

Full wwPDB X-ray Structure Validation Report (i)

Oct 10, 2023 – 01:46 AM EDT

PDB ID	:	7M50
Title	:	Crystallographic structure of a cubic crystal form of STMV grown from am-
		monium sulfate
Authors	:	McPherson, A.
Deposited on	:	2021-03-22
Resolution	:	2.31 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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.31 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$				
R _{free}	130704	5974(2.34-2.30)				
Clashscore	141614	6604 (2.34-2.30)				
Ramachandran outliers	138981	6523 (2.34-2.30)				
Sidechain outliers	138945	6523 (2.34-2.30)				
RSRZ outliers	127900	5855 (2.34-2.30)				
RNA backbone	3102	1031 (2.70-1.94)				

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 <=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	А	159	86%	6%	8%
1	В	159	84%	6%	10%
1	С	159	% 8 5%	5%	10%
1	D	159	% 	6%	9%



Mol	Chain	Length	Quality of chain	
1	Б	150	% •	
	E	109	82% %	9% 9%
1	F	159	87%	5% 8%
			%	
1	G	159	82%	9% • 8%
1	GG	159		F 0/ 00/
1	uu	105	3%	5% 9%
1	Н	159	84%	8% 8%
1	ттт	150		
	пп	109	87%	• 9%
1	Ι	159	87%	• 9%
		1 2 0	.% •	
	11	159	81%	8% • 10%
1	J	159	85%	8% 8%
			3%	
1	JJ	159	87%	6% 8%
1	K	150	4%	20/ 20/
1	11	105	<u>%</u>	070 070
1	KK	159	88%	• 9%
1	т	150	10%	
1	L	109	87%	10% ••
1	М	159	89%	• 9%
		1 7 0	4%	
1	N	159	85%	5% • 9%
1	0	159	80%	5% 6%
		100	88%	570 670
2	Р	8	62% 25%	12%
9	ΤT	0	88%	120/
	11	0	25% 12% 50% 75%	12%
2	V	8	62% 25%	12%
	G	0	67%	
3	S	6	67% 17%	17%
3	Т	6	17% 67%	17%
			80%	
4	UU	10	60% 10% 10%	20%
1	v	10	60%	20%
		10	80%	20%
4	bb	10	60% 30%	10%
~	3.7	-	86%	
6	Y	1	86%	14%



Mol	Chain	Length		Quality of	chain 🛛	
5	а	7	57	86%	200/	1.49/
	a		16	75%	29%	14 70
6	WW	12	17%	42%	25%	17%
6	е	12	42%	83%	42%	17%
			6	60%		
7	h	10	50%		30%	20%
0	:	0	22%			
0	1	9	33%	22%	44	%
8	11	9	44%	11%	44	%
			33%			
8	$\mathbf{q}\mathbf{q}$	9	569	%	44	1%
			50%			
9	kk	8		62%	12%	25%
			38%			
9	m	8		12% 12%		
			50%			
9	n	8		88%		12%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	MG	В	702	-	-	-	Х



2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 29786 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Δ	146	Total	С	Ν	0	S	0	0	0
	A	140	1130	709	201	214	6	0	0	0
1	D	149	Total	С	Ν	0	S	0	10	0
	D	140	1110	699	197	208	6	0	10	0
1	С	1/13	Total	С	Ν	0	S	0	14	0
1	U	140	1110	699	197	208	6	0	14	0
1	D 144	144	Total	С	Ν	Ο	\mathbf{S}	0	19	0
1		111	1118	703	199	210	6	0	12	0
1	E 145	145	Total	С	Ν	Ο	\mathbf{S}	0	12	0
		110	1126	707	200	213	6	0	12	0
1	F	147	Total	С	Ν	Ο	\mathbf{S}	0	10	0
	1	111	1137	713	202	216	6	0	10	0
1	G	146	Total	С	Ν	Ο	\mathbf{S}	0	8	0
	<u> </u>	110	1130	709	201	214	6	Ŭ	0	0
1	Н	147	Total	С	Ν	Ο	\mathbf{S}	0	10	0
			1137	713	202	216	6	Ŭ	10	
1	I	144	Total	С	Ν	0	S	0	8	0
	-		1118	703	199	210	6	Ŭ	<u> </u>	Ŭ
1	.J	147	Total	С	Ν	0	S	0	9	0
	, in the second		1137	713	202	216	6	, , , , , , , , , , , , , , , , , , ,	-	Ŭ
1	K	146	Total	С	N	0	S	0	8	0
		_	1130	709	201	214	<u>6</u>		_	_
1	L	157	Total	C	N	0	S	0	6	0
			1215	761	221	227	<u>6</u>			
1	М	144	Total	C	N	0	S	0	7	0
			1118	703	199	210	<u>6</u>			
1	Ν	144	Total	U 709	N 100	0	S	0	3	0
			1118	703	199	210	<u>6</u>			
1	1 0	150	Total	C	N	0	S	0	17	0
			1163	728	209	220	<u>6</u> C			
1	GG	144	Total	C	N	U 010	S	0	12	0
			1118	703	199	210	6			Ŭ

• Molecule 1 is a protein called Coat protein.



Mol	Chain	Residues		At	\mathbf{oms}			ZeroOcc	AltConf	Trace
1 HH	144	Total	С	Ν	0	S	0	0	0	
		1118	703	199	210	6	0	9	0	
1	II 142	Total	С	Ν	0	S	0	9	0	
	140	1110	699	197	208	6	0			
1	TT	1.47	Total	С	Ν	0	\mathbf{S}	0	19	0
1 11	147	1137	713	202	216	6	0	10	U	
1 KK	145	Total	С	Ν	0	S	0	0	0	
		1126	707	200	213	6	0	9	0	

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2 P	7	Total	С	Ν	Ο	Р	0	7	0	
	'	154	70	35	42	$\overline{7}$		1	0	
2	2 V	7	Total	С	Ν	Ο	Р	0	6	0
	1	154	70	35	42	7	0	0	0	
2 TT	7	Total	С	Ν	Ο	Р	0	6	0	
		154	70	35	42	7			0	

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3 S	5	Total	С	Ν	Ο	Р	0	5	0	
		110	50	25	30	5				
2	2 Т	E	Total	С	Ν	Ο	Р	0	5	0
0 1	5	110	50	25	30	5	0	5	U	

 Molecule 4 is a RNA chain called RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP)-3').

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
4		0	Total	С	Ν	Ο	Р	0	0	0
4 A	0	176	80	40	48	8	0	0	0	
4	4 1111	0	Total	С	Ν	Ο	Р	0	6	0
4 00	0	176	80	40	48	8	0	0	0	
4 bb	9	Total	С	Ν	Ο	Р	0	8	0	
		198	90	45	54	9			0	

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
Б	V	6	Total	С	Ν	Ο	Р	0	6	0
0	1	0	132	60	30	36	6	0		
5	0	6	Total	С	Ν	Ο	Р	0	6	0
5	a	0	132	60	30	36	6			U

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	0	19	Total	С	Ν	0	Р	0	10	0
0	е	12	240	108	24	96	12	0		
6	WW	10	Total	С	Ν	0	Р	0	2	0
	vv vv	10	200	90	20	80	10			

• Molecule 7 is a RNA chain called RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP)-3').

