[A]	U

There are no RNA pucker outliers to report.

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

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 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	LL	201[E]	4	4,4,4	1.02	0	6,6,6	0.45	0
5	PO4	LL	201[B]	4	4,4,4	1.01	0	6,6,6	0.46	0
5	PO4	N	201[C]	4	4,4,4	1.02	0	6,6,6	0.47	0
5	PO4	LL	201[A]	4	4,4,4	1.02	0	6,6,6	0.46	0
5	PO4	N	201[D]	4	4,4,4	1.03	0	6,6,6	0.46	0
5	PO4	A	202[B]	4	4,4,4	1.03	0	6,6,6	0.45	0
5	PO4	A	202[E]	4	4,4,4	1.02	0	6,6,6	0.46	0
6	SO4	E	202	-	4,4,4	0.27	0	6,6,6	0.15	0
5	PO4	A	202[A]	4	4,4,4	1.03	0	6,6,6	0.47	0
6	SO4	GG	201	-	4,4,4	0.22	0	6,6,6	0.13	0
5	PO4	G	202[E]	-	4,4,4	1.03	0	6,6,6	0.46	0
5	PO4	LL	201[C]	4	4,4,4	1.02	0	6,6,6	0.47	0
5	PO4	G	202[B]	-	4,4,4	1.02	0	6,6,6	0.45	0
5	PO4	GG	202[E]	4	4,4,4	1.01	0	6,6,6	0.46	0
5	PO4	GG	202[B]	-	4,4,4	1.02	0	6,6,6	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PO4	G	202[A]	-	4,4,4	1.03	0	6,6,6	0.47	0
5	PO4	LL	201[D]	4	4,4,4	1.01	0	6,6,6	0.45	0
5	PO4	GG	202[A]	-	4,4,4	1.03	0	6,6,6	0.46	0
5	PO4	DD	201[B]	-	4,4,4	1.02	0	6,6,6	0.47	0
5	PO4	A	202[C]	4	4,4,4	1.02	0	6,6,6	0.45	0
5	PO4	DD	201[E]	-	4,4,4	1.03	0	6,6,6	0.46	0
5	PO4	A	202[D]	4	4,4,4	1.04	0	6,6,6	0.46	0
6	SO4	FF	201	-	4,4,4	0.24	0	6,6,6	0.08	0
5	PO4	DD	201[A]	-	4,4,4	1.02	0	6,6,6	0.46	0
6	SO4	E	201	-	4,4,4	0.23	0	6,6,6	0.08	0
5	PO4	G	202[C]	4	4,4,4	1.02	0	6,6,6	0.46	0
5	PO4	GG	202[C]	-	4,4,4	1.01	0	6,6,6	0.45	0
5	PO4	G	202[D]	-	4,4,4	1.02	0	6,6,6	0.46	0
5	PO4	N	201[B]	4	4,4,4	1.02	0	6,6,6	0.47	0
5	PO4	GG	202[D]	-	4,4,4	1.02	0	6,6,6	0.45	0
5	PO4	N	201[E]	-	4,4,4	1.03	0	6,6,6	0.46	0
6	SO4	I	201	-	4,4,4	0.21	0	6,6,6	0.18	0
5	PO4	DD	201[C]	-	4,4,4	1.02	0	6,6,6	0.44	0
5	PO4	DD	201[D]	-	4,4,4	1.03	0	6,6,6	0.48	0
5	PO4	N	201[A]	-	4,4,4	1.03	0	6,6,6	0.47	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	G	202[B]	PO4	1	0
5	LL	201[D]	PO4	1	0
5	N	201[E]	PO4	1	0
6	I	201	SO4	0	1

4.7 Other polymers ⓘ

There are no such residues in this entry.

