



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:44 PM UTC

PDB ID : 7M57 / pdb_00007m57
Title : Crystallographic structure of a primitive orthorhombic crystal form of STMV
Authors : McPherson, A.
Deposited on : 2021-03-22
Resolution : 4.00 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 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

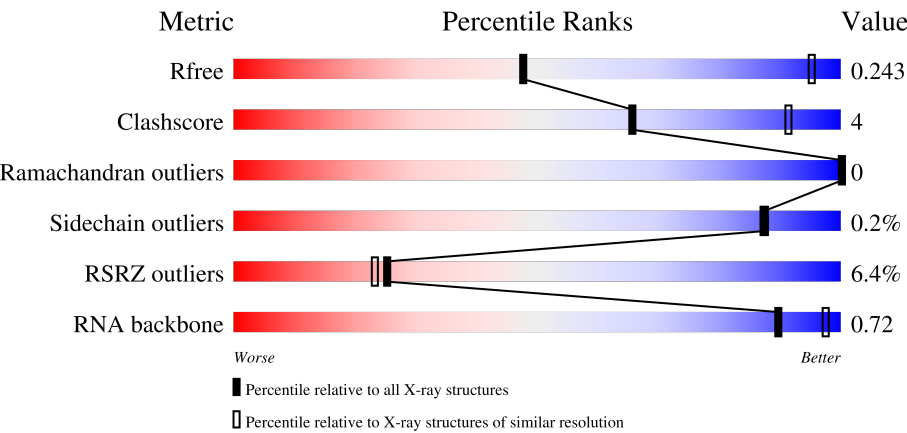
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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.



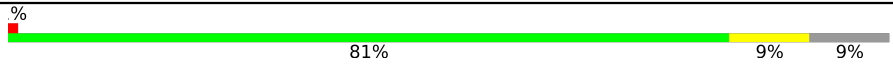
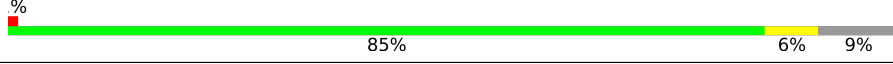
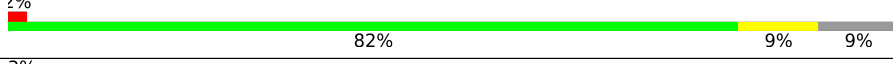
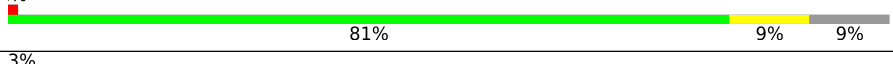
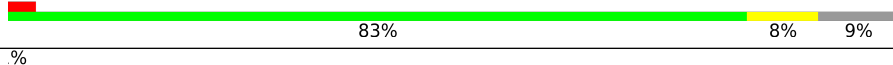
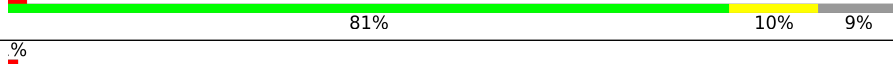
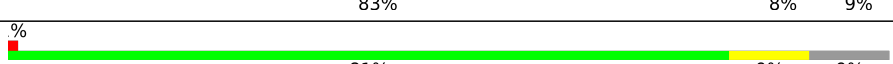
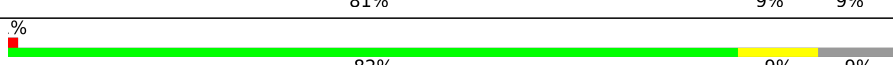
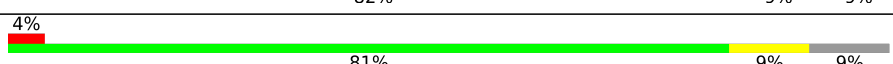
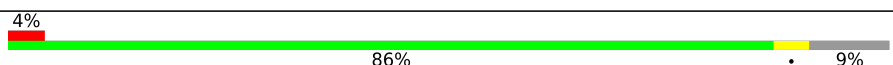
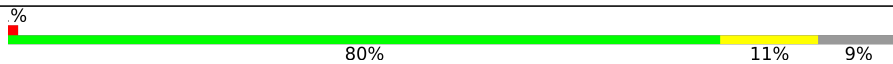
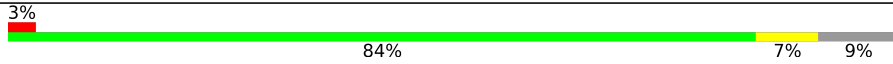
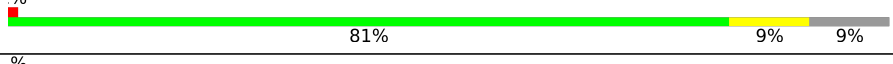
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)
RNA backbone	3983	1017 (4.84-3.10)

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	2% 79% 12% 9%
1	B	159	% 83% 8% 9%
1	BB	159	3% 82% 8% 9%
1	C	159	84% 6% 9%

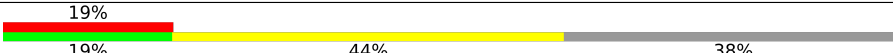
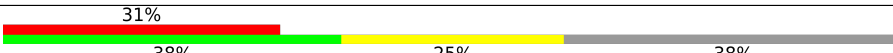
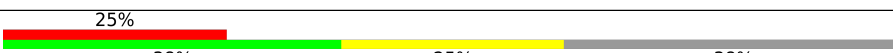
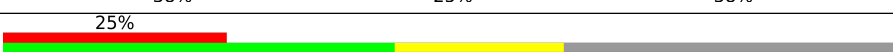
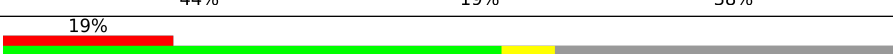
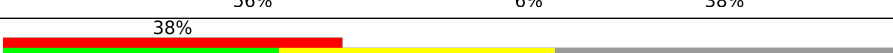
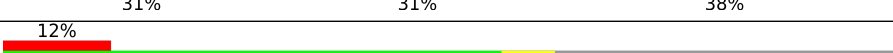
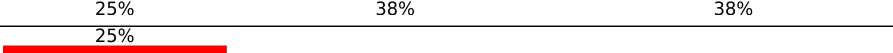
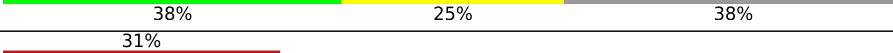
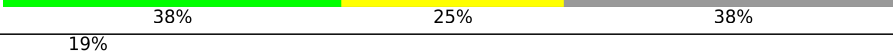
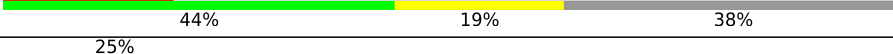
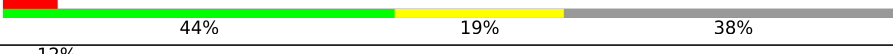
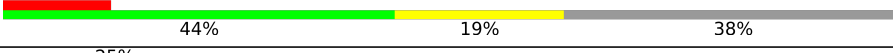
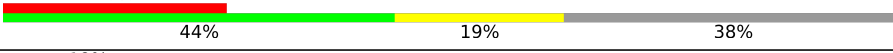
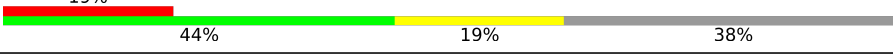
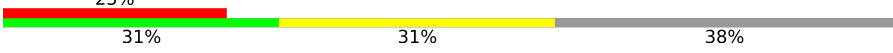
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Mol	Chain	Length	Quality of chain
1	CC	159	
1	D	159	
1	DD	159	
1	E	159	
1	EE	159	
1	F	159	
1	FF	159	
1	G	159	
1	GG	159	
1	H	159	
1	HH	159	
1	I	159	
1	II	159	
1	J	159	
1	JJ	159	
1	K	159	
1	KK	159	
1	L	159	
1	LL	159	
1	M	159	
1	MM	159	
1	N	159	
1	NN	159	
1	O	159	
1	OO	159	

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Mol	Chain	Length	Quality of chain
1	PP	159	
2	P	16	
2	Q	16	
2	QQ	16	
2	R	16	
2	RR	16	
2	S	16	
2	SS	16	
2	T	16	
2	TT	16	
2	U	16	
2	UU	16	
2	V	16	
2	VV	16	
2	W	16	
2	WW	16	
2	X	16	
2	Y	16	
2	YY	16	
2	Z	16	
2	ZZ	16	
2	a	16	
2	b	16	
2	bb	16	
2	c	16	

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Mol	Chain	Length	Quality of chain
2	cc	16	
2	d	16	
2	dd	16	
2	ee	16	
2	ff	16	
2	gg	16	
3	1	27	
3	2	27	
3	3	27	
3	4	27	
3	5	27	
3	6	27	
3	7	27	
3	8	27	
3	e	27	
3	f	27	
3	g	27	
3	h	27	
3	hh	27	
3	i	27	
3	ii	27	
3	j	27	
3	jj	27	
3	k	27	
3	kk	27	

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Mol	Chain	Length	Quality of chain
3	l	27	
3	ll	27	
3	m	27	
3	mm	27	
3	n	27	
3	nn	27	
3	o	27	
3	oo	27	
3	p	27	
3	pp	27	
3	q	27	
3	qq	27	
3	r	27	
3	rr	27	
3	s	27	
3	ss	27	
3	t	27	
3	tt	27	
3	u	27	
3	uu	27	
3	v	27	
3	vv	27	
3	w	27	
3	ww	27	
3	x	27	

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Mol	Chain	Length	Quality of chain
3	xx	27	7% 93%
3	y	27	7% 93%
3	yy	27	7% 93%
3	z	27	7% 93%
3	zz	27	7% 93%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 49953 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	19	0
			1224	778	212	226	8			
1	B	144	Total	C	N	O	S	0	17	0
			1201	761	209	222	9			
1	C	144	Total	C	N	O	S	0	19	0
			1226	779	213	225	9			
1	D	144	Total	C	N	O	S	0	21	0
			1226	778	212	228	8			
1	E	144	Total	C	N	O	S	0	20	0
			1223	775	214	226	8			
1	F	144	Total	C	N	O	S	0	19	0
			1225	775	214	228	8			
1	G	144	Total	C	N	O	S	0	18	0
			1208	764	212	224	8			
1	H	144	Total	C	N	O	S	0	20	0
			1222	775	213	225	9			
1	I	144	Total	C	N	O	S	0	16	0
			1196	754	208	225	9			
1	J	144	Total	C	N	O	S	0	17	0
			1204	764	208	224	8			
1	K	144	Total	C	N	O	S	6	20	0
			1221	772	213	227	9			
1	L	144	Total	C	N	O	S	0	18	0
			1206	762	210	225	9			
1	M	144	Total	C	N	O	S	0	15	0
			1186	751	207	220	8			
1	N	144	Total	C	N	O	S	0	17	0
			1209	767	211	223	8			
1	O	144	Total	C	N	O	S	0	20	0
			1218	773	212	224	9			
1	BB	144	Total	C	N	O	S	0	19	0
			1224	778	212	226	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	CC	144	Total 1201	C 761	N 209	O 222	S 9	0	17	0
1	DD	144	Total 1213	C 769	N 211	O 224	S 9	0	18	0
1	EE	144	Total 1240	C 790	N 215	O 227	S 8	0	21	0
1	FF	144	Total 1209	C 767	N 210	O 225	S 7	0	18	0
1	GG	144	Total 1218	C 771	N 213	O 226	S 8	0	18	0
1	HH	144	Total 1208	C 764	N 212	O 224	S 8	0	18	0
1	II	144	Total 1230	C 780	N 216	O 225	S 9	0	21	0
1	JJ	144	Total 1191	C 750	N 208	O 225	S 8	0	15	0
1	KK	144	Total 1211	C 769	N 209	O 225	S 8	0	18	0
1	LL	144	Total 1221	C 772	N 213	O 227	S 9	0	20	0
1	MM	144	Total 1206	C 762	N 210	O 225	S 9	0	18	0
1	NN	144	Total 1186	C 751	N 207	O 220	S 8	0	15	0
1	OO	144	Total 1223	C 775	N 215	O 224	S 9	0	19	0
1	PP	144	Total 1221	C 776	N 212	O 224	S 9	0	20	0

- | 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	C	N	O	P	0	10	0
			221	100	50	61	10			
2	ee	10	Total	C	N	O	P	0	10	0
			221	100	50	61	10			
2	ff	10	Total	C	N	O	P	0	10	0
			221	100	50	61	10			
2	gg	10	Total	C	N	O	P	0	10	0
			221	100	50	61	10			

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

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

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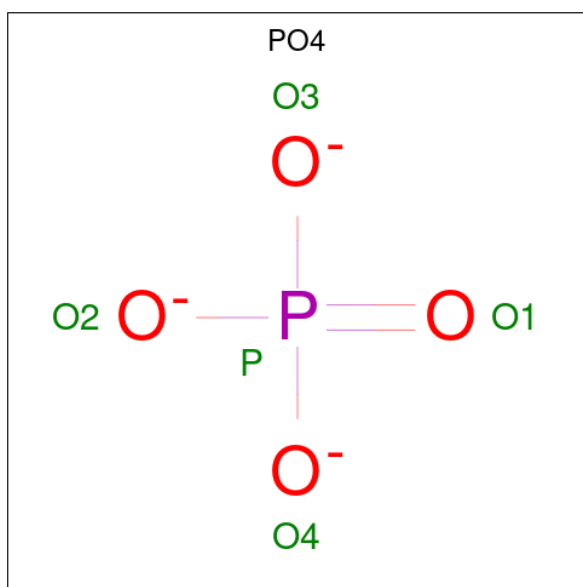
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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3	u	2	Total 26	C 10	N 2	O 12	P 2	0	2	0
3	v	2	Total 26	C 10	N 2	O 12	P 2	0	2	0
3	w	2	Total 26	C 10	N 2	O 12	P 2	0	2	0
3	x	2	Total 26	C 10	N 2	O 12	P 2	0	2	0
3	y	2	Total 26	C 10	N 2	O 12	P 2	0	2	0
3	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 286	C 110	N 22	O 132	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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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	10	Total	C	N	O	P	0	10	0
			201	90	20	81	10			
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 PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	P	0	1
			21	20	1		
4	F	1	Total	O	P	0	1
			21	20	1		
4	L	1	Total	O	P	0	1
			21	20	1		
4	DD	1	Total	O	P	0	1
			21	20	1		
4	KK	1	Total	O	P	0	1
			21	20	1		
4	LL	1	Total	O	P	0	1
			21	20	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	2	Total	O	0	0
			2	2		
5	H	1	Total	O	0	0
			1	1		
5	J	1	Total	O	0	0
			1	1		
5	L	1	Total	O	0	0
			1	1		
5	M	1	Total	O	0	0
			1	1		
5	a	1	Total	O	0	0
			1	1		