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
7	h	8	Total 160	С 72	N 16	O 64	Р 8	0	7	0

• Molecule 8 is a RNA chain called RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3').

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
e ;		5	Total	С	Ν	Ο	Р	0	5	0
0	1	0	100	45	10	40	5	0	0	0
8	11	5	Total	С	Ν	Ο	Р	0	5	0
0	11	5	100	45	10	40	5	0	5	0
0	aa	5	Total	С	Ν	Ο	Р	0	4	0
0	ЧЧ	5	100	45	10	40	5	0	4	0

• Molecule 9 is a RNA chain called RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP)-3').

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
0 m		7	Total	С	Ν	Ο	Р	0	7	0
9	111	1	140	63	14	56	7	0	4	0
0	n	7	Total	С	Ν	Ο	Р	0	7	0
9	11	1	140	63	14	56	7	0	1	0
0],],	6	Total	С	Ν	0	Р	0	6	0
9	KK K	0	120	54	12	48	6	0	U	U

• Molecule 10 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
10	Н	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
10	L	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
10	HH	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
10	II	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
10	R	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	В	1	Total Mg 1 1	0	0
11	G	1	Total Mg 1 1	0	0
11	Н	1	Total Mg 1 1	0	0
11	JJ	2	Total Mg 2 2	0	0

• Molecule 12 is CHLORIDE ION (three-letter code: CL) (formula: Cl).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	С	1	Total Cl 1 1	0	0



Mol	Chain	Residues	Ato	\mathbf{ms}		ZeroOcc	AltConf	
13	F	1	Total	0	\mathbf{S}	0	0	
10	1	I	5	4	1	0	0	
13	М	1	Total	Ο	\mathbf{S}	0	0	
10	111	I	5	4	1	0	0	
13	М	1	Total	Ο	\mathbf{S}	0	0	
10	101	1	5	4	1	0		
13	0	1	Total	Ο	\mathbf{S}	0	0	
10	U	1	5	4	1	0	0	
13	TT	1	Total	Ο	\mathbf{S}	0	0	
10	00	I	5	4	1	0	0	
13	KK	1	Total	Ο	\mathbf{S}	0	0	
10	1717	1	5	4	1			

• Molecule 14 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	А	128	Total O 128 128	0	0
14	В	149	Total O 149 149	0	1
14	С	118	Total O 118 118	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	D	177	Total O 177 177	0	1
14	Е	110	Total O 110 110	0	0
14	F	127	Total O 127 127	0	0
14	G	153	Total O 153 153	0	0
14	Н	149	Total O 149 149	0	0
14	Ι	105	Total O 105 105	0	0
14	J	155	Total O 155 155	0	0
14	К	198	Total O 198 198	0	0
14	L	138	Total O 138 138	0	0
14	М	150	Total O 150 150	0	1
14	Ν	96	Total O 96 96	0	0
14	О	252	Total O 252 252	0	0
14	Р	39	Total O 39 39	0	0
14	S	29	Total O 29 29	0	0
14	Т	22	Total O 22 22	0	0
14	V	61	Total O 61 61	0	0
14	Х	36	Total O 36 36	0	0
14	Y	55	Total O 55 55	0	0
14	a	67	Total O 67 67	0	0
14	е	193	Total O 193 193	0	0
14	h	64	Total O 64 64	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	i	17	Total O 17 17	0	0
14	m	39	Total O 39 39	0	0
14	n	48	$\begin{array}{cc} \text{Total} & \text{O} \\ 48 & 48 \end{array}$	0	0
14	GG	127	Total O 127 127	0	1
14	HH	188	Total O 188 188	0	0
14	II	271	Total O 271 271	0	0
14	JJ	125	Total O 125 125	0	0
14	KK	200	Total O 200 200	0	0
14	TT	46	Total O 46 46	0	0
14	UU	96	Total O 96 96	0	0
14	WW	76	Total O 76 76	0	0
14	bb	212	Total O 212 212	0	0
14	kk	65	Total O 65 65	0	0
14	11	24	TotalO2424	0	0
14	$\mathbf{q}\mathbf{q}$	13	Total O 13 13	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.



• Molecule 1: Coat protein

• Molecule 1: Coat protein







• Molecule 1: Coat protein		
Chain M:	89%	• 9%
MET AGC AGC AGC CTY CTYS ARC ARC ARC ACC ACC ACC ACC ACC ACC ACC	● ● 1130 1130 1130 1130	
• Molecule 1: Coat protein		
Chain N:	85%	5%•9%
MET GLIY ARG GLIY LYS LYS LYS PRO ARG ARG ARG ARG ARG ARG ARG ARG ARG ARG	E44 151 160 160 160 184 194 1116 1116 1116 1116 1116 1116 1116	A151 M159
• Molecule 1: Coat protein		
Chain O:	89%	5% 6%
MET GLY GLY ARG GLY LYS VAL LYS PRO ARD ASU ASU ASU ASU ASU ASU ASU ASU ASU ASU	872 R112 P127 V150 M159	
• Molecule 1: Coat protein		
Chain GG:	86%	5% 9%
MET ARG GLY ARG CLY LYS VAL LYS ASN ARG ASN ARG ASN ARG ASN ARG ARG ARG ARG ARG ARG ARG ARG ARG ARG	V81 112 1116 1116 8121 8121 0132 0133 0133 0133	
• Molecule 1: Coat protein		
Chain HH:	87%	• 9%
MET ARG GLY ARG CLY CLYS CLYS CLYS ARG ARG ARG ARG ARG ARG ARG ARG ARG ARG		
• Molecule 1: Coat protein		
Chain II:	81%	8% • 10%
MET ARG CLY CLYS CLYS CLYS CLYS CLYS CLYS ARG ARG ARG ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP	R39 R66 H81 H81 H81 H81 H81 H81 H81 R128 Q149 Q149 Q149 Q149 Q149 A151	891 120
• Molecule 1: Coat protein		
Chain JJ:	87%	6% 8%





• Molecule 4: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')