4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

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

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

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	A	144/159 (90%)	-1.78	0 100 100	7, 11, 34, 94	0
1	B	144/159 (90%)	-1.80	0 100 100	7, 11, 28, 84	0
1	BB	144/159 (90%)	-1.81	0 100 100	7, 12, 34, 91	0
1	C	144/159 (90%)	-1.79	0 100 100	7, 11, 32, 90	0
1	CC	144/159 (90%)	-1.79	0 100 100	7, 11, 27, 76	0
1	D	144/159 (90%)	-1.79	0 100 100	7, 11, 33, 80	0
1	DD	144/159 (90%)	-1.75	0 100 100	7, 12, 36, 91	1 (0%)
1	E	144/159 (90%)	-1.80	0 100 100	7, 11, 29, 85	0
1	EE	144/159 (90%)	-1.81	0 100 100	7, 11, 26, 76	0
1	F	144/159 (90%)	-1.83	0 100 100	7, 11, 26, 86	0
1	FF	144/159 (90%)	-1.79	0 100 100	7, 11, 34, 84	0
1	G	144/159 (90%)	-1.79	0 100 100	7, 11, 37, 83	1 (0%)
1	GG	144/159 (90%)	-1.83	0 100 100	8, 12, 31, 72	0
1	H	144/159 (90%)	-1.78	0 100 100	7, 11, 27, 81	0
1	HH	144/159 (90%)	-1.80	0 100 100	7, 12, 34, 83	0
1	I	144/159 (90%)	-1.80	0 100 100	7, 11, 35, 86	0
1	II	144/159 (90%)	-1.80	0 100 100	7, 11, 31, 83	0
1	J	144/159 (90%)	-1.80	0 100 100	7, 12, 32, 96	0
1	JJ	144/159 (90%)	-1.79	0 100 100	7, 12, 32, 82	0
1	K	144/159 (90%)	-1.77	0 100 100	7, 11, 31, 90	1 (0%)
1	KK	144/159 (90%)	-1.76	0 100 100	8, 12, 27, 92	0
1	L	144/159 (90%)	-1.82	0 100 100	8, 12, 30, 81	1 (0%)
1	LL	144/159 (90%)	-1.76	0 100 100	8, 12, 31, 88	1 (0%)
1	M	144/159 (90%)	-1.77	0 100 100	8, 13, 29, 75	1 (0%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	MM	144/159 (90%)	-1.81	0 100 100	8, 13, 29, 83	1 (0%)
1	N	144/159 (90%)	-1.79	0 100 100	8, 12, 26, 85	0
1	NN	144/159 (90%)	-1.77	0 100 100	8, 12, 28, 76	1 (0%)
1	O	144/159 (90%)	-1.79	0 100 100	7, 11, 31, 87	1 (0%)
1	OO	144/159 (90%)	-1.80	0 100 100	8, 12, 29, 78	0
1	PP	144/159 (90%)	-1.81	0 100 100	7, 11, 30, 90	0
2	P	10/12 (83%)	-0.02	0 100 100	18, 33, 58, 67	10 (100%)
2	Q	10/12 (83%)	-0.32	0 100 100	16, 33, 62, 62	10 (100%)
2	QQ	10/12 (83%)	0.74	2 (20%) 3 2	12, 20, 56, 69	10 (100%)
2	R	10/12 (83%)	-0.35	0 100 100	16, 34, 58, 60	10 (100%)
2	RR	10/12 (83%)	-0.13	0 100 100	16, 31, 61, 66	10 (100%)
2	S	10/12 (83%)	-0.03	0 100 100	17, 33, 65, 66	10 (100%)
2	SS	10/12 (83%)	-0.35	0 100 100	18, 34, 61, 68	10 (100%)
2	T	10/12 (83%)	0.05	0 100 100	17, 30, 56, 60	10 (100%)
2	TT	10/12 (83%)	-0.20	0 100 100	17, 31, 54, 57	10 (100%)
2	U	10/12 (83%)	0.65	1 (10%) 12 11	17, 25, 57, 68	10 (100%)
2	UU	10/12 (83%)	-0.21	0 100 100	17, 34, 61, 63	10 (100%)
2	V	10/12 (83%)	-0.28	0 100 100	17, 30, 61, 70	10 (100%)
2	VV	10/12 (83%)	0.14	0 100 100	17, 37, 62, 64	10 (100%)
2	W	10/12 (83%)	0.07	0 100 100	17, 33, 57, 63	10 (100%)
2	WW	10/12 (83%)	-0.16	0 100 100	18, 31, 62, 70	10 (100%)
2	X	10/12 (83%)	-0.36	0 100 100	16, 23, 63, 66	10 (100%)
2	Y	10/12 (83%)	0.01	0 100 100	16, 34, 66, 72	10 (100%)
2	YY	10/12 (83%)	-0.05	0 100 100	17, 33, 61, 67	10 (100%)
2	Z	10/12 (83%)	-0.05	0 100 100	16, 33, 58, 62	10 (100%)
2	ZZ	10/12 (83%)	-0.09	0 100 100	16, 34, 65, 68	10 (100%)
2	a	10/12 (83%)	-0.40	0 100 100	17, 29, 57, 63	10 (100%)
2	b	10/12 (83%)	0.11	0 100 100	18, 33, 62, 65	10 (100%)
2	bb	10/12 (83%)	-0.01	0 100 100	18, 31, 60, 67	10 (100%)
2	c	10/12 (83%)	-0.01	1 (10%) 12 11	15, 36, 58, 59	10 (100%)
