



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2023 – 03:33 AM EDT

PDB ID : 8DH4  
Title : T7 RNA polymerase elongation complex with unnatural base dPa-DsTP pair  
Authors : Oh, J.; Wang, D.  
Deposited on : 2022-06-24  
Resolution : 2.80 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
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) : 2.36

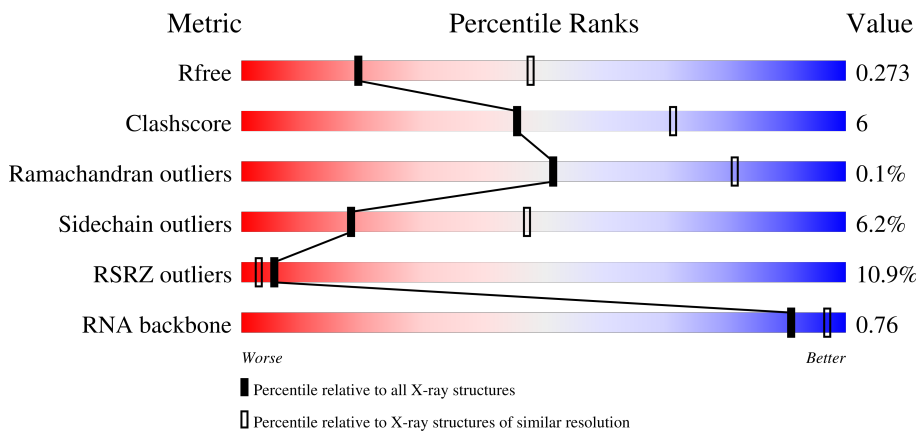
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)
RNA backbone	3102	1227 (3.10-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	B	883	4% (Poor fit) 81% (0 outliers) 15% (1 outlier) .. (2+ outliers)
1	E	883	11% (Poor fit) 76% (0 outliers) 16% (1 outlier) 7% (2+ outliers)
1	I	883	10% (Poor fit) 72% (0 outliers) 20% (1 outlier) 7% (2+ outliers)
1	M	883	14% (Poor fit) 70% (0 outliers) 22% (1 outlier) 7% (2+ outliers)

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Mol	Chain	Length	Quality of chain
2	A	18	
2	F	18	
2	J	18	
2	N	18	
3	C	12	
3	G	12	
3	K	12	
3	O	12	
4	D	9	
4	H	9	
4	L	9	
4	P	9	

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
6	MG	E	902	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 28446 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 T7 RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	856	Total 6728	C 4284	N 1169	O 1239	S 36	0	0	0
1	E	819	Total 6397	C 4086	N 1097	O 1181	S 33	0	0	0
1	I	821	Total 6429	C 4106	N 1112	O 1176	S 35	0	0	0
1	M	819	Total 6409	C 4090	N 1111	O 1176	S 32	0	0	0

- Molecule 2 is a DNA chain called Template strand DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	A	15	Total 303	C 145	N 55	O 88	P 15	0	0	0
2	F	17	Total 344	C 165	N 65	O 98	P 16	0	0	0
2	J	14	Total 282	C 135	N 50	O 83	P 14	0	0	0
2	N	15	Total 303	C 145	N 55	O 88	P 15	0	0	0

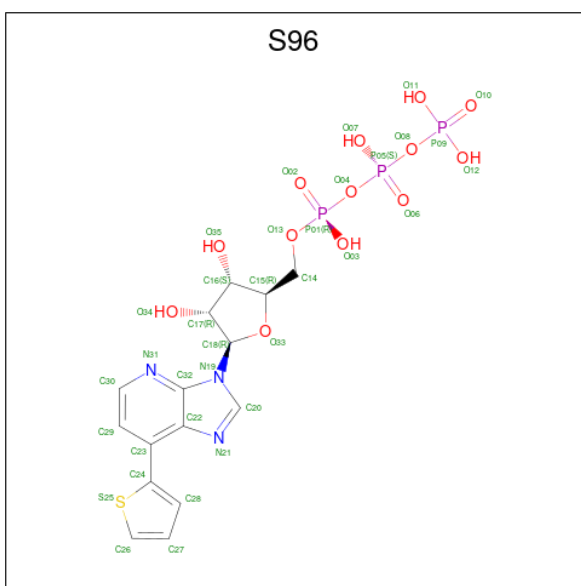
- Molecule 3 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	C	9	Total 193	C 86	N 35	O 63	P 9	0	0	0
3	G	8	Total 173	C 77	N 33	O 55	P 8	0	0	0
3	K	8	Total 173	C 77	N 33	O 55	P 8	0	0	0
3	O	8	Total 173	C 77	N 33	O 55	P 8	0	0	0

- Molecule 4 is a DNA chain called Non-template strand DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	D	6	Total	C	N	O	P	0	0	0
			122	59	19	38	6			
4	H	8	Total	C	N	O	P	0	0	0
			160	77	25	50	8			
4	L	3	Total	C	N	O	P	0	0	0
			63	30	12	18	3			
4	P	6	Total	C	N	O	P	0	0	0
			122	59	19	38	6			