	60%		
Chain X:	60%	20%	20%
A162 A163 A165 A165 A165 A169 A169 A169 A169 A169 A169 A169			
• Molecule 4: RNA	. (5'-R(P*UP*UP*UP*UP*U	UP*UP*UP*UP*UP*	UP*U)-3')
Chain UU:	80% 60%	10% 10%	20%
A160 A161 A162 A163 A163 A164 A166 A166 A167 A			
• Molecule 4: RNA	. (5'-R(P*UP*UP*UP*U	UP*UP*UP*UP*UP*	UP*U)-3')
	80%		
Chain bb:	60%	30%	10%
A160 A161 A162 A163 A164 A165 A165 A165 A165 A167 A168 A168			
• Molecule 5: RNA	. (5'-R(P*UP*UP*UP*U	UP*UP*UP*U)-3')	
	86%		
Chain Y:	86%		14%
A163 A164 A165 A165 A165 A166 A168 A168 A168			
• Molecule 5: RNA	. (5'-R(P*UP*UP*UP*U	UP*UP*UP*U)-3')	
	86%		
Chain a:	57%	29%	14%
A164 A165 A167 A167 A169 A169 A169 A169			
• Molecule 6: RNA	. (5'-R(P*UP*UP*UP*U	UP*UP*UP*UP*UP*	UP*UP*UP*U))-
Chain e:	42%	47%	17%
	1270	1270	1775
U179 U180 U182 U182 U185 U185 U186 U187 U187 U187 U189 U189			
• Molecule 6: RNA	(5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP	UP*UP*UP*UP*UP*	UP*UP*UP*U))-
Chain WW: 179	75% % 42%	25%	17%
165 1167 1167 1171 171 171 172 174 174			

D W I D E DATA BANK • Molecule 7: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3') 60% Chain h: 50% 30% 20% • Molecule 8: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3') 22% Chain i: 33% 22% 44% • Molecule 8: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3') 22% Chain ll: 44% 44% 11% • Molecule 8: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3') 33% Chain qq: 56% 44% • Molecule 9: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*U)-3') 38% Chain m: 75% 12% 12% • Molecule 9: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP)-3') 50% Chain n: 88% 12% • Molecule 9: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*U)-3') Chain kk: 62% 12% 25%







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 3	Depositor
Cell constants	234.05Å 234.05 Å 234.05 Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	74.01 - 2.31	Depositor
Resolution (A)	74.01 - 2.31	EDS
% Data completeness	86.0 (74.01-2.31)	Depositor
(in resolution range)	82.7(74.01-2.31)	EDS
R _{merge}	0.18	Depositor
R_{sym}	0.18	Depositor
$< I/\sigma(I) > 1$	4.71 (at 2.32Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
D D	0.246 , 0.271	Depositor
Λ, Λ_{free}	0.232 , 0.250	DCC
R_{free} test set	1918 reflections (1.25%)	wwPDB-VP
Wilson B-factor $(Å^2)$	3.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.30 , -5.7	EDS
L-test for twinning ²	$< L > = 0.28, < L^2 > = 0.13$	Xtriage
Estimated twinning fraction	0.147 for l,-k,h	Xtriage
F_o, F_c correlation	0.72	EDS
Total number of atoms	29786	wwPDB-VP
Average B, all atoms $(Å^2)$	9.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 1.96% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

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

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).

Mal	Chain	Bond lengths		Bond angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.24	0/1154	0.51	0/1572	
1	В	0.24	0/1134	0.51	0/1545	
1	С	0.24	0/1134	0.52	0/1545	
1	D	0.24	0/1142	0.51	0/1556	
1	Е	0.24	0/1150	0.51	0/1567	
1	F	0.24	0/1161	0.52	0/1582	
1	G	0.25	0/1154	0.54	0/1572	
1	GG	0.24	0/1142	0.51	0/1556	
1	Н	0.24	0/1161	0.51	0/1582	
1	HH	0.24	0/1142	0.51	0/1556	
1	Ι	0.24	0/1142	0.51	0/1556	
1	II	0.24	0/1134	0.52	0/1545	
1	J	0.24	0/1161	0.51	0/1582	
1	JJ	0.24	0/1161	0.52	0/1582	
1	K	0.24	0/1154	0.51	0/1572	
1	KK	0.24	0/1150	0.51	0/1567	
1	L	0.24	0/1240	0.51	0/1685	
1	М	0.24	0/1142	0.51	0/1556	
1	N	0.25	0/1142	0.52	0/1556	
1	0	0.24	0/1187	0.52	0/1615	
2	Р	0.19	0/174	0.72	0/269	
2	TT	0.19	0/174	1.23	3/269~(1.1%)	
2	V	0.19	0/174	0.70	0/269	
3	S	0.19	0/124	0.73	0/191	
3	Т	0.17	0/124	0.67	0/191	
4	UU	0.27	0/199	0.84	0/308	
4	Х	0.17	0/199	0.74	0/308	
4	bb	0.14	0/224	0.64	0/347	
5	Y	0.14	0/149	0.66	0/230	
5	a	0.32	0/149	0.88	0/230	
6	WW	0.25	0/219	1.17	3/336~(0.9%)	
6	е	0.23	0/263	1.16	4/404~(1.0%)	



Mal	Chain	Bond lengths		Bond angles		
	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5	
7	h	0.12	0/175	0.74	0/268	
8	i	0.20	0/109	0.76	0/166	
8	ll	0.13	0/109	0.73	0/166	
8	qq	0.18	0/109	1.00	0/166	
9	kk	0.13	0/131	0.72	0/200	
9	m	0.10	0/153	0.71	0/234	
9	n	0.10	0/153	0.71	0/234	
All	All	0.24	0/26198	0.57	10/36235~(0.0%)	

There are no bond length outliers.

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	TT	169[A]	A	OP1-P-O3'	-10.66	81.74	105.20
2	TT	169[A]	A	OP2-P-O3'	-9.45	84.41	105.20
2	TT	170[A]	А	OP1-P-OP2	8.29	132.04	119.60
6	WW	166[A]	U	C2-N1-C1'	7.63	126.86	117.70
6	WW	166[A]	U	N3-C2-O2	-7.08	117.24	122.20
6	е	185[A]	U	C2-N1-C1'	6.94	126.03	117.70
6	WW	166[A]	U	N1-C2-O2	6.88	127.61	122.80
6	е	181[A]	U	OP1-P-OP2	-6.76	109.45	119.60
6	е	181[A]	U	O4'-C1'-N1	6.13	113.10	108.20
6	е	185[A]	U	C6-N1-C1'	-5.34	113.73	121.20

All (10) bond angle outliers are listed below:

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	А	1130	0	1117	5	0
1	В	1110	0	1103	6	0
1	С	1110	0	1099	4	1
1	D	1118	0	1103	8	0
1	Е	1126	0	1108	11	0