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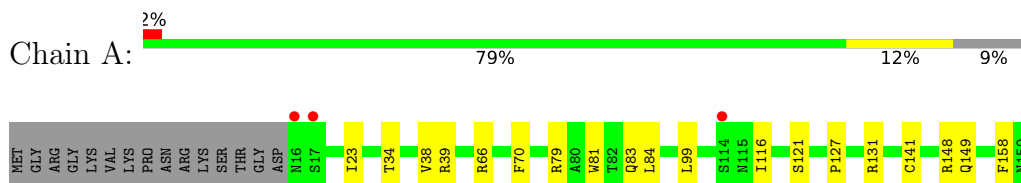
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	x	1	Total O 1 1	0	0
5	z	1	Total O 1 1	0	0
5	7	3	Total O 3 3	0	0
5	DD	1	Total O 1 1	0	0
5	FF	1	Total O 1 1	0	0
5	NN	1	Total O 1 1	0	0
5	PP	1	Total O 1 1	0	0

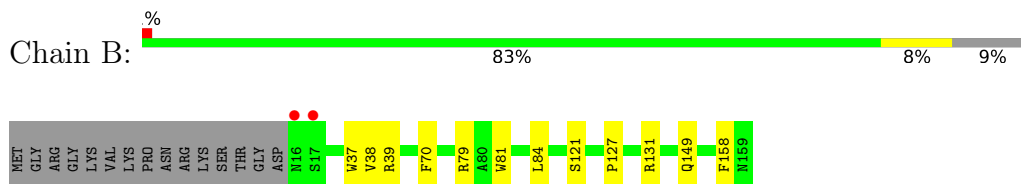
3 Residue-property plots [i](#)

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

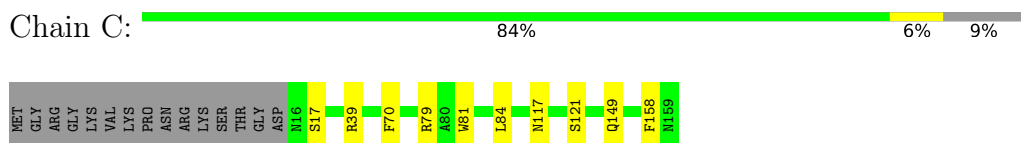
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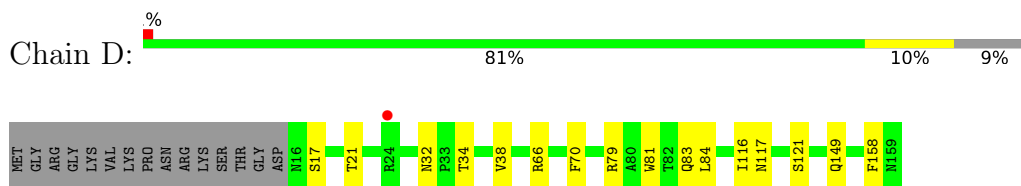
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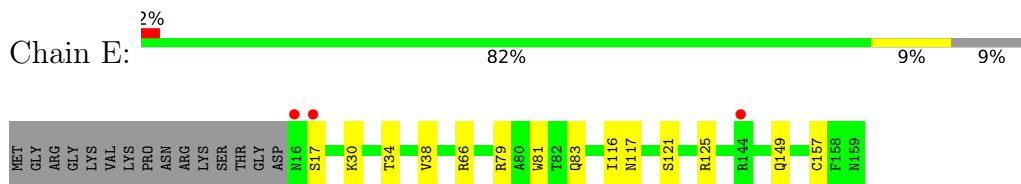
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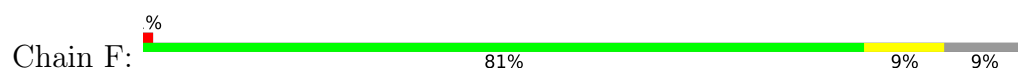
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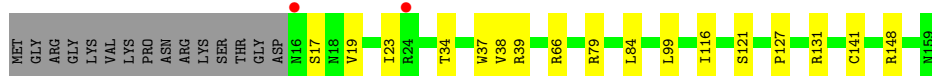
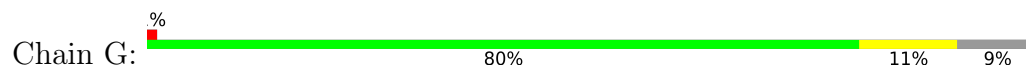
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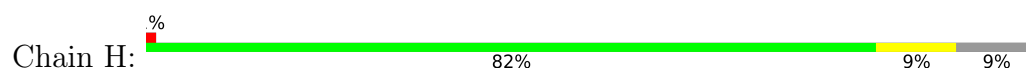
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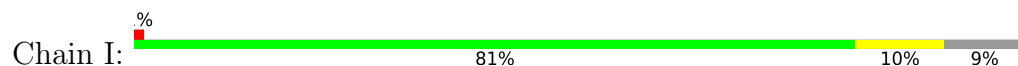
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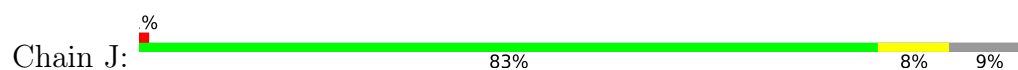
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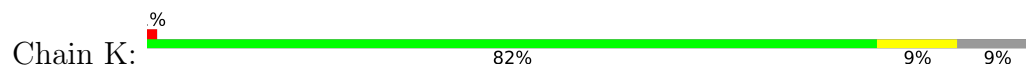
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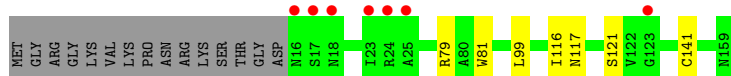
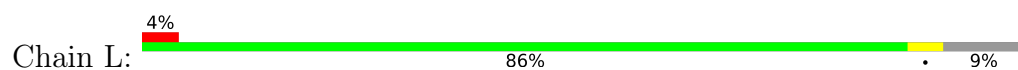
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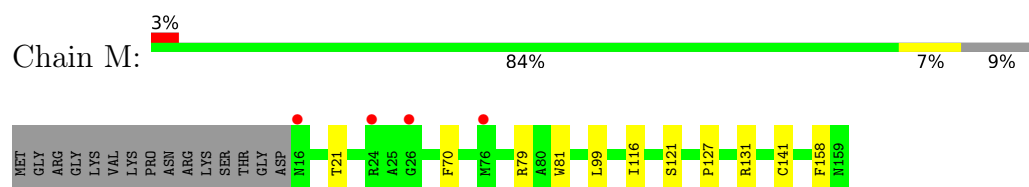
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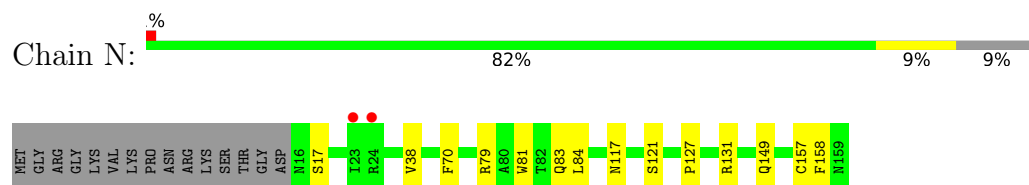
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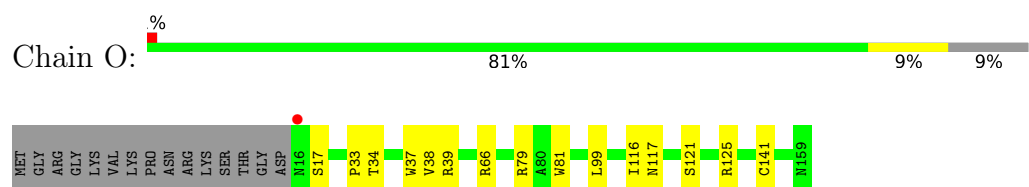
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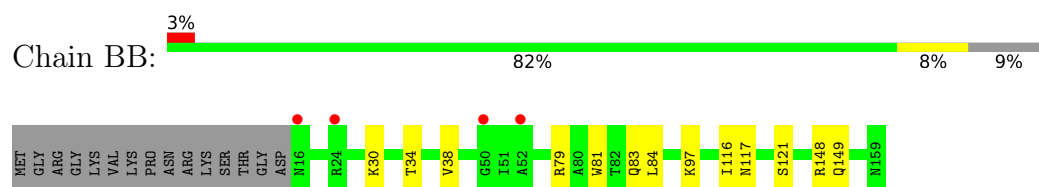
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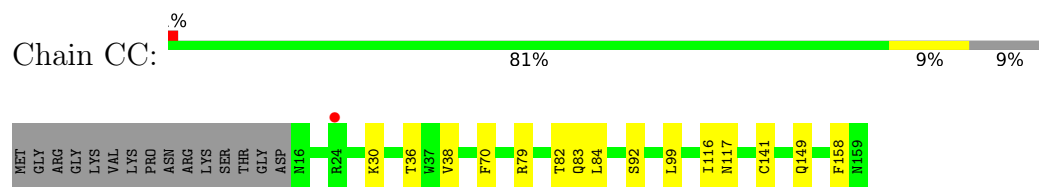
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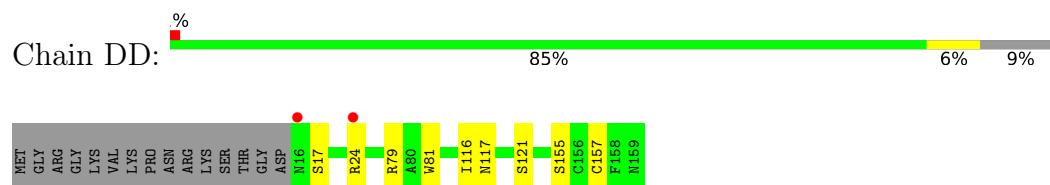
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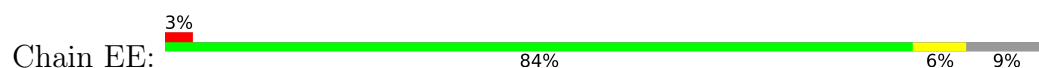
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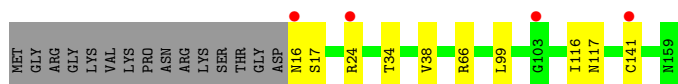


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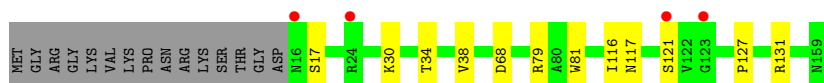
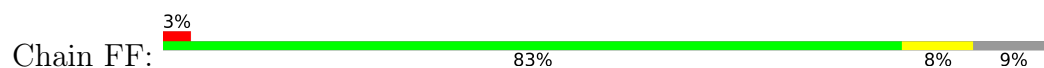


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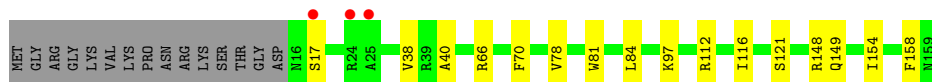
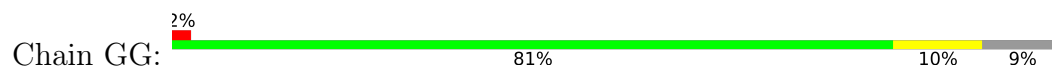