2	cc	10/12 (83%)	-0.08	0 100 100	17, 38, 63, 64	10 (100%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	d	10/12 (83%)	0.00	0 100 100	17, 34, 66, 67	10 (100%)
2	dd	10/12 (83%)	-0.02	0 100 100	19, 32, 60, 64	10 (100%)
2	ee	10/12 (83%)	0.12	1 (10%) 12 11	17, 36, 65, 67	10 (100%)
2	ff	10/12 (83%)	-0.18	0 100 100	18, 32, 63, 68	10 (100%)
2	gg	10/12 (83%)	0.27	1 (10%) 12 11	16, 33, 62, 64	10 (100%)
3	1	2/27 (7%)	-0.87	0 100 100	25, 25, 25, 41	2 (100%)
3	2	2/27 (7%)	-0.74	0 100 100	29, 29, 29, 42	2 (100%)
3	3	2/27 (7%)	-0.76	0 100 100	31, 31, 31, 42	2 (100%)
3	4	2/27 (7%)	-0.94	0 100 100	28, 28, 28, 38	2 (100%)
3	5	2/27 (7%)	-0.62	0 100 100	35, 35, 35, 38	2 (100%)
3	6	2/27 (7%)	-0.87	0 100 100	28, 28, 28, 41	2 (100%)
3	7	22/27 (81%)	-0.74	0 100 100	21, 34, 45, 47	22 (100%)
3	8	2/27 (7%)	-0.35	0 100 100	28, 28, 28, 39	2 (100%)
3	e	10/27 (37%)	-0.07	0 100 100	16, 34, 63, 66	10 (100%)
3	f	10/27 (37%)	-0.30	0 100 100	17, 35, 63, 65	10 (100%)
3	g	10/27 (37%)	-0.16	0 100 100	15, 37, 57, 60	10 (100%)
3	h	10/27 (37%)	-0.19	0 100 100	16, 32, 59, 69	10 (100%)
3	hh	10/27 (37%)	0.00	0 100 100	16, 32, 61, 66	10 (100%)
3	i	10/27 (37%)	0.51	1 (10%) 12 11	17, 27, 57, 73	10 (100%)
3	ii	10/27 (37%)	-0.14	0 100 100	16, 33, 62, 70	10 (100%)
3	j	10/27 (37%)	-0.02	0 100 100	17, 31, 52, 61	10 (100%)
3	jj	10/27 (37%)	-0.26	0 100 100	18, 32, 61, 67	10 (100%)
3	k	10/27 (37%)	-0.39	0 100 100	18, 33, 60, 66	10 (100%)
3	kk	10/27 (37%)	0.31	0 100 100	17, 34, 59, 68	10 (100%)
3	l	10/27 (37%)	-0.12	0 100 100	17, 31, 56, 61	10 (100%)
3	ll	10/27 (37%)	-0.12	0 100 100	17, 37, 66, 68	10 (100%)
3	m	10/27 (37%)	0.11	1 (10%) 12 11	17, 37, 67, 70	10 (100%)
3	mm	10/27 (37%)	-0.21	0 100 100	16, 35, 60, 64	10 (100%)
3	n	10/27 (37%)	-0.01	0 100 100	16, 35, 59, 63	10 (100%)
3	nn	10/27 (37%)	-0.34	0 100 100	17, 33, 61, 71	10 (100%)
3	o	10/27 (37%)	-0.05	0 100 100	16, 35, 64, 75	10 (100%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
3	oo	10/27 (37%)	-0.28	0	100 100	17, 33, 64, 67 10 (100%)
3	p	10/27 (37%)	-0.07	0	100 100	18, 33, 58, 68 10 (100%)
3	pp	10/27 (37%)	-0.12	0	100 100	18, 32, 61, 69 10 (100%)
3	q	10/27 (37%)	-0.10	0	100 100	16, 38, 65, 74 10 (100%)
3	qq	10/27 (37%)	-0.11	0	100 100	17, 38, 59, 66 10 (100%)
3	r	10/27 (37%)	-0.52	0	100 100	16, 31, 55, 62 10 (100%)
3	rr	10/27 (37%)	-0.15	0	100 100	17, 31, 58, 70 10 (100%)
3	s	10/27 (37%)	-0.18	0	100 100	18, 34, 58, 71 10 (100%)
3	ss	7/27 (25%)	-0.50	0	100 100	17, 21, 49, 62 7 (100%)
3	t	2/27 (7%)	-0.68	0	100 100	28, 28, 28, 39 2 (100%)
3	tt	10/27 (37%)	-0.48	0	100 100	16, 28, 60, 66 10 (100%)
3	u	2/27 (7%)	-0.18	0	100 100	25, 25, 25, 38 2 (100%)
3	uu	10/27 (37%)	-0.47	0	100 100	18, 35, 60, 72 10 (100%)
3	v	2/27 (7%)	-0.96	0	100 100	29, 29, 29, 50 2 (100%)
3	vv	10/27 (37%)	0.83	3 (30%)	1 1	11, 20, 56, 70 10 (100%)
3	w	2/27 (7%)	-0.56	0	100 100	26, 26, 26, 39 2 (100%)
3	ww	2/27 (7%)	-0.71	0	100 100	27, 27, 27, 43 2 (100%)
3	x	2/27 (7%)	-0.27	0	100 100	24, 24, 24, 40 2 (100%)
3	xx	2/27 (7%)	-0.32	0	100 100	29, 29, 29, 41 2 (100%)
3	y	2/27 (7%)	-1.23	0	100 100	24, 24, 24, 40 2 (100%)
3	yy	2/27 (7%)	-1.28	0	100 100	29, 29, 29, 39 2 (100%)
3	z	2/27 (7%)	0.21	0	100 100	28, 28, 28, 39 2 (100%)
3	zz	2/27 (7%)	-0.68	0	100 100	30, 30, 30, 45 2 (100%)
All	All	4975/6453 (77%)	-1.57	11 (0%)	91 90	7, 12, 53, 96 664 (13%)