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	Chain	Non H	II (model)	II(addad)	Clashag	Summ Clashes
	Chain	110 П-П			Clashes	Symm-Clasnes
	F	1137	0	1120	0	0
1	G CC	1130	0	1110	12	0
		1118	0	1103	0	0
		1137	0	1118	9	0
	HH	1118	0	1109	5	0
	l	1118	0	1106	5	0
		1110	0	1105	11	0
	J	1137	0	1122	9	0
1	11	1137	0	1118	7	0
	K	1130	0	1115	8	0
1	KK	1126	0	1110	4	0
1	L	1215	0	1216	12	0
1	М	1118	0	1109	3	0
1	N	1118	0	1112	7	0
1	0	1163	0	1146	6	0
2	Р	154	0	78	2	0
2	TT	154	0	78	2	0
2	V	154	0	78	1	0
3	S	110	0	56	0	0
3	Т	110	0	56	2	0
4	UU	176	0	89	2	0
4	Х	176	0	89	1	0
4	bb	198	0	100	0	0
5	Y	132	0	67	0	0
5	a	132	0	67	0	0
6	WW	200	0	95	1	0
6	e	240	0	121	0	0
7	h	160	0	81	0	0
8	i	100	0	51	0	0
8	11	100	0	51	0	0
8	qq	100	0	51	0	0
9	kk	120	0	61	0	0
9	m	140	0	71	0	0
9	n	140	0	71	0	0
10	В	5	0	0	0	0
10	Н	5	0	0	0	0
10	HH	5	0	0	0	0
10	II	5	0	0	0	0
10	L	5	0	0	0	0
10	R	5	0	0	0	0
11	В	1	0	0	0	0
11	G	1	0	0	0	0



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	Chain	Non-H	page H(model)	H(addad)	Clashes	Symm-Clashes
11	Ц	1				
11		1	0	0	0	0
12	00 00	1	0	0	0	0
13	F	5	0	0	0	0
13	II	5	0	0	0	0
13	KK K	5	0	0	0	0
13	M	10	0	0	0	0
13	0	5	0	0	0	0
14	A	128	0	0	2	0
14	B	149	0	0	0	0
14	С	118	0	0	0	0
14	D	177	0	0	1	0
14	Е	110	0	0	1	0
14	F	127	0	0	0	0
14	G	153	0	0	2	0
14	GG	127	0	0	0	0
14	Н	149	0	0	2	0
14	HH	188	0	0	0	0
14	Ι	105	0	0	1	0
14	II	271	0	0	1	0
14	J	155	0	0	1	0
14	JJ	125	0	0	2	0
14	Κ	198	0	0	0	0
14	KK	200	0	0	0	0
14	L	138	0	0	0	0
14	М	150	0	0	1	0
14	N	96	0	0	0	0
14	0	252	0	0	1	0
14	P	39	0	0	0	0
14	S	29	0	0	0	0
14	Т	22	0	0	0	0
14	TT TT	46	0	0	1	0
14		96	0	0	1	0
14	V	61	0	0		0
14	WW	76	0	0	1	0
14		30 FF	0	0		0
14	Y		0	0		0
14	a Ll	07	0	0		0
14	DD	212	0	0		0
14	e h	193 64	0	0		0
14	n :	04	0	0		0
14	1	11	U	U	0	U



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes			
14	kk	65	0	0	0	0			
14	ll	24	0	0	0	0			
14	m	39	0	0	0	0			
14	n	48	0	0	0	0			
14	qq	13	0	0	0	0			
All	All	29786	0	23765	118	1			

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 3.

All (118) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:L:12:SER:OG	1:L:16:ASN:O	2.15	0.65
1:JJ:79[A]:ARG:NH2	14:JJ:304:HOH:O	2.33	0.61
4:UU:162[A]:A:N6	14:UU:202:HOH:O	2.33	0.60
1:N:81:TRP:O	1:N:151:ALA:N	2.35	0.59
1:G:38:VAL:O	14:WW:201:HOH:O	2.17	0.58
1:G:48:GLN:NE2	14:G:306:HOH:O	2.37	0.58
1:G:16:ASN:N	1:G:17:SER:HB3	2.17	0.58
1:D:25:ALA:N	14:D:205:HOH:O	2.40	0.55
1:E:125:ARG:NH1	14:E:204:HOH:O	2.39	0.55
1:G:125:ARG:NH2	14:G:307:HOH:O	2.39	0.55
2:TT:168[A]:A:N6	14:TT:201:HOH:O	2.41	0.54
1:E:30:LYS:NZ	1:G:121:SER:O	2.35	0.53
4:X:168[A]:A:O2'	4:X:169[A]:A:OP1	2.27	0.53
1:J:148:ARG:NH1	14:J:207:HOH:O	2.42	0.52
1:H:13:THR:OG1	1:H:14:GLY:N	2.34	0.51
1:II:19:VAL:HG22	1:II:20:VAL:H	1.76	0.51
1:B:159:ASN:HD22	1:N:19:VAL:HG12	1.76	0.50
1:J:105:SER:HB3	1:J:107:GLU:OE1	2.12	0.50
1:I:112:ARG:NH2	14:I:209:HOH:O	2.44	0.49
1:KK:57:VAL:HG22	1:KK:140:VAL:HG13	1.93	0.49
1:A:34:THR:HB	1:O:66:ARG:NH2	2.28	0.48
1:E:129:ASN:O	1:II:132:GLN:NE2	2.43	0.48
1:GG:112:ARG:NH2	1:KK:44:GLU:OE2	2.36	0.48
2:V:164[A]:A:O2'	14:V:201:HOH:O	2.12	0.48
1:H:79:ARG:NH2	14:H:605:HOH:O	2.45	0.48
1:L:44:GLU:OE2	1:M:112:ARG:NH2	2.44	0.47
1:N:81:TRP:N	1:N:151:ALA:O	2.48	0.47
1:GG:74:THR:OG1	1:GG:133:ASN:OD1	2.33	0.47



			Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:JJ:44:GLU:OE2	1:KK:112:ARG:NH1	2.36	0.46
1:O:72:SER:N	14:O:502:HOH:O	2.48	0.46
1:K:117:ASN:HB3	1:L:116:ILE:HG12	1.98	0.46
1:GG:127:PRO:O	1:GG:131:ARG:HG3	2.16	0.46
1:H:121:SER:O	1:HH:30:LYS:NZ	2.41	0.46
1:E:34:THR:HB	1:F:66:ARG:NH2	2.31	0.46
1:II:81:TRP:O	1:II:151:ALA:N	2.41	0.45
1:L:48:GLN:HB2	1:L:51:ILE:HG22	1.97	0.45
1:L:11:LYS:HE2	1:L:21:THR:HB	1.97	0.45
1:H:44:GLU:OE2	1:I:112:ARG:NH2	2.40	0.45
1:J:66:ARG:NH2	1:K:34:THR:HB	2.31	0.45
3:T:165[A]:A:H2'	3:T:166[A]:A:C8	2.52	0.45
1:E:15:ASP:HB3	1:E:16:ASN:H	1.63	0.45
1:K:54:LYS:NZ	1:K:142:GLU:OE2	2.46	0.45
1:N:44:GLU:OE2	1:O:112:ARG:NH2	2.47	0.45
1:II:129:ASN:O	1:II:132:GLN:NE2	2.34	0.45
1:M:117:ASN:HB3	1:N:116:ILE:HG12	1.97	0.45
1:J:34:THR:HB	1:K:66:ARG:NH2	2.31	0.45
1:D:34:THR:HB	1:II:66:ARG:NH2	2.32	0.44
1:M:16:ASN:N	14:M:311:HOH:O	2.50	0.44
1:K:105:SER:HB2	1:K:107:GLU:OE1	2.18	0.44
1:D:127:PRO:O	1:D:131:ARG:HG3	2.17	0.44
1:C:84:LEU:HD12	1:C:148:ARG:HB2	2.00	0.44
1:D:30:LYS:NZ	1:JJ:121:SER:O	2.36	0.44
4:UU:162[A]:A:H2'	4:UU:163[A]:A:H8	1.83	0.44
1:E:16:ASN:HD21	1:F:125:ARG:HH22	1.64	0.44
1:H:148:ARG:NH2	14:H:607:HOH:O	2.50	0.44
1:G:34:THR:HB	1:HH:66:ARG:NH2	2.33	0.44
1:GG:116:ILE:HG12	1:KK:117:ASN:HB3	2.00	0.44
1:H:74:THR:OG1	1:H:133:ASN:OD1	2.31	0.43
1:H:127:PRO:O	1:H:131:ARG:HG3	2.18	0.43
1:A:148:ARG:NH2	14:A:205:HOH:O	2.51	0.43
1:B:105[A]:SER:HB3	1:B:107:GLU:OE1	2.18	0.43
1:JJ:127:PRO:O	1:JJ:131:ARG:HG3	2.18	0.43
1:I:81:TRP:O	1:I:151:ALA:N	2.45	0.43
1:0:127:PRO:0	1:O:131:ARG:HG3	2.19	0.43
1:G:125:ARG:HB2	1:HH:23:ILE:HD11	2.00	0.43
1:G:66:ARG:NH2	1:HH:34:THR:HB	2.33	0.43
1:II:84:LEU:HG	1:II:149[A]:GLN:HB2	2.01	0.43
1:A:66:ARG:NH2	1:O:34:THR:HB	2.33	0.43
1:G:127:PRO:O	1:G:131:ARG:HG3	2.19	0.43



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:II:129:ASN:OD1	14:II:301:HOH:O	2.22	0.43
1:D:83:GLN:HB3	1:D:149:GLN:HB3	2.01	0.42
1:F:81:TRP:CD1	1:F:121:SER:HB3	2.54	0.42
1:I:81:TRP:CD1	1:I:121:SER:HB3	2.54	0.42
1:F:44:GLU:OE2	1:G:112:ARG:NH1	2.42	0.42
1:F:127:PRO:O	1:F:131:ARG:HG3	2.19	0.42
1:C:81:TRP:O	1:C:151:ALA:N	2.41	0.42
1:K:112:ARG:NH2	1:O:44:GLU:OE2	2.47	0.42
6:WW:173:U:O2'	6:WW:174:U:O5'	2.36	0.42
1:B:127:PRO:O	1:B:131:ARG:HG3	2.18	0.42
1:E:127:PRO:O	1:E:131:ARG:HG3	2.19	0.42
1:J:81:TRP:CD1	1:J:121:SER:HB3	2.55	0.42
1:J:30:LYS:NZ	1:L:121:SER:O	2.41	0.42
1:E:66:ARG:NH2	1:F:34:THR:HB	2.34	0.42
1:L:99:LEU:HD11	1:L:142:GLU:HG3	2.02	0.42
1:JJ:112:ARG:NH2	14:JJ:307:HOH:O	2.53	0.42
1:B:68:ASP:OD1	1:B:68:ASP:N	2.53	0.42
1:B:117:ASN:HB3	1:C:116:ILE:HG12	2.00	0.42
1:D:117:ASN:HB3	1:E:116:ILE:HG12	2.02	0.42
1:I:117:ASN:HB3	1:J:116:ILE:HG12	2.01	0.42
1:J:99:LEU:HG	1:J:141:CYS:HA	2.01	0.41
1:JJ:97:LYS:HB3	1:JJ:142:GLU:HB2	2.00	0.41
1:A:127:PRO:O	1:A:131:ARG:HG3	2.20	0.41
1:K:127:PRO:O	1:K:131:ARG:HG3	2.20	0.41
1:L:6:VAL:O	1:L:7:LYS:HE2	2.20	0.41
1:N:121:SER:O	1:N:122:VAL:HG12	2.20	0.41
1:C:127:PRO:O	1:C:131:ARG:HG3	2.20	0.41
1:E:54:LYS:NZ	1:E:142:GLU:OE2	2.47	0.41
1:H:40:ALA:HB2	2:TT:167[A]:A:H4'	2.03	0.41
1:G:84:LEU:HG	1:G:149:GLN:HB2	2.03	0.41
1:H:99:LEU:HG	1:H:141:CYS:HA	2.03	0.41
1:D:66:ARG:NH2	1:II:34:THR:HB	2.35	0.41
1:K:81:TRP:CD1	1:K:121:SER:HB3	2.56	0.41
1:A:125:ARG:NH2	14:A:206:HOH:O	2.53	0.41
1:D:33:PRO:O	1:II:39:ARG:NH2	2.54	0.41
1:G:81:TRP:O	1:G:151:ALA:N	2.46	0.41
1:J:21:THR:HG22	2:P:165[A]:A:H5"	2.03	0.41
1:L:11:LYS:HG2	1:L:21:THR:HG21	2.03	0.41
1:L:127:PRO:O	1:L:131:ARG:HG3	2.21	0.41
1:II:117:ASN:HB3	1:JJ:116:ILE:HG12	2.02	0.41
1:N:84:LEU:HD12	1:N:148:ARG:HB2	2.02	0.41



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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:164[A]:A:H5'	1:HH:16:ASN:HB2	2.03	0.41
1:L:84:LEU:HG	1:L:149:GLN:HB3	2.03	0.40
2:P:164[A]:A:H2'	2:P:165[A]:A:C8	2.56	0.40
1:II:17:SER:OG	1:II:18:ASN:N	2.53	0.40
1:B:94:VAL:HG13	1:B:122:VAL:HG12	2.02	0.40
1:L:11:LYS:O	1:L:13:THR:N	2.55	0.40
1:GG:81:TRP:CD1	1:GG:121:SER:HB3	2.57	0.40

All (1) 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)
1:C:49[A]:SER:OG	1:C:49[A]:SER:OG[2_675]	2.14	0.06