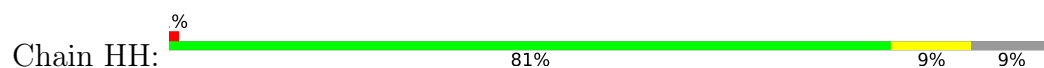
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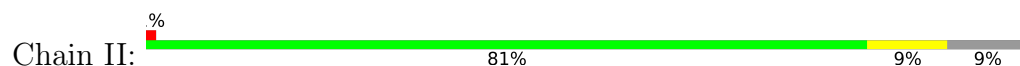
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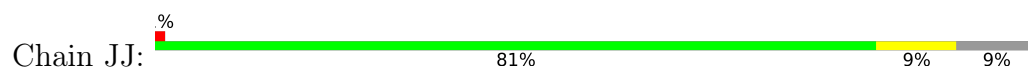
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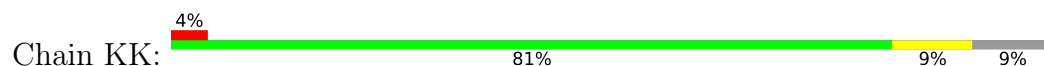
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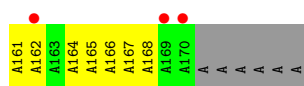
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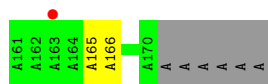
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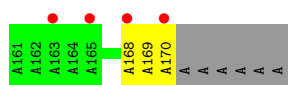
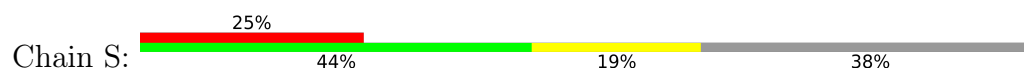
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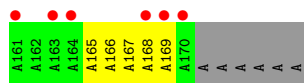
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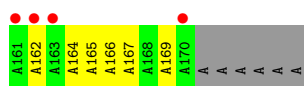
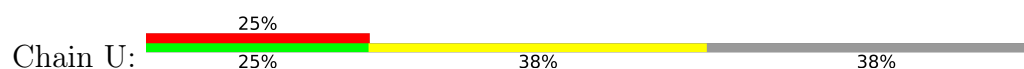
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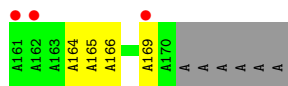
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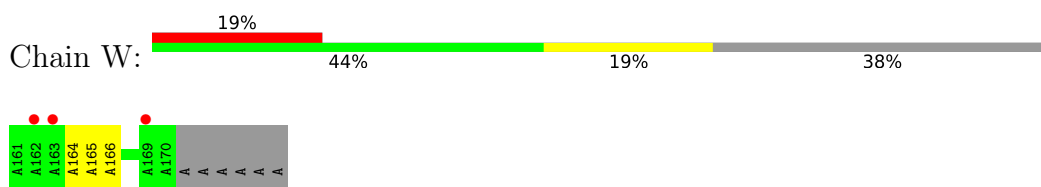
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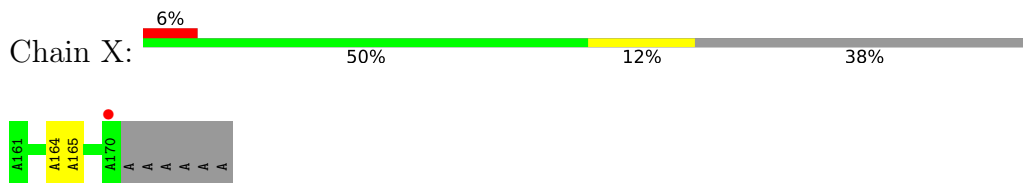
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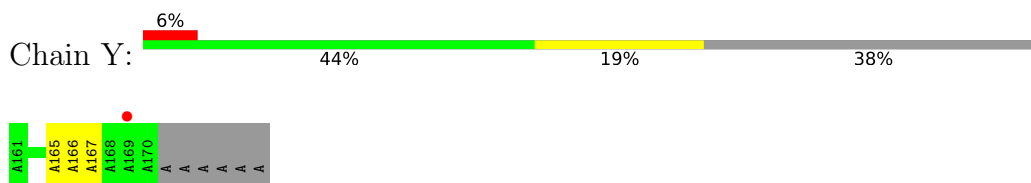
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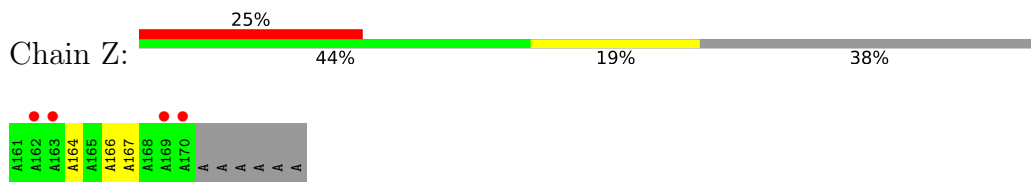
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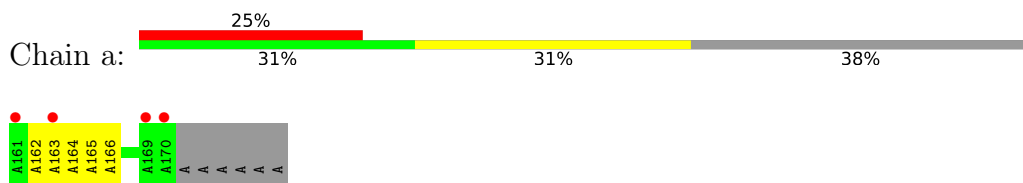
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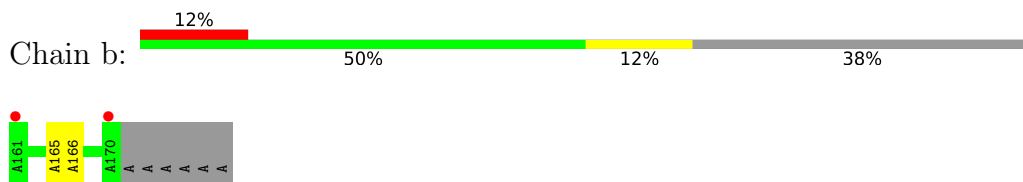
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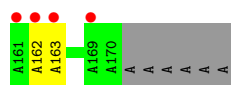
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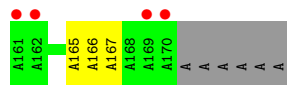
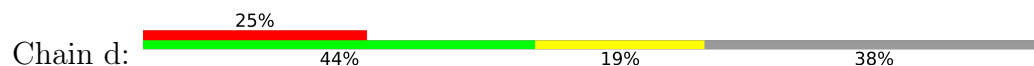
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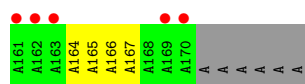
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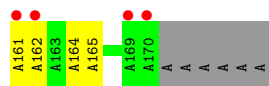
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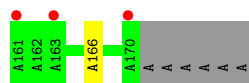
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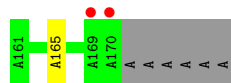
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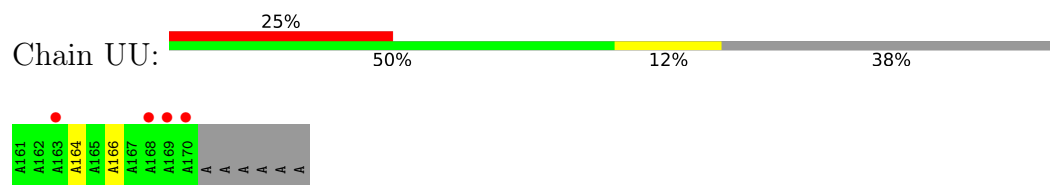
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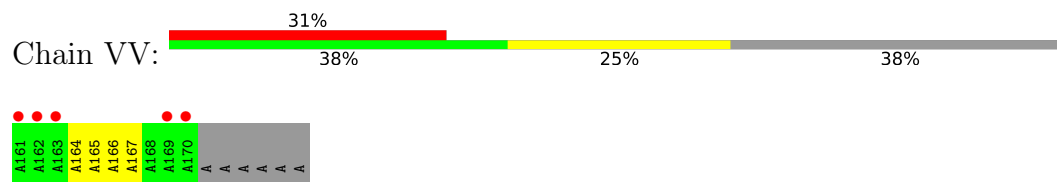
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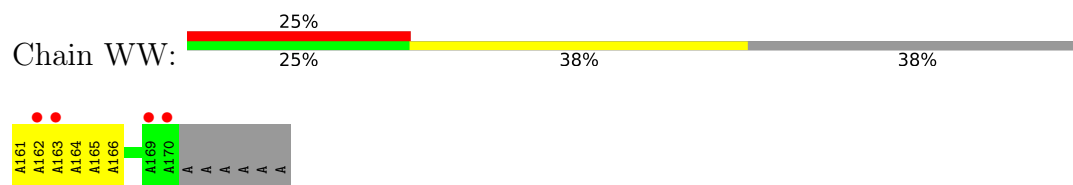
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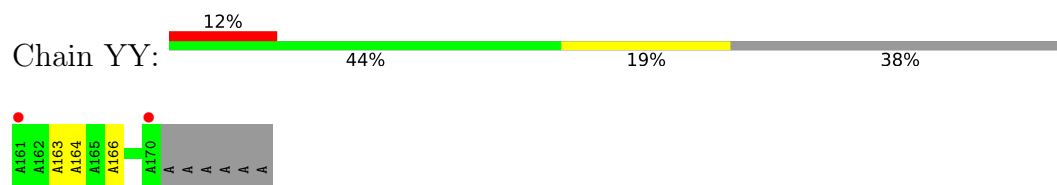
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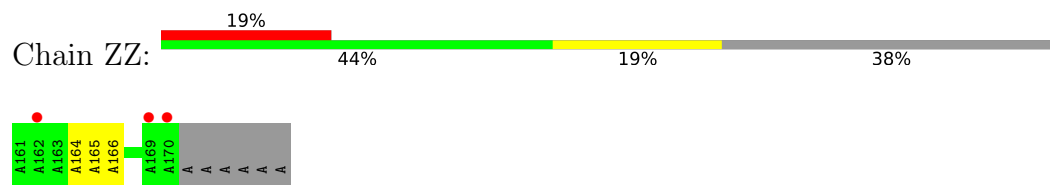
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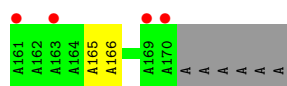


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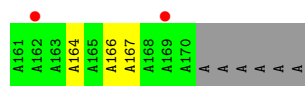
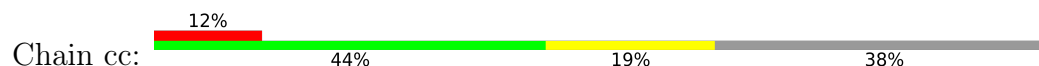


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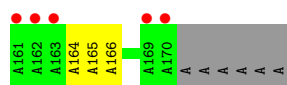
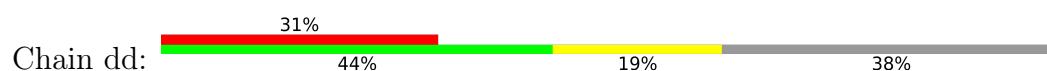




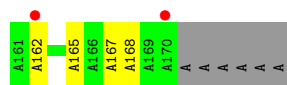
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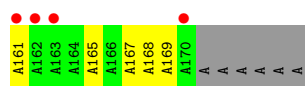
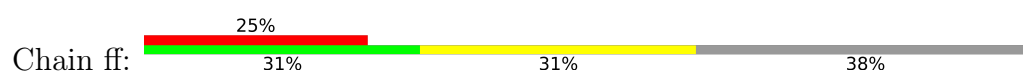
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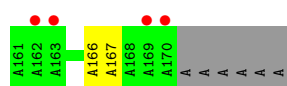
- Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')



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

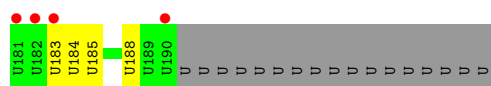


- Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')



- Molecule 3: RNA (27-mer)





- Molecule 3: RNA (27-mer)



- Molecule 3: RNA (27-mer)



- Molecule 3: RNA (27-mer)



- Molecule 3: RNA (27-mer)



- Molecule 3: RNA (27-mer)



- Molecule 3: RNA (27-mer)



- Molecule 3: RNA (27-mer)



• Molecule 3: RNA (27-mer)



• Molecule 3: RNA (27-mer)



• Molecule 3: RNA (27-mer)



• Molecule 3: RNA (27-mer)



• Molecule 3: RNA (27-mer)



• Molecule 3: RNA (27-mer)



● Molecule 3: RNA (27-mer)



● Molecule 3: RNA (27-mer)



● Molecule 3: RNA (27-mer)



● Molecule 3: RNA (27-mer)



● Molecule 3: RNA (27-mer)



● Molecule 3: RNA (27-mer)



● Molecule 3: RNA (27-mer)





- Molecule 3: RNA (27-mer)



- Molecule 3: RNA (27-mer)



- Molecule 3: RNA (27-mer)



- Molecule 3: RNA (27-mer)



- Molecule 3: RNA (27-mer)



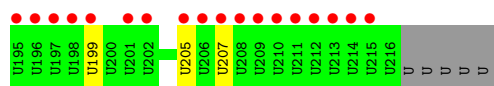
- Molecule 3: RNA (27-mer)



- Molecule 3: RNA (27-mer)



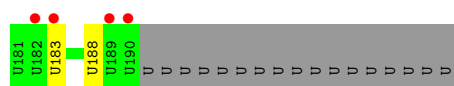
• Molecule 3: RNA (27-mer)



• Molecule 3: RNA (27-mer)



• Molecule 3: RNA (27-mer)



• Molecule 3: RNA (27-mer)



• Molecule 3: RNA (27-mer)



• Molecule 3: RNA (27-mer)



● Molecule 3: RNA (27-mer)



● Molecule 3: RNA (27-mer)



● Molecule 3: RNA (27-mer)



● Molecule 3: RNA (27-mer)



● Molecule 3: RNA (27-mer)

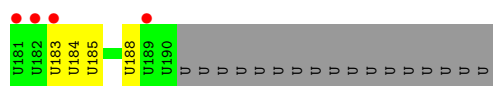


● Molecule 3: RNA (27-mer)



● Molecule 3: RNA (27-mer)





- Molecule 3: RNA (27-mer)



- Molecule 3: RNA (27-mer)



- Molecule 3: RNA (27-mer)



- Molecule 3: RNA (27-mer)



- Molecule 3: RNA (27-mer)



- Molecule 3: RNA (27-mer)



- Molecule 3: RNA (27-mer)



• Molecule 3: RNA (27-mer)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	192.08Å 202.29Å 177.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.00 – 4.00 60.00 – 4.00	Depositor EDS
% Data completeness (in resolution range)	81.8 (60.00-4.00) 81.7 (60.00-4.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.97 (at 3.99Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.200 , (Not available) 0.203 , 0.243	Depositor DCC
R_{free} test set	2416 reflections (4.08%)	wwPDB-VP
Wilson B-factor (Å ²)	26.6	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 23.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	49953	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.09	0/1301	0.25	0/1767
1	B	0.08	0/1269	0.24	0/1725
1	BB	0.08	0/1301	0.24	0/1767
1	C	0.08	0/1291	0.24	0/1755
1	CC	0.09	0/1269	0.26	0/1725
1	D	0.08	0/1297	0.24	0/1767
1	DD	0.09	0/1275	0.25	0/1734
1	E	0.10	0/1293	0.31	0/1759
1	EE	0.09	0/1317	0.25	0/1790
1	F	0.08	0/1292	0.24	0/1757
1	FF	0.09	0/1276	0.25	0/1737
1	G	0.08	0/1276	0.24	0/1735
1	GG	0.09	0/1285	0.24	0/1747
1	H	0.08	0/1292	0.25	0/1756
1	HH	0.08	0/1276	0.25	0/1735
1	I	0.09	0/1266	0.25	0/1721
1	II	0.09	0/1303	0.25	0/1770
1	J	0.09	0/1272	0.25	0/1731
1	JJ	0.09	0/1258	0.25	0/1711
1	K	0.08	0/1301	0.24	0/1768
1	KK	0.09	0/1280	0.25	0/1742
1	L	0.09	0/1276	0.24	0/1734
1	LL	0.08	0/1301	0.24	0/1768
1	M	0.09	0/1252	0.26	0/1702
1	MM	0.09	0/1276	0.23	0/1734
1	N	0.11	0/1279	0.27	0/1737
1	NN	0.09	0/1252	0.24	0/1702
1	O	0.08	0/1292	0.25	0/1756
1	OO	0.09	0/1296	0.25	0/1759
1	PP	0.08	0/1299	0.24	0/1766
2	P	0.08	0/250	0.24	0/386
2	Q	0.11	0/250	0.30	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	0.24	0/386
2	RR	0.09	0/250	0.21	0/386
2	S	0.07	0/250	0.21	0/386
2	SS	0.08	0/250	0.24	0/386
2	T	0.08	0/250	0.24	0/386
2	TT	0.07	0/250	0.22	0/386
2	U	0.08	0/250	0.24	0/386
2	UU	0.08	0/250	0.21	0/386
2	V	0.12	0/250	0.27	0/386
2	VV	0.08	0/250	0.24	0/386
2	W	0.08	0/250	0.22	0/386
2	WW	0.13	0/250	0.31	0/386
2	X	0.08	0/250	0.25	0/386
2	Y	0.08	0/250	0.24	0/386
2	YY	0.08	0/250	0.22	0/386
2	Z	0.08	0/250	0.25	0/386
2	ZZ	0.08	0/250	0.26	0/386
2	a	0.12	0/250	0.23	0/386
2	b	0.08	0/250	0.25	0/386
2	bb	0.07	0/250	0.22	0/386
2	c	0.08	0/250	0.21	0/386
2	cc	0.09	0/250	0.24	0/386
2	d	0.08	0/250	0.25	0/386
2	dd	0.14	0/250	0.36	0/386
2	ee	0.08	0/250	0.24	0/386
2	ff	0.09	0/250	0.25	0/386
2	gg	0.08	0/250	0.27	0/386
3	1	0.10	0/27	0.27	0/38
3	2	0.08	0/27	0.29	0/38
3	3	0.09	0/27	0.28	0/38
3	4	0.09	0/27	0.28	0/38
3	5	0.08	0/27	0.23	0/38
3	6	0.09	0/27	0.40	0/38
3	7	0.10	0/297	0.31	0/418
3	8	0.08	0/27	0.28	0/38
3	e	0.06	0/220	0.18	0/336
3	f	0.06	0/220	0.16	0/336
3	g	0.07	0/220	0.21	0/336
3	h	0.07	0/220	0.17	0/336
3	hh	0.07	0/220	0.17	0/336
3	i	0.07	0/220	0.17	0/336
3	ii	0.07	0/220	0.16	0/336