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	i	190[A]	U	5.0
2	U	170[B]	A	3.6
2	QQ	170[A]	A	3.2
3	vv	190[B]	U	2.8
3	m	183[A]	U	2.6

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 oligosaccharides 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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	LL	202	1/1	0.97	0.08	53,53,53,53	0
4	MG	JJ	201	1/1	0.98	0.05	59,59,59,59	0
4	MG	A	201	1/1	0.98	0.15	76,76,76,76	0
6	SO4	FF	201	5/5	0.98	0.05	87,92,135,185	0
4	MG	G	201	1/1	0.99	0.08	45,45,45,45	0
4	MG	L	201	1/1	0.99	0.10	50,50,50,50	0
6	SO4	E	201	5/5	0.99	0.05	87,118,148,213	0
6	SO4	E	202	5/5	0.99	0.06	74,99,108,168	0
6	SO4	I	201	5/5	0.99	0.13	51,58,99,165	0
4	MG	EE	201	1/1	0.99	0.10	53,53,53,53	0
6	SO4	GG	201	5/5	0.99	0.07	63,101,161,208	0
5	PO4	G	202[A]	5/5	1.00	0.05	6,6,6,6	5
5	PO4	G	202[B]	5/5	1.00	0.05	6,6,6,6	5
5	PO4	G	202[C]	5/5	1.00	0.05	6,6,6,6	5
5	PO4	G	202[D]	5/5	1.00	0.05	6,6,6,6	5
5	PO4	G	202[E]	5/5	1.00	0.05	6,6,6,6	5
5	PO4	N	201[A]	5/5	1.00	0.06	7,7,7,7	5
5	PO4	N	201[B]	5/5	1.00	0.06	7,7,7,7	5
5	PO4	N	201[C]	5/5	1.00	0.06	7,7,7,7	5
5	PO4	N	201[D]	5/5	1.00	0.06	7,7,7,7	5
5	PO4	N	201[E]	5/5	1.00	0.06	7,7,7,7	5
5	PO4	DD	201[A]	5/5	1.00	0.05	7,7,7,7	5
5	PO4	DD	201[B]	5/5	1.00	0.05	7,7,7,7	5
5	PO4	DD	201[C]	5/5	1.00	0.05	7,7,7,7	5
5	PO4	DD	201[D]	5/5	1.00	0.05	7,7,7,7	5
5	PO4	DD	201[E]	5/5	1.00	0.05	7,7,7,7	5
5	PO4	GG	202[A]	5/5	1.00	0.04	7,7,7,7	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	PO4	GG	202[B]	5/5	1.00	0.04	7,7,7,7	5
5	PO4	GG	202[C]	5/5	1.00	0.04	7,7,7,7	5
5	PO4	GG	202[D]	5/5	1.00	0.04	7,7,7,7	5
5	PO4	GG	202[E]	5/5	1.00	0.04	7,7,7,7	5
5	PO4	LL	201[A]	5/5	1.00	0.06	7,7,8,8	5
5	PO4	LL	201[B]	5/5	1.00	0.06	7,7,7,8	5
5	PO4	LL	201[C]	5/5	1.00	0.06	7,7,7,8	5
5	PO4	LL	201[D]	5/5	1.00	0.06	7,7,7,8	5
5	PO4	LL	201[E]	5/5	1.00	0.06	7,7,8,8	5
5	PO4	A	202[A]	5/5	1.00	0.05	6,6,6,6	5
5	PO4	A	202[B]	5/5	1.00	0.05	6,6,6,6	5
5	PO4	A	202[C]	5/5	1.00	0.05	6,6,6,6	5
5	PO4	A	202[D]	5/5	1.00	0.05	6,6,6,6	5
5	PO4	A	202[E]	5/5	1.00	0.05	6,6,6,6	5

5.5 Other polymers [i](#)

There are no such residues in this entry.