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
1	А	144/159~(91%)	135 (94%)	6 (4%)	3(2%)	7	5
1	В	141/159~(89%)	134 (95%)	6 (4%)	1 (1%)	22	26
1	С	141/159~(89%)	134 (95%)	7 (5%)	0	100	100
1	D	142/159~(89%)	132 (93%)	10 (7%)	0	100	100
1	Е	143/159~(90%)	136 (95%)	7 (5%)	0	100	100
1	F	145/159~(91%)	133 (92%)	12 (8%)	0	100	100
1	G	144/159~(91%)	135 (94%)	8 (6%)	1 (1%)	22	26
1	GG	142/159~(89%)	133 (94%)	9 (6%)	0	100	100
1	Н	145/159~(91%)	137 (94%)	8 (6%)	0	100	100
1	HH	142/159~(89%)	135 (95%)	7 (5%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
1	Ι	142/159~(89%)	134 (94%)	8 (6%)	0	100	100
1	II	141/159~(89%)	129 (92%)	11 (8%)	1 (1%)	22	26
1	J	145/159~(91%)	135~(93%)	10 (7%)	0	100	100
1	JJ	145/159~(91%)	137 (94%)	8 (6%)	0	100	100
1	Κ	144/159~(91%)	133~(92%)	11 (8%)	0	100	100
1	KK	143/159~(90%)	137~(96%)	6 (4%)	0	100	100
1	L	155/159~(98%)	137 (88%)	16 (10%)	2(1%)	12	12
1	М	142/159~(89%)	132 (93%)	10 (7%)	0	100	100
1	Ν	142/159~(89%)	131 (92%)	10 (7%)	1 (1%)	22	26
1	Ο	148/159~(93%)	138 (93%)	9 (6%)	1 (1%)	22	26
All	All	2876/3180~(90%)	2687 (93%)	179 (6%)	10 (0%)	41	50

All (10) Ramachandran outliers are listed below:

Mol	Chain	\mathbf{Res}	Type
1	Ν	122	VAL
1	II	129	ASN
1	L	12	SER
1	L	16	ASN
1	А	17	SER
1	В	37	TRP
1	G	17	SER
1	0	12	SER
1	А	15	ASP
1	А	16	ASN

5.3.2Protein sidechains (i)

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	Perce	ntiles
1	А	129/140~(92%)	129 (100%)	0	100	100
1	В	127/140~(91%)	127 (100%)	0	100	100



Mol	Chain	Analysed	Rotameric	Outliers	Perce	\mathbf{ntiles}
1	\mathbf{C}	127/140~(91%)	127~(100%)	0	100	100
1	D	128/140~(91%)	128 (100%)	0	100	100
1	Ε	129/140~(92%)	128 (99%)	1 (1%)	81	90
1	F	130/140~(93%)	130 (100%)	0	100	100
1	G	129/140~(92%)	129 (100%)	0	100	100
1	GG	128/140~(91%)	128 (100%)	0	100	100
1	Н	130/140~(93%)	130 (100%)	0	100	100
1	HH	128/140~(91%)	128 (100%)	0	100	100
1	Ι	128/140~(91%)	128 (100%)	0	100	100
1	II	127/140~(91%)	127 (100%)	0	100	100
1	J	130/140~(93%)	130 (100%)	0	100	100
1	JJ	130/140~(93%)	130 (100%)	0	100	100
1	Κ	129/140~(92%)	129 (100%)	0	100	100
1	KK	129/140~(92%)	129 (100%)	0	100	100
1	L	138/140~(99%)	138 (100%)	0	100	100
1	М	128/140~(91%)	128 (100%)	0	100	100
1	Ν	128/140~(91%)	127 (99%)	1 (1%)	81	90
1	О	133/140~(95%)	133 (100%)	0	100	100
All	All	2585/2800 (92%)	2583 (100%)	2 (0%)	93	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Е	159	ASN
1	Ν	122	VAL

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

Mol	Chain	Res	Type
1	D	48	GLN
1	G	48	GLN
1	J	117	ASN
1	L	9	ASN



5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	Р	6/8~(75%)	0	0
2	TT	6/8~(75%)	5(83%)	0
2	V	6/8~(75%)	1 (16%)	0
3	S	4/6~(66%)	1 (25%)	0
3	Т	4/6~(66%)	1 (25%)	0
4	UU	7/10~(70%)	1 (14%)	0
4	Х	7/10~(70%)	1 (14%)	1 (14%)
4	bb	8/10~(80%)	3~(37%)	0
5	Y	5/7~(71%)	0	0
5	a	5/7~(71%)	2 (40%)	0
6	WW	10/12~(83%)	7 (70%)	2(20%)
6	е	11/12~(91%)	7~(63%)	0
7	h	7/10~(70%)	3 (42%)	0
8	i	4/9~(44%)	2(50%)	0
8	11	4/9~(44%)	1 (25%)	0
8	qq	4/9~(44%)	0	0
9	kk	5/8~(62%)	1 (20%)	0
9	m	6/8~(75%)	1 (16%)	0
9	n	6/8~(75%)	0	0
All	All	115/165~(69%)	37 (32%)	3(2%)

All (37) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	S	164[A]	А
3	Т	168[A]	А
2	V	169[A]	А
4	Х	169[A]	А
5	a	168[A]	А
5	a	169[A]	А
6	е	180	U
6	е	181[A]	U
6	е	182[A]	U
6	е	183[A]	U
6	е	184[A]	U
6	е	185[A]	U
6	е	186[A]	U
7	h	184[A]	U
7	h	186[A]	U
7	h	187[A]	U
8	i	185[A]	U



	9	1	1 0
Mol	Chain	Res	Type
8	i	186[A]	U
9	m	188[A]	U
2	TT	166[A]	А
2	TT	167[A]	А
2	TT	168[A]	А
2	TT	169[A]	А
2	TT	170[A]	А
4	UU	162[A]	А
6	WW	166[A]	U
6	WW	167[A]	U
6	WW	168	U
6	WW	171	U
6	WW	172	U
6	WW	173	U
6	WW	174	U
4	bb	161[A]	А
4	bb	163[A]	А
4	bb	168[A]	А
9	kk	184[A]	U
8	11	188[A]	U

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All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	Х	168[A]	А
6	WW	165	U
6	WW	173	U

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 for Mogul analysis.



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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).

Mal	Tuno	Chain	Dog	Tink	B	ond leng	gths	E	Bond ang	gles
	туре	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
13	SO4	KK	201	-	4,4,4	0.14	0	6,6,6	1.59	1 (16%)
13	SO4	0	201	-	4,4,4	0.14	0	6,6,6	0.06	0
13	SO4	F	201	-	4,4,4	0.14	0	6,6,6	1.32	1 (16%)
13	SO4	М	202	-	4,4,4	0.14	0	6,6,6	0.12	0
10	PO4	HH	401	-	4,4,4	0.92	0	6,6,6	0.43	0
10	PO4	R	1	-	4,4,4	0.91	0	6,6,6	0.44	0
10	PO4	Н	501	-	4,4,4	0.92	0	6,6,6	0.42	0
13	SO4	JJ	203	-	4,4,4	0.14	0	6,6,6	0.05	0
13	SO4	М	201	-	4,4,4	0.14	0	6,6,6	0.07	0
10	PO4	В	701	-	4,4,4	0.92	0	6,6,6	0.43	0
10	PO4	L	901	-	4,4,4	0.92	0	6,6,6	0.43	0
10	PO4	II	201	-	4,4,4	0.90	0	6,6,6	1.09	0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
13	KK	201	SO4	03-S-01	3.27	126.37	109.31
13	F	201	SO4	O4-S-O3	2.14	118.21	109.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.