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	j	0.07	0/220	0.17	0/336
3	jj	0.06	0/220	0.20	0/336
3	k	0.08	0/220	0.22	0/336
3	kk	0.07	0/220	0.17	0/336
3	l	0.07	0/220	0.16	0/336
3	ll	0.07	0/220	0.17	0/336
3	m	0.07	0/220	0.17	0/336
3	mm	0.07	0/220	0.17	0/336
3	n	0.06	0/220	0.18	0/336
3	nn	0.08	0/220	0.21	0/336
3	o	0.06	0/220	0.16	0/336
3	oo	0.06	0/220	0.17	0/336
3	p	0.07	0/220	0.17	0/336
3	pp	0.06	0/220	0.16	0/336
3	q	0.06	0/220	0.15	0/336
3	qq	0.06	0/220	0.17	0/336
3	r	0.07	0/220	0.16	0/336
3	rr	0.06	0/220	0.16	0/336
3	s	0.07	0/220	0.19	0/336
3	ss	0.07	0/220	0.18	0/336
3	t	0.09	0/27	0.35	0/38
3	tt	0.07	0/220	0.15	0/336
3	u	0.11	0/27	0.46	0/38
3	uu	0.07	0/220	0.16	0/336
3	v	0.14	0/27	0.41	0/38
3	vv	0.07	0/220	0.18	0/336
3	w	0.11	0/27	0.46	0/38
3	ww	0.07	0/27	0.25	0/38
3	x	0.11	0/27	0.41	0/38
3	xx	0.10	0/27	0.30	0/38
3	y	0.08	0/27	0.24	0/38
3	yy	0.08	0/27	0.26	0/38
3	z	0.11	0/27	0.37	0/38
3	zz	0.08	0/27	0.27	0/38
All	All	0.09	0/53396	0.24	0/75119

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1224	0	1272	14	0
1	B	1201	0	1236	7	0
1	BB	1224	0	1271	12	0
1	C	1226	0	1261	7	0
1	CC	1201	0	1236	13	1
1	D	1226	0	1249	13	0
1	DD	1213	0	1242	7	0
1	E	1223	0	1252	12	0
1	EE	1240	0	1282	10	0
1	F	1225	0	1250	13	0
1	FF	1209	0	1235	12	0
1	G	1208	0	1241	13	0
1	GG	1218	0	1243	13	0
1	H	1222	0	1260	11	0
1	HH	1208	0	1241	14	0
1	I	1196	0	1217	12	1
1	II	1230	0	1273	12	0
1	J	1204	0	1234	11	0
1	JJ	1191	0	1208	11	0
1	K	1221	0	1246	12	0
1	KK	1211	0	1240	14	0
1	L	1206	0	1233	8	0
1	LL	1221	0	1246	14	0
1	M	1186	0	1220	7	0
1	MM	1206	0	1233	4	0
1	N	1209	0	1248	11	1
1	NN	1186	0	1220	6	0
1	O	1218	0	1256	13	0
1	OO	1223	0	1265	14	0
1	PP	1221	0	1263	10	0
2	P	221	0	104	3	0
2	Q	221	0	111	6	1
2	QQ	221	0	108	4	0
2	R	221	0	111	2	0
2	RR	221	0	111	4	0
2	S	221	0	104	2	0
2	SS	221	0	111	0	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	T	221	0	107	4	0
2	TT	221	0	102	1	0
2	U	221	0	106	7	0
2	UU	221	0	105	2	0
2	V	221	0	104	5	0
2	VV	221	0	105	4	0
2	W	221	0	107	3	0
2	WW	221	0	105	6	0
2	X	221	0	111	2	0
2	Y	221	0	103	4	0
2	YY	221	0	109	3	0
2	Z	221	0	104	3	0
2	ZZ	221	0	111	5	0
2	a	221	0	111	6	0
2	b	221	0	111	1	1
2	bb	221	0	104	2	0
2	c	221	0	111	2	0
2	cc	221	0	106	3	0
2	d	221	0	109	3	0
2	dd	221	0	111	3	0
2	ee	221	0	111	3	0
2	ff	221	0	111	6	0
2	gg	221	0	109	2	0
3	1	26	0	10	1	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	286	0	110	3	0
3	8	26	0	10	0	0
3	e	201	0	92	2	0
3	f	201	0	101	1	0
3	g	201	0	101	3	0
3	h	201	0	94	2	0
3	hh	201	0	91	1	0
3	i	201	0	96	1	0
3	ii	201	0	101	1	0
3	j	201	0	95	3	0
3	jj	201	0	101	3	0
3	k	201	0	91	1	0
3	kk	201	0	91	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	l	201	0	91	2	0
3	ll	201	0	92	1	0
3	m	201	0	101	2	0
3	mm	201	0	90	1	0
3	n	201	0	92	2	0
3	nn	201	0	90	1	0
3	o	201	0	94	2	0
3	oo	201	0	90	2	0
3	p	201	0	101	4	0
3	pp	201	0	101	1	0
3	q	201	0	101	1	0
3	qq	201	0	96	2	0
3	r	201	0	101	1	0
3	rr	201	0	94	2	0
3	s	201	0	92	3	0
3	ss	201	0	101	1	0
3	t	26	0	10	0	0
3	tt	201	0	101	1	0
3	u	26	0	10	0	0
3	uu	201	0	101	4	0
3	v	26	0	10	0	0
3	vv	201	0	93	3	0
3	w	26	0	10	1	0
3	ww	26	0	10	0	0
3	x	26	0	10	4	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	B	21	0	0	0	0
4	DD	21	0	0	0	0
4	F	21	0	0	0	0
4	KK	21	0	0	1	0
4	L	21	0	0	1	0
4	LL	21	0	0	1	0
5	7	3	0	0	2	0
5	DD	1	0	0	0	0
5	FF	1	0	0	0	0
5	G	2	0	0	0	0
5	H	1	0	0	0	0
5	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	L	1	0	0	0	0
5	M	1	0	0	0	0
5	NN	1	0	0	0	0
5	PP	1	0	0	0	0
5	a	1	0	0	0	0
5	x	1	0	0	0	0
5	z	1	0	0	0	0
All	All	49953	0	43772	335	3

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 4.

All (335) 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)
2:U:162[B]:A:H61	3:j:188[B]:U:H3	1.34	0.76
1:BB:79[A]:ARG:NH2	3:hh:188[A]:U:OP1	2.19	0.75
1:BB:38:VAL:O	2:gg:166[B]:A:O2'	2.05	0.74
1:KK:79[A]:ARG:NH2	3:qq:188[A]:U:OP1	2.19	0.74
1:O:17:SER:HA	2:U:164[B]:A:H4'	1.68	0.73
2:W:164[B]:A:H4'	1:GG:17:SER:HA	1.72	0.71
2:ff:169[B]:A:H61	3:uu:181[B]:U:H3	1.39	0.71
1:FF:79[A]:ARG:NH2	3:ll:188[A]:U:OP1	2.22	0.70
1:A:79[A]:ARG:NH2	3:e:188[A]:U:OP1	2.25	0.70
1:J:79[A]:ARG:NH2	3:n:188[A]:U:OP1	2.26	0.69
1:PP:38:VAL:O	2:QQ:166[A]:A:O2'	2.10	0.68
1:PP:17:SER:HA	2:VV:164[B]:A:H4'	1.75	0.68
2:X:164[A]:A:H4'	1:DD:17:SER:HA	1.74	0.68
1:KK:38:VAL:O	2:cc:166[B]:A:O2'	2.11	0.67
1:A:83:GLN:HB3	1:A:149[B]:GLN:HB3	1.75	0.67
1:I:79[A]:ARG:NH2	3:m:188[A]:U:OP1	2.24	0.67
2:W:166[B]:A:O2'	1:EE:38:VAL:O	2.15	0.66
1:N:17:SER:HA	2:Q:164[A]:A:H4'	1.78	0.65
1:EE:17:SER:HA	2:WW:164[A]:A:H4'	1.78	0.65
3:7:205[A]:U:OP2	5:7:301:HOH:O	2.15	0.64
1:D:79[A]:ARG:NH2	3:h:188[A]:U:OP1	2.31	0.63
1:BB:83:GLN:HB3	1:BB:149[B]:GLN:HB3	1.80	0.63
1:D:32:ASN:O	1:II:39[B]:ARG:NH2	2.32	0.62
1:F:17:SER:HA	2:YY:164[B]:A:H4'	1.83	0.61
1:KK:83:GLN:HB3	1:KK:149[B]:GLN:HB3	1.81	0.61
2:a:163[A]:A:H2'	2:a:164[A]:A:C8	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:83:GLN:HB3	1:J:149[B]:GLN:HB3	1.82	0.61
1:K:38:VAL:O	2:Y:166[A]:A:O2'	2.17	0.60
1:DD:79[A]:ARG:NH2	3:jj:188[A]:U:OP1	2.35	0.60
1:LL:38:VAL:O	2:bb:166[A]:A:O2'	2.18	0.60
1:D:38:VAL:O	2:YY:166[B]:A:O2'	2.18	0.59
1:PP:79[B]:ARG:NH2	3:vv:188[B]:U:O3'	2.36	0.59
1:C:79[A]:ARG:NH2	3:g:188[A]:U:OP1	2.36	0.58
1:JJ:83:GLN:HB3	1:JJ:149[B]:GLN:HB3	1.84	0.58
1:J:38:VAL:O	2:Z:166[B]:A:O2'	2.20	0.58
1:CC:36:THR:HG21	1:OO:19:VAL:HG11	1.86	0.58
1:E:79[A]:ARG:NH2	3:i:188[A]:U:OP1	2.36	0.58
1:E:17:SER:HA	2:Z:164[B]:A:H4'	1.86	0.57
2:V:166[A]:A:H2	2:WW:164[A]:A:N1	2.02	0.57
1:N:79[B]:ARG:NH2	3:r:189[B]:U:OP1	2.38	0.57
1:O:38:VAL:O	2:P:166[A]:A:O2'	2.24	0.56
1:L:117:ASN:ND2	4:L:201[C]:PO4:O3	2.35	0.55
1:M:79[B]:ARG:NH2	3:q:188[B]:U:O3'	2.40	0.55
2:P:165[A]:A:H2'	2:P:166[A]:A:H8	1.71	0.55
1:E:38:VAL:O	2:U:166[B]:A:O2'	2.24	0.55
1:GG:38:VAL:O	2:UU:166[A]:A:O2'	2.24	0.55
2:U:169[B]:A:H5''	3:x:195[B]:U:H4'	1.88	0.54
1:F:38:VAL:HG23	2:U:165[B]:A:H1'	1.88	0.54
1:CC:79[B]:ARG:NH2	3:ii:188[B]:U:O3'	2.41	0.54
1:MM:79[B]:ARG:NH2	3:ss:188[B]:U:O3'	2.40	0.54
2:ee:162[B]:A:H61	3:tt:188[B]:U:H3	1.53	0.54
1:FF:38:VAL:O	2:VV:166[B]:A:O2'	2.23	0.54
1:LL:84:LEU:HD12	1:LL:148:ARG:HB2	1.89	0.53
2:Q:161[A]:A:H2'	2:Q:162[A]:A:H8	1.73	0.53
1:JJ:117:ASN:HB3	1:KK:116:ILE:HG12	1.90	0.53
2:QQ:165[A]:A:H2'	2:QQ:166[A]:A:H8	1.74	0.53
2:ff:169[B]:A:N6	3:uu:181[B]:U:H3	2.05	0.53
1:JJ:35:PRO:HB2	2:ZZ:166[A]:A:H5''	1.91	0.53
1:JJ:36:THR:OG1	2:ZZ:165[A]:A:O3'	2.27	0.53
1:D:17:SER:HA	2:V:164[A]:A:H4'	1.90	0.53
1:D:117:ASN:HB3	1:E:116:ILE:HG12	1.91	0.53
2:RR:164[A]:A:H2'	2:RR:165[A]:A:H8	1.74	0.53
1:HH:38:VAL:HG23	2:WW:165[A]:A:H1'	1.91	0.52
1:F:38:VAL:HG12	2:T:167[A]:A:H4'	1.92	0.52
1:A:38:VAL:HG12	2:d:167[B]:A:H4'	1.91	0.52
2:RR:164[A]:A:H2'	2:RR:165[A]:A:C8	2.45	0.52
2:U:169[B]:A:C5'	3:x:195[B]:U:H4'	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:54[A]:LYS:NZ	1:H:142:GLU:OE2	2.43	0.51
2:T:165[A]:A:H2'	2:T:166[A]:A:H8	1.76	0.51
1:LL:116:ILE:HG12	1:PP:117:ASN:HB3	1.92	0.51
1:B:38:VAL:HG23	2:Q:165[A]:A:H1'	1.92	0.51
1:I:17:SER:HA	2:a:164[A]:A:H4'	1.91	0.51
1:II:81:TRP:CD1	1:II:121:SER:HB3	2.46	0.51
2:ff:161[B]:A:H61	3:uu:189[B]:U:H3	1.57	0.51
1:EE:117:ASN:HB3	1:FF:116:ILE:HG12	1.92	0.51
1:FF:30:LYS:NZ	1:HH:121:SER:O	2.43	0.51
1:N:70:PHE:CD1	1:N:158:PHE:HB3	2.47	0.51
1:E:30:LYS:NZ	1:G:121:SER:O	2.38	0.50
3:7:199[B]:U:OP2	5:7:302:HOH:O	2.19	0.50
1:BB:30:LYS:NZ	1:LL:121:SER:O	2.36	0.50
1:C:84:LEU:HG	1:C:149[A]:GLN:HB2	1.93	0.50
1:D:66:ARG:NH2	1:II:34:THR:HB	2.26	0.50
1:F:117:ASN:HB3	1:G:116:ILE:HG12	1.93	0.50
1:BB:117:ASN:HB3	1:CC:116:ILE:HG12	1.93	0.50
1:PP:38:VAL:HG12	2:QQ:167[A]:A:H4'	1.93	0.50
1:I:83:GLN:HB3	1:I:149[B]:GLN:HB3	1.93	0.50
2:c:162[B]:A:H2'	2:c:163[B]:A:H8	1.76	0.50
1:II:117:ASN:HB3	1:JJ:116:ILE:HG12	1.93	0.50
1:FF:17:SER:HA	2:cc:164[B]:A:H4'	1.93	0.50
1:FF:81:TRP:CD1	1:FF:121:SER:HB3	2.46	0.50
1:H:117:ASN:HB3	1:I:116:ILE:HG12	1.93	0.50
1:K:81:TRP:CD1	1:K:121:SER:HB3	2.47	0.50
1:NN:81:TRP:CD1	1:NN:121:SER:HB3	2.46	0.50
1:OO:79[B]:ARG:HH22	3:uu:189[B]:U:P	2.35	0.49
1:I:84:LEU:HG	1:I:149[A]:GLN:HB2	1.94	0.49
1:O:79[B]:ARG:NH2	3:s:189[B]:U:OP2	2.40	0.49
1:GG:84:LEU:HD12	1:GG:148:ARG:HB2	1.94	0.49
1:A:38:VAL:O	2:d:166[B]:A:O2'	2.29	0.49
1:BB:38:VAL:HG12	2:gg:167[B]:A:H4'	1.94	0.49
1:N:70:PHE:CG	1:N:158:PHE:HB3	2.48	0.49
1:F:155[B]:SER:OG	3:j:187[B]:U:O2'	2.30	0.49
2:S:169[A]:A:HO2'	2:S:170[A]:A:H5'	1.78	0.49
1:KK:81:TRP:CD1	1:KK:121:SER:HB3	2.48	0.49
2:dd:165[A]:A:H2'	2:dd:166[A]:A:C8	2.48	0.49
1:J:66:ARG:NH2	1:K:34:THR:HB	2.28	0.49
1:II:97[B]:LYS:HB3	1:II:142:GLU:HB2	1.94	0.49
1:JJ:81:TRP:CD1	1:JJ:121:SER:HB3	2.48	0.49
2:V:169[A]:A:O2'	2:WW:161[A]:A:N1	2.36	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:GLN:HB3	1:D:149[B]:GLN:HB3	1.95	0.48
1:N:79[B]:ARG:HD3	1:N:81:TRP:HH2	1.77	0.48
1:I:117:ASN:HB3	1:J:116:ILE:HG12	1.95	0.48
1:HH:99:LEU:HD11	1:HH:142:GLU:HG3	1.95	0.48
1:HH:117:ASN:HB3	1:II:116:ILE:HG12	1.94	0.48
1:J:34:THR:HB	1:K:66:ARG:NH2	2.27	0.48
1:KK:34:THR:HB	1:LL:66:ARG:NH2	2.27	0.48
2:ff:167[B]:A:H2'	2:ff:168[B]:A:H8	1.79	0.48
2:T:168[A]:A:HO2'	2:T:169[A]:A:H5'	1.78	0.48
3:qq:184[A]:U:H2'	3:qq:185[A]:U:C6	2.49	0.48
1:A:34:THR:HB	1:O:66:ARG:NH2	2.29	0.48
1:G:17:SER:HA	2:UU:164[A]:A:H4'	1.96	0.47
3:1:195[A]:U:N3	1:EE:16:ASN:OD1	2.43	0.47
3:pp:184[A]:U:H2'	3:pp:185[A]:U:C6	2.49	0.47
1:HH:79[B]:ARG:NH2	3:nn:189[B]:U:OP1	2.46	0.47
3:n:184[A]:U:H2'	3:n:185[A]:U:C6	2.50	0.47
1:JJ:99:LEU:HG	1:JJ:141:CYS:HA	1.96	0.47
1:E:125:ARG:HE	3:x:195[B]:U:H3'	1.79	0.47
1:H:155[B]:SER:HB2	3:l:188[B]:U:H5'	1.97	0.47
2:ee:167[B]:A:H2'	2:ee:168[B]:A:H8	1.79	0.47
1:N:84:LEU:HG	1:N:149[A]:GLN:HB2	1.97	0.47
1:D:84:LEU:HG	1:D:149[A]:GLN:HB2	1.96	0.47
1:OO:19:VAL:HG12	1:OO:20:VAL:N	2.29	0.47
1:OO:82:THR:O	1:OO:119:ARG:NH1	2.48	0.47
1:I:38:VAL:HG23	2:X:165[A]:A:H1'	1.97	0.47
1:B:79[B]:ARG:NH2	3:f:189[B]:U:OP1	2.48	0.47
1:BB:34:THR:HB	1:PP:66:ARG:NH2	2.30	0.47
1:CC:70:PHE:CD1	1:CC:158:PHE:HB3	2.51	0.46
1:FF:38:VAL:HG12	2:VV:167[B]:A:H4'	1.96	0.46
2:ZZ:165[A]:A:H2'	2:ZZ:166[A]:A:H8	1.79	0.46
1:J:38:VAL:HG12	2:Z:167[B]:A:H4'	1.97	0.46
2:T:165[A]:A:H2'	2:T:166[A]:A:C8	2.51	0.46
3:w:195[B]:U:O4	1:II:17:SER:HB2	2.16	0.46
1:FF:34:THR:HB	1:GG:66:ARG:NH2	2.30	0.46
1:LL:79[B]:ARG:NH2	3:rr:188[B]:U:O3'	2.49	0.46
1:L:79[B]:ARG:HH22	3:p:189[B]:U:P	2.38	0.46
1:CC:99:LEU:HG	1:CC:141:CYS:HA	1.97	0.46
1:D:34:THR:HB	1:II:66:ARG:NH2	2.31	0.46
2:Q:161[A]:A:H2'	2:Q:162[A]:A:C8	2.50	0.46
1:NN:117:ASN:HB3	1:OO:116:ILE:HG12	1.97	0.46
2:P:165[A]:A:H2'	2:P:166[A]:A:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:38:VAL:HG12	2:U:167[B]:A:H4'	1.98	0.45
2:a:165[A]:A:H2'	2:a:166[A]:A:C8	2.51	0.45
1:II:79[B]:ARG:HH22	3:oo:189[B]:U:P	2.38	0.45
2:YY:163[B]:A:H2'	2:YY:164[B]:A:H8	1.81	0.45
1:N:81:TRP:CD1	1:N:121:SER:HB3	2.52	0.45
1:B:70:PHE:CD1	1:B:158:PHE:HB3	2.52	0.45
1:GG:40:ALA:HB2	3:mm:187[B]:U:H4'	1.99	0.45
1:C:81:TRP:CD1	1:C:121:SER:HB3	2.51	0.45
2:R:165[A]:A:H2'	2:R:166[A]:A:C8	2.52	0.45
1:F:17:SER:HB2	3:x:195[B]:U:O4	2.16	0.45
1:G:84:LEU:HD12	1:G:148:ARG:HB2	1.98	0.45
1:LL:84:LEU:HG	1:LL:149[A]:GLN:HB2	1.98	0.45
1:HH:117:ASN:ND2	4:KK:201[B]:PO4:O1	2.48	0.45
1:H:30:LYS:NZ	1:FF:121:SER:O	2.44	0.45
1:BB:116:ILE:HG12	1:FF:117:ASN:HB3	1.98	0.45
1:A:66:ARG:NH2	1:O:34:THR:HB	2.32	0.45
1:G:23:ILE:HG21	1:HH:79[B]:ARG:HH21	1.82	0.45
1:K:38:VAL:HG12	2:Y:167[A]:A:H4'	1.98	0.45
1:O:37:TRP:CE2	1:O:39:ARG:HD3	2.52	0.45
1:F:79[B]:ARG:HH22	3:j:189[B]:U:P	2.39	0.45
1:G:66:ARG:NH2	1:HH:34:THR:HB	2.31	0.45
1:O:81:TRP:CD1	1:O:121:SER:HB3	2.51	0.45
1:CC:30:LYS:HG3	1:OO:24:ARG:HG2	1.99	0.45
1:L:81:TRP:CD1	1:L:121:SER:HB3	2.52	0.44
1:M:99:LEU:HG	1:M:141:CYS:HA	1.99	0.44
1:E:81:TRP:CD1	1:E:121:SER:HB3	2.52	0.44
1:CC:117:ASN:HB3	1:DD:116:ILE:HG12	1.99	0.44
1:GG:81:TRP:CD1	1:GG:121:SER:HB3	2.53	0.44
1:JJ:16:ASN:C	2:dd:164[A]:A:H4'	2.42	0.44
1:I:70:PHE:CD1	1:I:158:PHE:HB3	2.52	0.44
2:S:168[A]:A:HO2'	2:S:169[A]:A:H5'	1.82	0.44
1:NN:84:LEU:HD12	1:NN:148:ARG:HB2	2.00	0.44
1:PP:40:ALA:HB2	3:vv:187[B]:U:H4'	1.99	0.44
1:G:38:VAL:HG23	2:V:165[A]:A:H1'	1.99	0.44
1:A:84:LEU:HD12	1:A:148:ARG:HB2	2.00	0.44
1:KK:38:VAL:HG12	2:cc:167[B]:A:H4'	1.99	0.44
1:HH:84:LEU:HG	1:HH:149[A]:GLN:HB2	1.99	0.44
1:H:34:THR:HB	1:EE:66:ARG:NH2	2.33	0.44
1:II:83:GLN:HB3	1:II:149[B]:GLN:HB3	1.99	0.44
1:J:21:THR:HG22	3:s:185[B]:U:H5''	1.99	0.44
1:HH:81:TRP:CD1	1:HH:121:SER:HB3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LL:117:ASN:ND2	4:LL:201[B]:PO4:O3	2.39	0.44
1:MM:84:LEU:HG	1:MM:149[A]:GLN:HB2	2.00	0.44
1:II:127:PRO:O	1:II:131:ARG:HG3	2.18	0.43
2:ff:167[B]:A:H2'	2:ff:168[B]:A:C8	2.52	0.43
1:KK:38:VAL:HG22	1:KK:157[A]:CYS:SG	2.58	0.43
1:I:30:LYS:HG3	1:DD:24:ARG:HG2	2.00	0.43
1:GG:38:VAL:HG23	2:VV:165[B]:A:H1'	2.00	0.43
1:GG:84:LEU:HG	1:GG:149[A]:GLN:HB2	2.00	0.43
1:H:81:TRP:CD1	1:H:121:SER:HB3	2.54	0.43
1:K:99:LEU:HG	1:K:141:CYS:HA	1.99	0.43
1:CC:84:LEU:HG	1:CC:149[A]:GLN:HB2	2.00	0.43
1:DD:81:TRP:CD1	1:DD:121:SER:HB3	2.52	0.43
1:MM:81:TRP:CD1	1:MM:121:SER:HB3	2.53	0.43
1:M:81:TRP:CD1	1:M:121:SER:HB3	2.53	0.43
1:CC:84:LEU:HG	1:CC:149[B]:GLN:HB2	1.99	0.43
1:A:99:LEU:HG	1:A:141:CYS:HA	2.01	0.43
1:H:38:VAL:HG23	2:W:165[B]:A:H1'	2.00	0.43
1:II:79[B]:ARG:NH2	3:oo:189[B]:U:OP2	2.38	0.43
1:H:66:ARG:NH2	1:EE:34:THR:HB	2.33	0.43
1:GG:116:ILE:HG12	1:KK:117:ASN:HB3	1.99	0.43
1:OO:83:GLN:HB3	1:OO:149[B]:GLN:HB3	2.00	0.43
1:OO:117:ASN:HB3	1:PP:116:ILE:HG12	2.01	0.43
1:E:83:GLN:HB3	1:E:149[B]:GLN:HB3	2.01	0.43
1:K:79[B]:ARG:NH2	3:o:188[B]:U:O3'	2.52	0.43
1:N:17:SER:CA	2:Q:164[A]:A:H4'	2.48	0.43
1:N:83:GLN:HB3	1:N:149[B]:GLN:HB3	1.99	0.43
3:s:184[B]:U:H2'	3:s:185[B]:U:C6	2.53	0.43
1:LL:127:PRO:O	1:LL:131:ARG:HG3	2.19	0.43
1:G:99:LEU:HG	1:G:141:CYS:HA	2.01	0.43
1:I:70:PHE:CG	1:I:158:PHE:HB3	2.54	0.43
2:c:162[B]:A:H2'	2:c:163[B]:A:C8	2.54	0.43
1:GG:78:VAL:HG13	1:GG:154:ILE:HG12	2.01	0.43
1:KK:84:LEU:HG	1:KK:149[A]:GLN:HB2	2.01	0.43
1:LL:82:THR:HG21	1:LL:92:SER:HB3	2.01	0.43
1:PP:81:TRP:CD1	1:PP:121:SER:HB3	2.53	0.43
1:J:38:VAL:HG23	2:Y:165[A]:A:H1'	2.01	0.42
1:J:81:TRP:CD1	1:J:121:SER:HB3	2.54	0.42
1:K:116:ILE:HG12	1:O:117:ASN:HB3	2.00	0.42
1:O:99:LEU:HG	1:O:141:CYS:HA	2.00	0.42
3:g:184[A]:U:H2'	3:g:185[A]:U:C6	2.54	0.42
1:JJ:17:SER:HA	2:dd:164[A]:A:H4'	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81:TRP:CD1	1:D:121:SER:HB3	2.55	0.42
1:H:79[B]:ARG:NH2	3:l:189[B]:U:OP2	2.33	0.42
1:K:84:LEU:HG	1:K:149[A]:GLN:HB2	2.01	0.42
1:PP:127:PRO:O	1:PP:131:ARG:HG3	2.19	0.42
1:A:81:TRP:CD1	1:A:121:SER:HB3	2.54	0.42
2:b:165[B]:A:H2'	2:b:166[B]:A:H8	1.84	0.42
1:BB:30:LYS:HG3	1:KK:24:ARG:HG2	2.00	0.42
1:OO:36:THR:OG1	2:ff:165[B]:A:O2'	2.37	0.42
2:RR:161[A]:A:H2'	2:RR:162[A]:A:C8	2.54	0.42
2:ZZ:165[A]:A:H2'	2:ZZ:166[A]:A:C8	2.54	0.42
1:A:127:PRO:O	1:A:131:ARG:HG3	2.19	0.42
1:B:127:PRO:O	1:B:131:ARG:HG3	2.18	0.42
1:KK:84:LEU:HD12	1:KK:148:ARG:HB2	2.01	0.42
1:F:70:PHE:CD1	1:F:158:PHE:HB3	2.54	0.42
1:F:84:LEU:HG	1:F:149[A]:GLN:HB2	2.01	0.42
1:J:99:LEU:HG	1:J:141:CYS:HA	2.01	0.42
1:M:70:PHE:CD1	1:M:158:PHE:HB3	2.54	0.42
2:a:162[A]:A:H2'	2:a:163[A]:A:C8	2.54	0.42
2:a:162[A]:A:H2'	2:a:163[A]:A:H8	1.85	0.42
1:BB:81:TRP:CD1	1:BB:121:SER:HB3	2.54	0.42
1:BB:84:LEU:HD12	1:BB:148:ARG:HB2	2.00	0.42
1:KK:66:ARG:NH2	1:LL:34:THR:HB	2.35	0.42
1:OO:70:PHE:CD1	1:OO:158:PHE:HB3	2.54	0.42
2:RR:161[A]:A:H2'	2:RR:162[A]:A:H8	1.84	0.42
2:R:165[A]:A:H2'	2:R:166[A]:A:H8	1.85	0.42
1:OO:70:PHE:CG	1:OO:158:PHE:HB3	2.54	0.42
1:C:17:SER:HA	2:ZZ:164[A]:A:H5''	2.00	0.42
1:N:117:ASN:HB3	1:O:116:ILE:HG12	2.02	0.42
1:E:34:THR:HB	1:F:66:ARG:NH2	2.34	0.42
3:m:184[A]:U:H2'	3:m:185[A]:U:C6	2.54	0.42
1:FF:127:PRO:O	1:FF:131:ARG:HG3	2.20	0.42
1:LL:117:ASN:HB3	1:MM:116:ILE:HG12	2.02	0.42
3:kk:184[A]:U:H2'	3:kk:185[A]:U:C6	2.54	0.42
1:CC:82:THR:HG21	1:CC:92:SER:HB3	2.01	0.42
1:HH:78:VAL:HG13	1:HH:154:ILE:HG12	2.02	0.42
1:KK:17:SER:HA	2:QQ:164[A]:A:H4'	2.02	0.42
1:OO:81:TRP:CD1	1:OO:121:SER:HB3	2.54	0.42
3:e:184[A]:U:H2'	3:e:185[A]:U:C6	2.55	0.42
1:HH:38:VAL:HG22	1:HH:157[A]:CYS:SG	2.60	0.42
1:D:21:THR:HG21	2:V:165[A]:A:OP1	2.20	0.41
1:D:70:PHE:CD1	1:D:158:PHE:HB3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:81:TRP:CD1	1:I:121:SER:HB3	2.54	0.41
1:L:79[B]:ARG:HH12	3:p:189[B]:U:P	2.41	0.41
3:vv:184[B]:U:H2'	3:vv:185[B]:U:C6	2.55	0.41
1:G:38:VAL:O	2:WW:166[A]:A:O2'	2.36	0.41
1:O:38:VAL:HG23	2:d:165[B]:A:H1'	2.01	0.41
3:p:184[B]:U:H2'	3:p:185[B]:U:C6	2.56	0.41
1:LL:70:PHE:CD1	1:LL:158:PHE:HB3	2.54	0.41
2:bb:165[A]:A:H2'	2:bb:166[A]:A:H8	1.84	0.41
2:WW:162[A]:A:H2'	2:WW:163[A]:A:H8	1.84	0.41
1:A:39:ARG:NH2	1:O:33:PRO:O	2.53	0.41
1:H:97[B]:LYS:HB3	1:H:142:GLU:HB2	2.02	0.41
2:a:163[A]:A:H2'	2:a:164[A]:A:H8	1.83	0.41
1:GG:70:PHE:CD1	1:GG:158:PHE:HB3	2.56	0.41
1:L:117:ASN:HB3	1:M:116:ILE:HG12	2.02	0.41
1:M:70:PHE:CG	1:M:158:PHE:HB3	2.55	0.41
1:NN:127:PRO:O	1:NN:131:ARG:HG3	2.20	0.41
1:A:70:PHE:CD1	1:A:158:PHE:HB3	2.56	0.41
1:C:70:PHE:CD1	1:C:158:PHE:HB3	2.55	0.41
1:G:34:THR:HB	1:HH:66:ARG:NH2	2.34	0.41
1:CC:83:GLN:HB3	1:CC:149[B]:GLN:HB3	2.03	0.41
1:NN:57:VAL:HG22	1:NN:140:VAL:HG22	2.02	0.41
1:OO:84:LEU:HG	1:OO:149[A]:GLN:HB2	2.02	0.41
1:E:66:ARG:NH2	1:F:34:THR:HB	2.35	0.41
1:G:79[B]:ARG:NH2	3:k:188[B]:U:O3'	2.53	0.41
1:G:127:PRO:O	1:G:131:ARG:HG3	2.21	0.41
1:L:79[B]:ARG:NH2	3:p:189[B]:U:OP2	2.51	0.41
1:I:127:PRO:O	1:I:131:ARG:HG3	2.20	0.41
1:K:79[B]:ARG:NH2	3:o:189[B]:U:OP1	2.52	0.41
2:Q:167[A]:A:H2'	2:Q:168[A]:A:C8	2.56	0.41
1:GG:112:ARG:HD2	1:LL:28:TYR:CE2	2.56	0.41
1:NN:38:VAL:HG23	2:ee:165[B]:A:H1'	2.03	0.41
1:B:84:LEU:HG	1:B:149[B]:GLN:HB2	2.01	0.41
1:F:65:PHE:O	1:F:67:THR:HG23	2.21	0.41
1:G:37:TRP:CE2	1:G:39:ARG:HD3	2.56	0.41
1:L:99:LEU:HG	1:L:141:CYS:HA	2.03	0.41
1:M:127:PRO:O	1:M:131:ARG:HG3	2.21	0.41
1:N:127:PRO:O	1:N:131:ARG:HG3	2.20	0.41
1:DD:117:ASN:HB3	1:EE:116:ILE:HG12	2.03	0.41
1:DD:155[A]:SER:OG	3:jj:188[A]:U:H5'	2.21	0.41
1:EE:24:ARG:HG2	1:HH:30:LYS:HG3	2.03	0.41
1:JJ:82:THR:HG21	1:JJ:92:SER:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:rr:184[B]:U:H2'	3:rr:185[B]:U:C6	2.55	0.41
1:A:116:ILE:HG12	1:E:117:ASN:HB3	2.03	0.41
1:F:127:PRO:O	1:F:131:ARG:HG3	2.21	0.41
3:h:184[A]:U:H2'	3:h:185[A]:U:C6	2.56	0.41
1:CC:70:PHE:CG	1:CC:158:PHE:HB3	2.56	0.41
1:B:81:TRP:CD1	1:B:121:SER:HB3	2.57	0.40
1:H:70:PHE:CD1	1:H:158:PHE:HB3	2.55	0.40
1:EE:38:VAL:HG23	2:TT:165[A]:A:H1'	2.03	0.40
3:jj:184[A]:U:H2'	3:jj:185[A]:U:C6	2.56	0.40
1:K:97[B]:LYS:HB3	1:K:142:GLU:HB2	2.03	0.40
1:K:117:ASN:HB3	1:L:116:ILE:HG12	2.03	0.40
1:CC:36:THR:HG21	1:OO:19:VAL:CG1	2.49	0.40
1:C:39:ARG:HD2	3:g:186[A]:U:O2'	2.21	0.40
1:C:117:ASN:HB3	1:D:116:ILE:HG12	2.02	0.40
1:A:23:ILE:HD11	1:O:125:ARG:HB2	2.02	0.40
1:B:37:TRP:CE2	1:B:39:ARG:HD3	2.57	0.40
2:Y:165[A]:A:H2'	2:Y:166[A]:A:H8	1.86	0.40
3:7:207[B]:U:H3'	1:JJ:125:ARG:HE	1.86	0.40
1:EE:99:LEU:HG	1:EE:141:CYS:HA	2.04	0.40