5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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, 95^{th} 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	А	146/159~(91%)	0.33	5 (3%) 45 52	4, 7, 11, 19	0
1	В	143/159~(89%)	0.32	1 (0%) 87 91	4,6,9,11	0
1	С	143/159~(89%)	0.27	1 (0%) 87 91	3, 4, 7, 19	0
1	D	144/159~(90%)	0.16	1 (0%) 87 91	2, 4, 7, 14	0
1	Ε	145/159~(91%)	0.26	1 (0%) 87 91	4, 5, 8, 15	0
1	F	147/159~(92%)	0.42	2 (1%) 75 80	4, 8, 10, 17	0
1	G	146/159~(91%)	0.32	1 (0%) 87 91	3, 6, 10, 12	0
1	GG	144/159~(90%)	0.28	3 (2%) 63 70	2, 3, 7, 14	0
1	Н	147/159~(92%)	0.35	5 (3%) 45 52	5, 7, 10, 18	0
1	HH	144/159~(90%)	0.22	0 100 100	3, 4, 7, 15	0
1	Ι	144/159~(90%)	0.38	2 (1%) 75 80	7, 10, 12, 19	0
1	II	143/159~(89%)	0.22	2 (1%) 75 80	2, 4, 7, 12	0
1	J	147/159~(92%)	0.43	4 (2%) 54 62	8, 10, 13, 22	0
1	JJ	147/159~(92%)	0.36	4 (2%) 54 62	2, 4, 8, 18	0
1	K	146/159~(91%)	0.50	6 (4%) 37 44	7, 9, 13, 23	0
1	KK	145/159~(91%)	0.17	1 (0%) 87 91	2, 3, 7, 16	0
1	L	157/159~(98%)	0.77	16 (10%) 6 10	9, 11, 17, 22	0
1	М	144/159~(90%)	0.57	5 (3%) 44 51	10, 11, 15, 21	0
1	Ν	144/159~(90%)	0.53	7 (4%) 29 37	6, 10, 14, 16	0
1	О	150/159~(94%)	0.45	6 (4%) 38 45	5, 8, 13, 26	0
2	Р	7/8~(87%)	3.46	7 (100%) 0 0	16, 18, 23, 28	0
2	TT	7/8~(87%)	5.29	$7\ (100\%)\ 0\ 0$	17, 20, 24, 29	0
2	V	7/8 (87%)	3.16	6 (85%) 0 0	14, 17, 22, 23	0
3	S	5/6~(83%)	3.06	4 (80%) 0 0	15, 16, 19, 21	0



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Mol	Chain	Analysed	$\langle RSRZ \rangle$	# RSRZ >	·2	$OWAB(Å^2)$	Q<0.9
3	Т	5/6~(83%)	1.78	2~(40%) 0	0	16, 17, 18, 19	0
4	UU	8/10~(80%)	4.72	8 (100%) 0	0	17, 18, 26, 26	0
4	Х	8/10~(80%)	3.28	6~(75%) 0	0	21, 22, 26, 26	0
4	bb	9/10~(90%)	5.30	8 (88%) 0	0	14, 19, 25, 27	0
5	Y	6/7~(85%)	3.41	6 (100%) 0	0	20, 22, 23, 23	0
5	a	6/7~(85%)	5.67	6 (100%) 0	0	20, 23, 29, 31	0
6	WW	10/12~(83%)	3.90	9~(90%) 0	0	16, 24, 29, 30	0
6	е	12/12~(100%)	3.75	10 (83%) 0	0	19, 23, 28, 28	0
7	h	8/10 (80%)	2.95	6~(75%) 0	0	14, 17, 24, 26	0
8	i	5/9~(55%)	1.47	2(40%) 0	0	15, 15, 19, 23	0
8	11	5/9~(55%)	2.17	2(40%) 0	0	16, 16, 22, 23	0
8	qq	5/9~(55%)	2.12	3~(60%) 0	0	14, 15, 22, 22	0
9	kk	6/8~(75%)	2.66	4 (66%) 0	0	17, 19, 23, 28	0
9	m	7/8~(87%)	2.80	3~(42%) 0	0	17, 20, 28, 28	0
9	n	7/8~(87%)	2.63	4 (57%) 0	0	19, 20, 24, 25	0
All	All	3049/3345~(91%)	0.50	176 (5%) 23	29	2, 7, 16, 31	0

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All (176) RSRZ outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	RSRZ
1	L	6	VAL	10.0
1	J	13	THR	9.7
4	bb	161[A]	А	8.9
2	TT	168[A]	А	8.7
2	TT	169[A]	А	8.5
4	bb	162[A]	А	8.1
5	a	168[A]	А	8.1
4	bb	160	А	8.0
4	UU	161	А	7.7
4	UU	162[A]	А	7.7
6	WW	171	U	7.5
3	S	163[A]	А	7.5
6	е	180	U	7.4
1	Κ	14	GLY	7.2
5	a	$1\overline{67[A]}$	А	6.7
5	a	164[A]	А	6.7
4	bb	163[A]	А	6.4



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Mol	Chain	Res	Type	RSRZ
4		160	A	6.1
2		170[A]	A	6.0
1	J	15	ASP	6.0
5	a	169[A]	A	6.0
2	Р	169[A]	A	5.9
6	WW	173	U	5.8
6	е	190[A]	U	5.7
4	bb	168[A]	A	5.6
1	F	13	THR	5.6
2	V	169[A]	А	5.6
6	е	181[A]	U	5.5
9	kk	183[A]	U	5.5
6	WW	172	U	5.5
9	m	182[A]	U	5.4
9	m	188[A]	U	5.4
5	Y	163[A]	А	5.4
6	WW	174	U	5.3
1	Н	15	ASP	5.3
1	0	11	LYS	5.2
1	JJ	13	THR	5.1
6	е	189[A]	U	5.1
4	Х	169[A]	А	5.1
9	n	188[A]	U	5.0
7	h	190[A]	U	4.9
1	II	17	SER	4.7
2	V	163	A	4.7
2	Р	163[A]	A	4.7
2	TT	164[A]	A	4.6
1	L	15	ASP	4.6
7	h	183	U	4.5
1	A	15	ASP	4.5
8	11	188[A]	U	4.5
7	h	184[A]	Ū	4.4
4	X	162[A]	Ā	4.3
4	UU	167[A]	A	4.3
1	L	16	ASN	4.3
1	I.	13	THR	4.3
1		15	ASP	1.0 <u>1</u> 2
6	90 	170	II	ч.5 Д 9
1	I.	19	SEP	1.2 1.2
1	Г Г	12		4.2 1 9
		167[A]	ЛЭГ	4.2
\mathbf{G}	L X	$10/ \mathbf{A} $	A	4.1