All (3) 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)
2:Q:166[A]:A:O2'	1:CC:38:VAL:O[2_575]	2.12	0.08
1:N:38:VAL:O	2:SS:166[A]:A:O2'[2_575]	2.13	0.07
1:I:38:VAL:O	2:b:166[B]:A:O2'[2_575]	2.15	0.05

5.3 Torsion angles ⓘ

5.3.1 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	163/159 (102%)	156 (96%)	7 (4%)	0	100	100
1	B	159/159 (100%)	150 (94%)	9 (6%)	0	100	100
1	BB	163/159 (102%)	157 (96%)	6 (4%)	0	100	100
1	C	162/159 (102%)	155 (96%)	7 (4%)	0	100	100
1	CC	159/159 (100%)	152 (96%)	7 (4%)	0	100	100
1	D	163/159 (102%)	155 (95%)	8 (5%)	0	100	100
1	DD	160/159 (101%)	152 (95%)	8 (5%)	0	100	100
1	E	162/159 (102%)	155 (96%)	7 (4%)	0	100	100
1	EE	165/159 (104%)	157 (95%)	8 (5%)	0	100	100
1	F	162/159 (102%)	156 (96%)	6 (4%)	0	100	100
1	FF	160/159 (101%)	153 (96%)	7 (4%)	0	100	100
1	G	160/159 (101%)	153 (96%)	7 (4%)	0	100	100
1	GG	161/159 (101%)	155 (96%)	6 (4%)	0	100	100
1	H	162/159 (102%)	155 (96%)	7 (4%)	0	100	100
1	HH	160/159 (101%)	153 (96%)	7 (4%)	0	100	100
1	I	159/159 (100%)	153 (96%)	6 (4%)	0	100	100
1	II	163/159 (102%)	157 (96%)	6 (4%)	0	100	100
1	J	160/159 (101%)	155 (97%)	5 (3%)	0	100	100
1	JJ	158/159 (99%)	151 (96%)	7 (4%)	0	100	100
1	K	163/159 (102%)	158 (97%)	5 (3%)	0	100	100
1	KK	161/159 (101%)	153 (95%)	8 (5%)	0	100	100
1	L	160/159 (101%)	155 (97%)	5 (3%)	0	100	100
1	LL	163/159 (102%)	157 (96%)	6 (4%)	0	100	100
1	M	157/159 (99%)	150 (96%)	7 (4%)	0	100	100
1	MM	160/159 (101%)	153 (96%)	7 (4%)	0	100	100
1	N	160/159 (101%)	153 (96%)	7 (4%)	0	100	100
1	NN	157/159 (99%)	151 (96%)	6 (4%)	0	100	100
1	O	162/159 (102%)	157 (97%)	5 (3%)	0	100	100
1	OO	162/159 (102%)	154 (95%)	8 (5%)	0	100	100
1	PP	163/159 (102%)	157 (96%)	6 (4%)	0	100	100
All	All	4829/4770 (101%)	4628 (96%)	201 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	149/140 (106%)	149 (100%)	0	100	100
1	B	145/140 (104%)	145 (100%)	0	100	100
1	BB	149/140 (106%)	149 (100%)	0	100	100
1	C	148/140 (106%)	148 (100%)	0	100	100
1	CC	145/140 (104%)	145 (100%)	0	100	100
1	D	149/140 (106%)	149 (100%)	0	100	100
1	DD	146/140 (104%)	144 (99%)	2 (1%)	59	71
1	E	148/140 (106%)	146 (99%)	2 (1%)	59	71
1	EE	151/140 (108%)	151 (100%)	0	100	100
1	F	148/140 (106%)	148 (100%)	0	100	100
1	FF	146/140 (104%)	146 (100%)	0	100	100
1	G	146/140 (104%)	145 (99%)	1 (1%)	76	79
1	GG	147/140 (105%)	147 (100%)	0	100	100
1	H	148/140 (106%)	148 (100%)	0	100	100
1	HH	146/140 (104%)	146 (100%)	0	100	100
1	I	145/140 (104%)	143 (99%)	2 (1%)	59	71
1	II	149/140 (106%)	149 (100%)	0	100	100
1	J	146/140 (104%)	146 (100%)	0	100	100
1	JJ	144/140 (103%)	144 (100%)	0	100	100
1	K	149/140 (106%)	149 (100%)	0	100	100
1	KK	147/140 (105%)	147 (100%)	0	100	100
1	L	146/140 (104%)	146 (100%)	0	100	100
1	LL	149/140 (106%)	149 (100%)	0	100	100
1	M	143/140 (102%)	142 (99%)	1 (1%)	76	79
1	MM	146/140 (104%)	146 (100%)	0	100	100
1	N	146/140 (104%)	145 (99%)	1 (1%)	76	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	NN	143/140 (102%)	143 (100%)	0	100	100
1	O	148/140 (106%)	148 (100%)	0	100	100
1	OO	148/140 (106%)	148 (100%)	0	100	100
1	PP	149/140 (106%)	149 (100%)	0	100	100
All	All	4409/4200 (105%)	4400 (100%)	9 (0%)	87	87

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	157[A]	CYS
1	E	157[B]	CYS
1	G	19	VAL
1	I	157[A]	CYS
1	I	157[B]	CYS
1	M	21	THR
1	N	157	CYS
1	DD	157[A]	CYS
1	DD	157[B]	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	32	ASN
1	FF	32	ASN
1	GG	117	ASN
1	II	89	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	P	9/16 (56%)	0	0
2	Q	9/16 (56%)	0	0
2	QQ	9/16 (56%)	0	0
2	R	9/16 (56%)	0	0
2	RR	9/16 (56%)	0	0
2	S	9/16 (56%)	0	0
2	SS	9/16 (56%)	0	0
2	T	9/16 (56%)	0	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	TT	9/16 (56%)	0	0
2	U	9/16 (56%)	0	0
2	UU	9/16 (56%)	0	0
2	V	9/16 (56%)	0	0
2	VV	9/16 (56%)	0	0
2	W	9/16 (56%)	0	0
2	WW	9/16 (56%)	0	0
2	X	9/16 (56%)	0	0
2	Y	9/16 (56%)	0	0
2	YY	9/16 (56%)	0	0
2	Z	9/16 (56%)	0	0
2	ZZ	9/16 (56%)	0	0
2	a	9/16 (56%)	0	0
2	b	9/16 (56%)	0	0
2	bb	9/16 (56%)	0	0
2	c	9/16 (56%)	0	0
2	cc	9/16 (56%)	0	0
2	d	9/16 (56%)	0	0
2	dd	9/16 (56%)	0	0
2	ee	9/16 (56%)	0	0
2	ff	9/16 (56%)	0	0
2	gg	9/16 (56%)	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%)	2 (22%)	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	9/27 (33%)	1 (11%)	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	540/1803 (29%)	31 (5%)	0

All (31) 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	182[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	ss	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

30 ligands are modelled in this entry.

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
4	PO4	F	201[B]	-	4,4,4	0.98	0	6,6,6	0.46	0
4	PO4	F	201[D]	-	4,4,4	0.97	0	6,6,6	0.46	0
4	PO4	L	201[B]	-	4,4,4	0.98	0	6,6,6	0.46	0
4	PO4	B	201[B]	-	4,4,4	0.97	0	6,6,6	0.47	0
4	PO4	B	201[D]	-	4,4,4	0.97	0	6,6,6	0.46	0
4	PO4	DD	201[B]	-	4,4,4	0.98	0	6,6,6	0.47	0
4	PO4	DD	201[D]	-	4,4,4	0.98	0	6,6,6	0.46	0
4	PO4	KK	201[B]	-	4,4,4	0.97	0	6,6,6	0.45	0
4	PO4	KK	201[D]	-	4,4,4	0.97	0	6,6,6	0.46	0
4	PO4	L	201[D]	-	4,4,4	0.97	0	6,6,6	0.47	0
4	PO4	LL	201[E]	-	4,4,4	0.98	0	6,6,6	0.46	0
4	PO4	L	201[A]	-	4,4,4	0.98	0	6,6,6	0.46	0
4	PO4	F	201[E]	-	4,4,4	0.98	0	6,6,6	0.47	0
4	PO4	B	201[E]	-	4,4,4	0.97	0	6,6,6	0.47	0
4	PO4	DD	201[E]	-	4,4,4	0.98	0	6,6,6	0.46	0
4	PO4	L	201[E]	-	4,4,4	0.97	0	6,6,6	0.45	0
4	PO4	KK	201[E]	-	4,4,4	0.97	0	6,6,6	0.47	0
4	PO4	LL	201[A]	-	4,4,4	0.97	0	6,6,6	0.47	0
4	PO4	LL	201[C]	-	4,4,4	0.97	0	6,6,6	0.47	0
4	PO4	F	201[A]	-	4,4,4	0.98	0	6,6,6	0.46	0
4	PO4	F	201[C]	-	4,4,4	0.97	0	6,6,6	0.46	0
4	PO4	LL	201[B]	-	4,4,4	0.98	0	6,6,6	0.46	0
4	PO4	LL	201[D]	-	4,4,4	0.98	0	6,6,6	0.47	0
4	PO4	B	201[C]	-	4,4,4	0.97	0	6,6,6	0.47	0
4	PO4	B	201[A]	-	4,4,4	0.97	0	6,6,6	0.46	0
4	PO4	DD	201[A]	-	4,4,4	0.97	0	6,6,6	0.47	0
4	PO4	KK	201[A]	-	4,4,4	0.97	0	6,6,6	0.46	0
4	PO4	KK	201[C]	-	4,4,4	0.98	0	6,6,6	0.45	0
4	PO4	L	201[C]	-	4,4,4	0.98	0	6,6,6	0.47	0
4	PO4	DD	201[C]	-	4,4,4	0.97	0	6,6,6	0.46	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.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	KK	201[B]	PO4	1	0
4	LL	201[B]	PO4	1	0
4	L	201[C]	PO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.26	3 (2%) 63 47	8, 18, 29, 73	19 (13%)
1	B	144/159 (90%)	0.23	2 (1%) 73 55	9, 19, 30, 69	17 (11%)
1	BB	144/159 (90%)	0.38	4 (2%) 55 40	9, 20, 33, 61	19 (13%)
1	C	144/159 (90%)	0.26	0 100 100	9, 20, 34, 62	19 (13%)
1	CC	144/159 (90%)	0.30	1 (0%) 84 68	10, 19, 36, 60	17 (11%)
1	D	144/159 (90%)	0.21	1 (0%) 84 68	9, 20, 28, 65	21 (14%)
1	DD	144/159 (90%)	0.29	2 (1%) 73 55	9, 19, 31, 73	18 (12%)
1	E	144/159 (90%)	0.33	3 (2%) 63 47	9, 19, 31, 64	20 (13%)
1	EE	144/159 (90%)	0.33	4 (2%) 55 40	8, 19, 24, 73	21 (14%)
1	F	144/159 (90%)	0.38	2 (1%) 73 55	9, 18, 28, 54	19 (13%)
1	FF	144/159 (90%)	0.34	4 (2%) 55 40	9, 20, 33, 62	18 (12%)
1	G	144/159 (90%)	0.31	2 (1%) 73 55	9, 19, 32, 75	18 (12%)
1	GG	144/159 (90%)	0.31	3 (2%) 63 47	8, 20, 33, 74	18 (12%)
1	H	144/159 (90%)	0.30	2 (1%) 73 55	9, 19, 32, 69	20 (13%)
1	HH	144/159 (90%)	0.24	2 (1%) 73 55	9, 20, 31, 63	18 (12%)
1	I	144/159 (90%)	0.34	1 (0%) 84 68	9, 19, 31, 86	16 (11%)
1	II	144/159 (90%)	0.35	1 (0%) 84 68	9, 20, 36, 72	21 (14%)
1	J	144/159 (90%)	0.29	1 (0%) 84 68	9, 19, 31, 100	17 (11%)
1	JJ	144/159 (90%)	0.38	2 (1%) 73 55	10, 20, 34, 75	15 (10%)
1	K	144/159 (90%)	0.29	2 (1%) 73 55	8, 18, 26, 78	20 (13%)
1	KK	144/159 (90%)	0.36	6 (4%) 40 31	10, 20, 34, 59	18 (12%)
1	L	144/159 (90%)	0.33	7 (4%) 35 29	9, 19, 33, 68	18 (12%)
1	LL	144/159 (90%)	0.33	2 (1%) 73 55	9, 20, 34, 66	20 (13%)
1	M	144/159 (90%)	0.32	4 (2%) 55 40	9, 18, 33, 73	15 (10%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	MM	144/159 (90%)	0.34	5 (3%)	47 35	10, 20, 32, 68	18 (12%)
1	N	144/159 (90%)	0.39	2 (1%)	73 55	8, 18, 30, 63	17 (11%)
1	NN	144/159 (90%)	0.30	4 (2%)	55 40	10, 20, 33, 58	15 (10%)
1	O	144/159 (90%)	0.31	1 (0%)	84 68	9, 18, 32, 75	20 (13%)
1	OO	144/159 (90%)	0.35	2 (1%)	73 55	9, 20, 30, 76	19 (13%)
1	PP	144/159 (90%)	0.27	0	100 100	9, 19, 32, 61	20 (13%)
2	P	10/16 (62%)	1.73	3 (30%)	1 3	17, 24, 31, 37	10 (100%)
2	Q	10/16 (62%)	1.17	3 (30%)	1 3	14, 24, 52, 57	10 (100%)
2	QQ	10/16 (62%)	1.87	5 (50%)	0 1	14, 24, 44, 45	10 (100%)
2	R	10/16 (62%)	1.29	1 (10%)	12 15	16, 19, 32, 42	10 (100%)
2	RR	10/16 (62%)	1.55	4 (40%)	1 1	19, 26, 42, 55	10 (100%)
2	S	10/16 (62%)	1.79	4 (40%)	1 1	14, 27, 39, 40	10 (100%)
2	SS	10/16 (62%)	1.47	3 (30%)	1 3	15, 19, 34, 42	10 (100%)
2	T	10/16 (62%)	2.18	6 (60%)	0 1	10, 18, 54, 56	10 (100%)
2	TT	10/16 (62%)	1.54	2 (20%)	3 5	18, 27, 34, 44	10 (100%)
2	U	10/16 (62%)	1.76	4 (40%)	1 1	15, 22, 44, 50	10 (100%)
2	UU	10/16 (62%)	1.50	4 (40%)	1 1	18, 26, 44, 46	10 (100%)
2	V	10/16 (62%)	1.57	3 (30%)	1 3	16, 21, 30, 48	10 (100%)
2	VV	10/16 (62%)	1.96	5 (50%)	0 1	13, 21, 38, 48	10 (100%)
2	W	10/16 (62%)	1.33	3 (30%)	1 3	14, 21, 49, 49	10 (100%)
2	WW	10/16 (62%)	1.79	4 (40%)	1 1	16, 25, 30, 46	10 (100%)
2	X	10/16 (62%)	1.11	1 (10%)	12 15	11, 20, 31, 40	10 (100%)
2	Y	10/16 (62%)	1.25	1 (10%)	12 15	13, 24, 37, 49	10 (100%)
2	YY	10/16 (62%)	1.33	2 (20%)	3 5	18, 28, 43, 50	10 (100%)
2	Z	10/16 (62%)	1.47	4 (40%)	1 1	13, 21, 38, 45	10 (100%)
2	ZZ	10/16 (62%)	1.34	3 (30%)	1 3	9, 17, 31, 49	10 (100%)
2	a	10/16 (62%)	1.56	4 (40%)	1 1	10, 19, 28, 57	10 (100%)
2	b	10/16 (62%)	1.25	2 (20%)	3 5	14, 20, 49, 49	10 (100%)
2	bb	10/16 (62%)	1.46	4 (40%)	1 1	14, 19, 46, 55	10 (100%)
2	c	10/16 (62%)	1.77	4 (40%)	1 1	11, 19, 38, 41	10 (100%)
2	cc	10/16 (62%)	1.68	2 (20%)	3 5	11, 19, 40, 41	10 (100%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	d	10/16 (62%)	1.37	4 (40%) 1 1	14, 22, 41, 42	10 (100%)
2	dd	10/16 (62%)	1.72	5 (50%) 0 1	12, 20, 36, 44	10 (100%)
2	ee	10/16 (62%)	1.17	2 (20%) 3 5	16, 23, 32, 41	10 (100%)
2	ff	10/16 (62%)	1.61	4 (40%) 1 1	16, 20, 31, 34	10 (100%)
2	gg	10/16 (62%)	1.72	4 (40%) 1 1	15, 23, 34, 38	10 (100%)
3	1	2/27 (7%)	3.08	2 (100%) 0 0	42, 42, 42, 47	2 (100%)
3	2	2/27 (7%)	3.19	2 (100%) 0 0	27, 27, 27, 37	2 (100%)
3	3	2/27 (7%)	2.32	1 (50%) 0 1	33, 33, 33, 33	2 (100%)
3	4	2/27 (7%)	2.68	2 (100%) 0 0	34, 34, 34, 42	2 (100%)
3	5	2/27 (7%)	3.56	2 (100%) 0 0	22, 22, 22, 26	2 (100%)
3	6	2/27 (7%)	3.08	2 (100%) 0 0	36, 36, 36, 40	2 (100%)
3	7	22/27 (81%)	2.78	18 (81%) 0 0	16, 27, 41, 46	22 (100%)
3	8	2/27 (7%)	3.25	2 (100%) 0 0	38, 38, 38, 38	2 (100%)
3	e	10/27 (37%)	1.79	4 (40%) 1 1	18, 21, 32, 50	10 (100%)
3	f	10/27 (37%)	1.16	1 (10%) 12 15	15, 23, 47, 48	10 (100%)
3	g	10/27 (37%)	1.46	2 (20%) 3 5	12, 18, 29, 44	10 (100%)
3	h	10/27 (37%)	1.83	4 (40%) 1 1	14, 17, 50, 52	10 (100%)
3	hh	10/27 (37%)	1.78	4 (40%) 1 1	18, 22, 38, 45	10 (100%)
3	i	10/27 (37%)	1.81	6 (60%) 0 1	16, 18, 43, 51	10 (100%)
3	ii	10/27 (37%)	1.01	1 (10%) 12 15	12, 22, 65, 65	10 (100%)
3	j	10/27 (37%)	1.17	0 100 100	22, 24, 55, 70	10 (100%)
3	jj	10/27 (37%)	1.23	3 (30%) 1 3	13, 19, 43, 55	10 (100%)
3	k	10/27 (37%)	1.73	4 (40%) 1 1	13, 23, 37, 39	10 (100%)
3	kk	10/27 (37%)	1.43	1 (10%) 12 15	13, 26, 51, 56	10 (100%)
3	l	10/27 (37%)	1.46	3 (30%) 1 3	16, 23, 47, 72	10 (100%)
3	ll	10/27 (37%)	1.40	3 (30%) 1 3	19, 22, 31, 69	10 (100%)
3	m	10/27 (37%)	1.30	1 (10%) 12 15	12, 19, 32, 50	10 (100%)
3	mm	10/27 (37%)	1.82	3 (30%) 1 3	18, 26, 51, 55	10 (100%)
3	n	10/27 (37%)	1.45	4 (40%) 1 1	11, 21, 35, 47	10 (100%)
3	nn	10/27 (37%)	1.58	2 (20%) 3 5	10, 17, 31, 40	10 (100%)
3	o	10/27 (37%)	1.37	4 (40%) 1 1	12, 19, 25, 44	10 (100%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
3	oo	10/27 (37%)	1.57	3 (30%) 1 3	25, 28, 43, 57	10 (100%)
3	p	10/27 (37%)	1.19	3 (30%) 1 3	13, 18, 29, 51	10 (100%)
3	pp	10/27 (37%)	1.40	4 (40%) 1 1	9, 17, 41, 48	10 (100%)
3	q	10/27 (37%)	1.09	2 (20%) 3 5	13, 17, 38, 54	10 (100%)
3	qq	10/27 (37%)	1.73	5 (50%) 0 1	12, 22, 39, 47	10 (100%)
3	r	10/27 (37%)	1.41	3 (30%) 1 3	11, 19, 36, 52	10 (100%)
3	rr	10/27 (37%)	1.77	4 (40%) 1 1	13, 21, 38, 50	10 (100%)
3	s	10/27 (37%)	1.84	5 (50%) 0 1	18, 21, 35, 58	10 (100%)
3	ss	10/27 (37%)	1.62	4 (40%) 1 1	10, 16, 35, 40	10 (100%)
3	t	2/27 (7%)	3.17	2 (100%) 0 0	18, 18, 18, 33	2 (100%)
3	tt	10/27 (37%)	0.94	2 (20%) 3 5	15, 21, 39, 41	10 (100%)
3	u	2/27 (7%)	3.11	2 (100%) 0 0	23, 23, 23, 33	2 (100%)
3	uu	10/27 (37%)	1.02	1 (10%) 12 15	15, 21, 28, 54	10 (100%)
3	v	2/27 (7%)	2.92	2 (100%) 0 0	26, 26, 26, 38	2 (100%)
3	vv	10/27 (37%)	1.99	5 (50%) 0 1	22, 24, 41, 50	10 (100%)
3	w	2/27 (7%)	4.06	2 (100%) 0 0	40, 40, 40, 44	2 (100%)
3	ww	2/27 (7%)	3.07	1 (50%) 0 1	24, 24, 24, 31	2 (100%)
3	x	2/27 (7%)	2.78	2 (100%) 0 0	14, 14, 14, 18	2 (100%)
3	xx	2/27 (7%)	5.19	2 (100%) 0 0	15, 15, 15, 17	2 (100%)
3	y	2/27 (7%)	3.27	2 (100%) 0 0	26, 26, 26, 31	2 (100%)
3	yy	2/27 (7%)	2.81	2 (100%) 0 0	27, 27, 27, 39	2 (100%)
3	z	2/27 (7%)	3.27	2 (100%) 0 0	23, 23, 23, 40	2 (100%)
3	zz	2/27 (7%)	3.11	2 (100%) 0 0	29, 29, 29, 31	2 (100%)
All	All	4978/6573 (75%)	0.49	318 (6%) 25 23	8, 19, 38, 100	1209 (24%)