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Mol	Chain	Res	Type	RSRZ	
1	Κ	15	ASP	3.9	
1	L	7	LYS	3.9	
1	JJ	14	GLY	3.8	
2	TT	165	А	3.8	
5	a	165[A]	А	3.7	
1	А	24	ARG	3.7	
9	m	183[A]	U	3.7	
1	А	14	GLY	3.7	
1	0	15	ASP	3.6	
4	UU	163[A]	А	3.6	
4	Х	163[A]	А	3.6	
4	bb	164[A]	А	3.6	
6	WW	170	U	3.6	
6	е	182[A]	U	3.6	
4	Х	168[A]	А	3.5	
8	qq	185[A]	U	3.5	
5	Y	168[A]	А	3.5	
1	Ν	43	PHE	3.5	
2	TT	166[A]	А	3.4	
1	Ν	51	ILE	3.4	
1	K	60	LEU	3.3	
1	Е	15	ASP	3.3	
1	II	128	THR	3.3	
3	Т	168[A]	А	3.2	
1	0	10	ARG	3.2	
6	е	185[A]	U	3.2	
1	L	10	ARG	3.2	
8	qq	183	U	3.2	
1	Н	14	GLY	3.2	
2	Р	167[A]	А	3.2	
1	J	24	ARG	3.2	
9	n	187[A]	U	3.2	
4	UU	165[A]	A	3.2	
9	kk	184[A]	U	3.1	
4	X	167[A]	A	3.1	
1	K	$\overline{38}$	VAL	3.1	
6	WW	165	U	3.1	
1	0	150	VAL	3.1	
4	UU	164[A]	A	3.1	
1	Н	13	THR	3.0	
8	i	188[A]	U	3.0	
1	Ν	81	TRP	3.0	



Mol	Chain	Res	Type	RSRZ	
1	0	12	SER	3.0	
9	kk	188[A]	U	2.9	
1	М	24	ARG	2.9	
2	V	168[A]	А	2.9	
4	Х	165[A]	А	2.9	
5	a	166[A]	А	2.9	
1	М	16	ASN	2.8	
2	Р	166[A]	А	2.8	
1	L	14	GLY	2.8	
4	bb	166[A]	А	2.8	
9	n	186[A]	U	2.8	
5	Y	164[A]	A	2.7	
6	е	188[A]	U	2.7	
1	Ι	16	ASN	2.7	
2	Р	165[A]	A	2.7	
1	0	14	GLY	2.7	
1	А	16	ASN	2.6	
1	L	4	GLY	2.6	
7	h	187[A]	U	2.6	
2	Р	168[A]	A	2.6	
2	V	166[A]	A	2.6	
5	Y	166[A]	A	2.6	
1	L	52	ALA	2.6	
1	N	60	LEU	2.6	
1	G	14	GLY	2.5	
7	h	189[A]	U	2.5	
1	L	3	ARG	2.5	
1	GG	48	GLN	2.5	
8	ll	184[A]	U	2.5	
1	Н	19	VAL	2.5	
1	L	9	ASN	2.5	
2	V	164[A]	A	2.5	
1	М	45	VAL	2.4	
1	K	16	ASN	2.4	
3	S	164[A]	A	2.4	
9	n	182[A]	U	2.4	
9	kk	186[A]	U	2.4	
1	JJ	16	ASN	2.4	
1	J	14	GLY	2.4	
2	Р	164[A]	A	2.4	
8	qq	187[A]	U	2.4	
1	GG	16	ASN	2.4	



Mol	Chain	Res	Type	RSRZ	
6	е	183[A]	U	2.3	
2	V	167[A]	А	2.3	
1	Н	24	ARG	2.3	
8	i	184[A]	U	2.3	
6	е	187[A]	U	2.3	
1	В	24	ARG	2.3	
4	bb	167[A]	А	2.3	
1	L	28	TYR	2.2	
1	KK	19	VAL	2.2	
1	GG	24[A]	ARG	2.2	
6	WW	166[A]	U	2.2	
1	L	116	ILE	2.2	
1	А	48	GLN	2.2	
6	WW	169	U	2.2	
1	Ι	148	ARG	2.2	
1	М	149	GLN	2.2	
3	S	165[A]	А	2.1	
5	Y	165[A]	А	2.1	
1	N	31	VAL	2.1	
1	L	11	LYS	2.1	
1	D	16	ASN	2.1	
6	WW	167[A]	U	2.1	
7	h	186[A]	U	2.1	
1	С	52	ALA	2.1	
1	М	130	LEU	2.1	
1	L	5	LYS	2.1	
4	UU	166[A]	А	2.1	
1	N	70	PHE	2.1	
3	S	167[A]	А	2.0	
1	N	94	VAL	2.0	
1	K	49[A]	SER	2.0	
2	TT	167[A]	А	2.0	
3	Т	164[A]	А	2.0	

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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 monosaccharides 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, 95^{th} 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
10	PO4	II	201	5/5	0.76	0.37	$23,\!26,\!26,\!33$	5
11	MG	В	702	1/1	0.80	0.57	4,4,4,4	0
13	SO4	JJ	203	5/5	0.83	0.48	9,9,12,18	5
13	SO4	М	202	5/5	0.89	0.18	31,31,34,39	5
13	SO4	0	201	5/5	0.90	0.49	30,30,31,34	5
13	SO4	М	201	5/5	0.90	0.51	$35,\!40,\!44,\!45$	5
13	SO4	F	201	5/5	0.93	0.21	11,12,13,14	5
12	CL	С	201	1/1	0.94	0.09	13,13,13,13	0
11	MG	G	201	1/1	0.94	0.66	14,14,14,14	0
11	MG	JJ	202	1/1	0.94	0.33	4,4,4,4	0
10	PO4	HH	401	5/5	0.95	0.17	2,2,2,2	0
13	SO4	KK	201	5/5	0.95	0.55	24,28,29,30	5
10	PO4	L	901	5/5	0.96	0.11	$9,\!10,\!11,\!15$	0
11	MG	JJ	201	1/1	0.96	0.24	$6,\!6,\!6,\!6$	0
10	PO4	Н	501	5/5	0.97	0.11	7,7,7,7	0
10	PO4	В	701	5/5	0.97	0.15	3,4,4,4	0
11	MG	Н	502	1/1	0.97	0.10	7,7,7,7	0
10	PO4	R	1	5/5	0.99	0.35	42,49,49,49	5

6.5 Other polymers (i)

There are no such residues in this entry.