All (318) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	xx	196[B]	U	5.3
3	xx	195[B]	U	5.1
3	7	208[B]	U	4.7
3	5	195[A]	U	4.6
3	7	214[A]	U	4.4
2	TT	170[A]	A	4.3

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Mol	Chain	Res	Type	RSRZ
3	w	196[B]	U	4.3
3	7	207[B]	U	4.2
1	G	16	ASN	4.2
3	ww	195[B]	U	4.2
3	rr	182[B]	U	4.1
1	FF	123	GLY	4.0
2	QQ	169[A]	A	4.0
3	vv	182[B]	U	3.9
3	w	195[B]	U	3.9
1	GG	24	ARG	3.8
3	y	195[A]	U	3.8
1	J	16	ASN	3.7
3	u	195[A]	U	3.7
1	OO	24	ARG	3.7
3	z	195[A]	U	3.7
1	K	16	ASN	3.7
3	hh	189[A]	U	3.7
3	1	196[A]	U	3.7
2	T	170[A]	A	3.7
1	M	24	ARG	3.6
1	KK	24	ARG	3.6
3	2	195[B]	U	3.6
3	7	198[A]	U	3.6
2	cc	169[B]	A	3.6
2	gg	169[B]	A	3.5
3	e	182[A]	U	3.5
3	8	195[A]	U	3.5
2	VV	169[B]	A	3.5
1	EE	24	ARG	3.4
3	hh	182[A]	U	3.4
3	7	210[A]	U	3.4
2	dd	161[A]	A	3.4
2	U	162[B]	A	3.3
1	F	16	ASN	3.3
1	MM	24	ARG	3.3
2	b	170[B]	A	3.3
2	gg	170[B]	A	3.3
2	YY	170[B]	A	3.3
1	NN	24	ARG	3.3
3	t	196[B]	U	3.3
2	c	161[B]	A	3.2
3	7	201[B]	U	3.2

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Mol	Chain	Res	Type	RSRZ
3	ss	181[B]	U	3.2
1	KK	27[A]	SER	3.2
3	6	195[A]	U	3.2
2	S	163[A]	A	3.2
3	v	195[B]	U	3.2
3	zz	196[B]	U	3.1
2	T	169[A]	A	3.1
1	JJ	16	ASN	3.1
3	3	196[B]	U	3.1
2	SS	170[A]	A	3.1
3	rr	183[B]	U	3.1
3	g	189[A]	U	3.1
3	i	181[A]	U	3.1
1	L	24	ARG	3.1
2	UU	169[A]	A	3.1
3	t	195[B]	U	3.1
3	7	195[A]	U	3.1
3	zz	195[B]	U	3.1
2	VV	170[B]	A	3.1
1	BB	16	ASN	3.1
3	ss	189[B]	U	3.1
3	7	197[A]	U	3.0
3	qq	183[A]	U	3.0
3	7	205[A]	U	3.0
3	8	196[A]	U	3.0
2	T	164[A]	A	3.0
2	c	162[B]	A	3.0
2	WW	169[A]	A	3.0
3	7	213[A]	U	3.0
3	6	196[A]	U	3.0
3	7	209[A]	U	3.0
3	7	211[A]	U	3.0
1	I	16	ASN	3.0
3	l	183[B]	U	2.9
3	7	196[A]	U	2.9
2	c	163[B]	A	2.9
1	NN	19	VAL	2.9
3	ss	183[B]	U	2.9
2	SS	161[A]	A	2.9
3	r	190[B]	U	2.9
2	ff	170[B]	A	2.9
3	x	195[B]	U	2.9

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Mol	Chain	Res	Type	RSRZ
1	L	17	SER	2.9
2	Z	169[B]	A	2.9
2	RR	161[A]	A	2.9
3	yy	196[A]	U	2.9
1	MM	17	SER	2.9
1	B	16	ASN	2.9
2	V	169[A]	A	2.8
1	O	16	ASN	2.8
3	h	183[A]	U	2.8
3	z	196[A]	U	2.8
2	RR	170[A]	A	2.8
1	II	39[A]	ARG	2.8
3	ll	190[A]	U	2.8
3	2	196[B]	U	2.8
2	ZZ	169[A]	A	2.8
3	y	196[A]	U	2.8
3	yy	195[A]	U	2.8
2	V	162[A]	A	2.8
2	X	170[A]	A	2.8
2	WW	162[A]	A	2.8
3	n	182[A]	U	2.7
2	P	170[A]	A	2.7
2	RR	162[A]	A	2.7
3	mm	182[B]	U	2.7
3	pp	189[A]	U	2.7
1	MM	23	ILE	2.7
2	QQ	170[A]	A	2.7
2	SS	163[A]	A	2.7
2	dd	163[A]	A	2.7
3	k	190[B]	U	2.7
1	N	23	ILE	2.7
2	d	169[B]	A	2.7
2	dd	170[A]	A	2.7
2	ff	162[B]	A	2.7
3	r	183[B]	U	2.7
1	KK	16	ASN	2.7
2	QQ	163[A]	A	2.7
3	4	195[A]	U	2.7
3	nn	181[B]	U	2.7
3	oo	181[B]	U	2.7
3	h	189[A]	U	2.7
3	v	196[B]	U	2.7

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Mol	Chain	Res	Type	RSRZ
3	x	196[B]	U	2.7
3	ss	182[B]	U	2.7
2	Y	169[A]	A	2.7
3	4	196[A]	U	2.7
3	ll	182[A]	U	2.7
2	Z	170[B]	A	2.7
1	FF	16	ASN	2.6
3	k	181[B]	U	2.6
3	q	189[B]	U	2.6
1	B	17	SER	2.6
3	e	190[A]	U	2.6
3	h	190[A]	U	2.6
3	r	182[B]	U	2.6
3	rr	181[B]	U	2.6
3	7	212[A]	U	2.6
1	NN	16	ASN	2.6
1	DD	24	ARG	2.6
3	rr	189[B]	U	2.6
3	i	184[A]	U	2.6
3	n	184[A]	U	2.6
3	5	196[A]	U	2.6
1	L	123	GLY	2.6
1	K	24	ARG	2.6
2	d	170[B]	A	2.6
3	vv	184[B]	U	2.6
3	vv	181[B]	U	2.5
1	F	22[A]	MET	2.5
3	7	206[A]	U	2.5
3	qq	189[A]	U	2.5
2	ZZ	170[A]	A	2.5
3	1	195[A]	U	2.5
3	nn	190[B]	U	2.5
3	u	196[A]	U	2.5
1	KK	125	ARG	2.5
3	ii	182[B]	U	2.5
2	VV	163[B]	A	2.4
2	ee	170[B]	A	2.4
3	kk	181[A]	U	2.4
3	mm	190[B]	U	2.4
3	tt	189[B]	U	2.4
1	E	17	SER	2.4
1	CC	24	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
3	l	189[B]	U	2.4
3	qq	182[A]	U	2.4
2	a	170[A]	A	2.4
2	bb	163[A]	A	2.4
3	pp	182[A]	U	2.4
1	BB	52	ALA	2.4
2	T	163[A]	A	2.4
2	WW	163[A]	A	2.4
3	s	190[B]	U	2.4
1	LL	16	ASN	2.4
3	e	181[A]	U	2.4
2	S	165[A]	A	2.4
2	W	162[B]	A	2.4
2	c	169[B]	A	2.4
2	dd	162[A]	A	2.4
2	ee	162[B]	A	2.4
1	A	16	ASN	2.4
2	S	170[A]	A	2.4
2	a	169[A]	A	2.4
3	e	183[A]	U	2.3
3	l	190[B]	U	2.3
3	s	183[B]	U	2.3
3	qq	190[A]	U	2.3
2	R	163[A]	A	2.3
2	QQ	162[A]	A	2.3
1	M	16	ASN	2.3
3	i	189[A]	U	2.3
2	T	161[A]	A	2.3
2	VV	162[B]	A	2.3
3	k	189[B]	U	2.3
2	gg	162[B]	A	2.3
1	LL	35[A]	PRO	2.3
3	k	182[B]	U	2.3
3	p	189[B]	U	2.3
2	U	161[B]	A	2.3
2	YY	161[B]	A	2.3
2	ff	161[B]	A	2.3
2	gg	163[B]	A	2.3
1	H	24	ARG	2.3
1	A	17	SER	2.3
1	DD	16	ASN	2.3
1	MM	16	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
3	o	189[B]	U	2.3
3	pp	181[A]	U	2.3
1	L	23	ILE	2.3
1	HH	17	SER	2.3
1	D	24	ARG	2.3
1	JJ	24	ARG	2.3
2	U	170[B]	A	2.2
2	d	161[B]	A	2.2
1	KK	30	LYS	2.2
1	KK	50	GLY	2.2
3	hh	183[A]	U	2.2
2	S	168[A]	A	2.2
2	T	168[A]	A	2.2
2	UU	163[A]	A	2.2
1	EE	141	CYS	2.2
1	M	26	GLY	2.2
1	EE	103	GLY	2.2
3	s	182[B]	U	2.2
3	jj	189[A]	U	2.2
3	jj	190[A]	U	2.2
2	QQ	161[A]	A	2.2
2	bb	161[A]	A	2.2
1	GG	25	ALA	2.2
2	P	163[A]	A	2.2
2	VV	161[B]	A	2.2
2	WW	170[A]	A	2.2
1	MM	25	ALA	2.2
3	f	190[B]	U	2.2
3	hh	190[A]	U	2.2
2	U	163[B]	A	2.2
2	ZZ	162[A]	A	2.2
2	dd	169[A]	A	2.2
2	ff	163[B]	A	2.2
1	M	76	MET	2.2
3	jj	181[A]	U	2.2
1	OO	95[A]	ARG	2.2
2	Q	170[A]	A	2.2
3	m	181[A]	U	2.2
3	s	184[B]	U	2.2
3	mm	183[B]	U	2.2
1	G	24	ARG	2.2
2	W	169[B]	A	2.2

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Mol	Chain	Res	Type	RSRZ
2	bb	169[A]	A	2.2
3	n	189[A]	U	2.1
3	tt	190[B]	U	2.1
1	E	16	ASN	2.1
2	bb	170[A]	A	2.1
1	L	25	ALA	2.1
3	i	190[A]	U	2.1
1	HH	22[A]	MET	2.1
2	a	161[A]	A	2.1
3	h	182[A]	U	2.1
3	uu	190[B]	U	2.1
3	vv	189[B]	U	2.1
1	E	144[A]	ARG	2.1
1	BB	24	ARG	2.1
3	o	182[B]	U	2.1
3	7	199[B]	U	2.1
3	oo	189[B]	U	2.1
2	UU	170[A]	A	2.1
2	cc	162[B]	A	2.1
2	Q	162[A]	A	2.1
2	W	163[B]	A	2.1
2	TT	169[A]	A	2.1
3	n	190[A]	U	2.1
3	o	181[B]	U	2.1
3	7	202[B]	U	2.1
1	H	129	ASN	2.1
1	L	16	ASN	2.1
1	L	18[A]	ASN	2.1
2	P	161[A]	A	2.1
2	Q	169[A]	A	2.1
2	a	163[A]	A	2.1
3	i	182[A]	U	2.1
3	s	181[B]	U	2.1
3	pp	190[A]	U	2.1
1	BB	50	GLY	2.1
1	GG	17	SER	2.1
3	p	181[B]	U	2.1
3	oo	182[B]	U	2.1
2	Z	162[B]	A	2.0
1	EE	16	ASN	2.0
1	A	114	SER	2.0
1	NN	17	SER	2.0

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Mol	Chain	Res	Type	RSRZ
3	p	190[B]	U	2.0
1	FF	24	ARG	2.0
2	b	161[B]	A	2.0
2	d	162[B]	A	2.0
3	g	182[A]	U	2.0
3	o	183[B]	U	2.0
3	7	215[A]	U	2.0
3	vv	183[B]	U	2.0
1	N	24	ARG	2.0
1	FF	121	SER	2.0
2	V	161[A]	A	2.0
2	Z	163[B]	A	2.0
2	RR	169[A]	A	2.0
2	UU	168[A]	A	2.0
3	i	188[A]	U	2.0
3	q	182[B]	U	2.0
3	ll	183[A]	U	2.0
3	qq	181[A]	U	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 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(Å ²)	Q<0.9
4	PO4	KK	201[A]	5/5	0.79	0.37	19,19,19,19	5
4	PO4	KK	201[B]	5/5	0.79	0.37	19,19,19,19	5
4	PO4	KK	201[C]	5/5	0.79	0.37	19,19,19,19	5
4	PO4	KK	201[D]	5/5	0.79	0.37	19,19,19,19	5
4	PO4	KK	201[E]	5/5	0.79	0.37	19,19,19,19	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PO4	F	201[A]	5/5	0.82	0.37	18,18,18,18	5
4	PO4	F	201[B]	5/5	0.82	0.37	18,18,18,18	5
4	PO4	F	201[C]	5/5	0.82	0.37	18,18,18,18	5
4	PO4	F	201[D]	5/5	0.82	0.37	18,18,18,18	5
4	PO4	F	201[E]	5/5	0.82	0.37	18,18,18,18	5
4	PO4	L	201[A]	5/5	0.83	0.30	17,17,17,17	5
4	PO4	L	201[B]	5/5	0.83	0.30	17,17,17,17	5
4	PO4	L	201[C]	5/5	0.83	0.30	17,17,17,17	5
4	PO4	L	201[D]	5/5	0.83	0.30	17,17,17,17	5
4	PO4	L	201[E]	5/5	0.83	0.30	17,17,17,17	5
4	PO4	LL	201[A]	5/5	0.86	0.32	19,19,19,19	5
4	PO4	LL	201[B]	5/5	0.86	0.32	19,19,19,19	5
4	PO4	LL	201[C]	5/5	0.86	0.32	19,19,19,19	5
4	PO4	LL	201[D]	5/5	0.86	0.32	19,19,19,19	5
4	PO4	LL	201[E]	5/5	0.86	0.32	19,19,19,19	5
4	PO4	B	201[A]	5/5	0.93	0.23	18,18,18,18	5
4	PO4	B	201[B]	5/5	0.93	0.23	18,18,18,18	5
4	PO4	B	201[C]	5/5	0.93	0.23	18,18,18,18	5
4	PO4	B	201[D]	5/5	0.93	0.23	18,18,18,18	5
4	PO4	B	201[E]	5/5	0.93	0.23	18,18,18,18	5
4	PO4	DD	201[A]	5/5	0.97	0.24	18,18,18,18	5
4	PO4	DD	201[B]	5/5	0.97	0.24	18,18,18,18	5
4	PO4	DD	201[C]	5/5	0.97	0.24	18,18,18,18	5
4	PO4	DD	201[D]	5/5	0.97	0.24	18,18,18,18	5
4	PO4	DD	201[E]	5/5	0.97	0.24	18,18,18,18	5

6.5 Other polymers

There are no such residues in this entry.