- Molecule 5 is (7P)-3-{5-O-[(R)-hydroxy{[(S)-hydroxy(phosphonoxy)phosphoryl]oxy}phosphoryl]-beta-D-ribofuranosyl}-7-(thiophen-2-yl)-3H-imidazo[4,5-b]pyridine (three-letter code: S96) (formula: C<sub>15</sub>H<sub>18</sub>N<sub>3</sub>O<sub>13</sub>P<sub>3</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
5	B	1	Total	C	N	O	P	S	0	0
			35	15	3	13	3	1		
5	E	1	Total	C	N	O	P	S	0	0
			35	15	3	13	3	1		

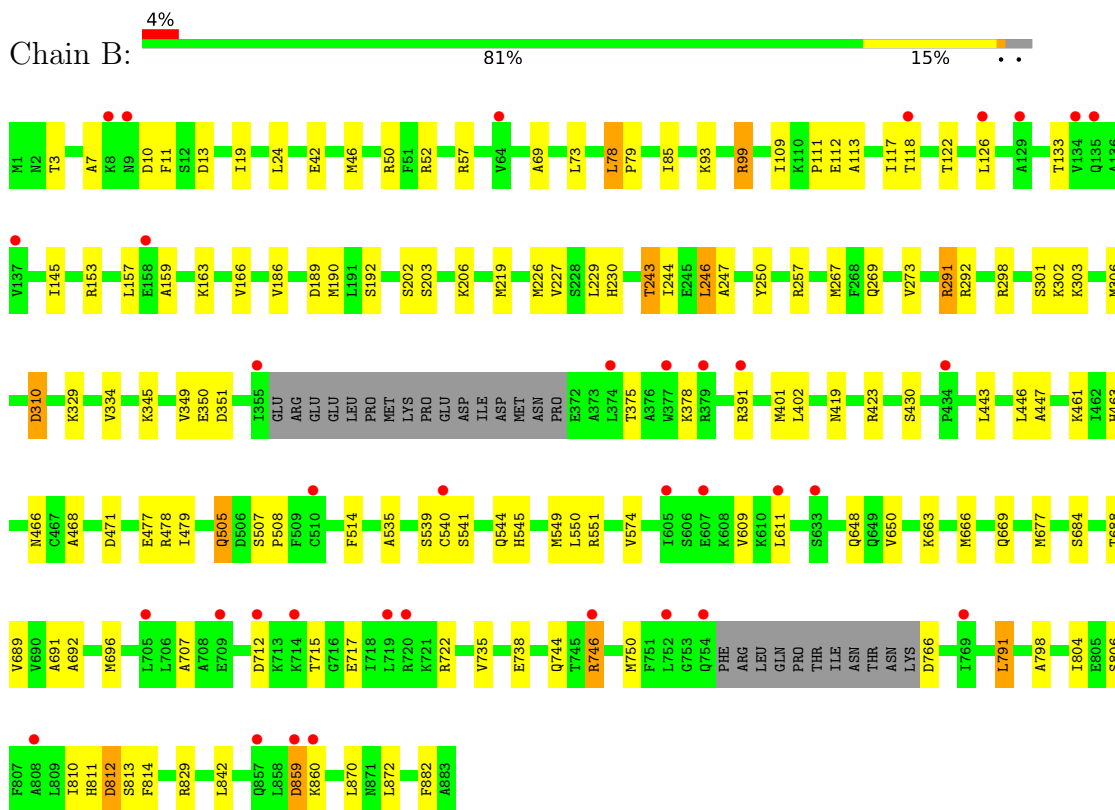
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
6	B	1	Total	Mg	0	0
			1	1		
6	E	1	Total	Mg	0	0
			1	1		

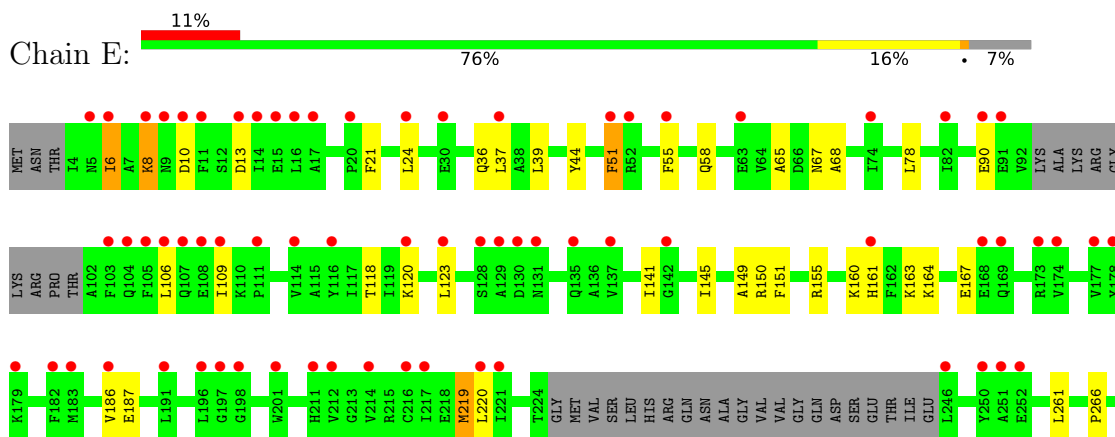
### 3 Residue-property plots i

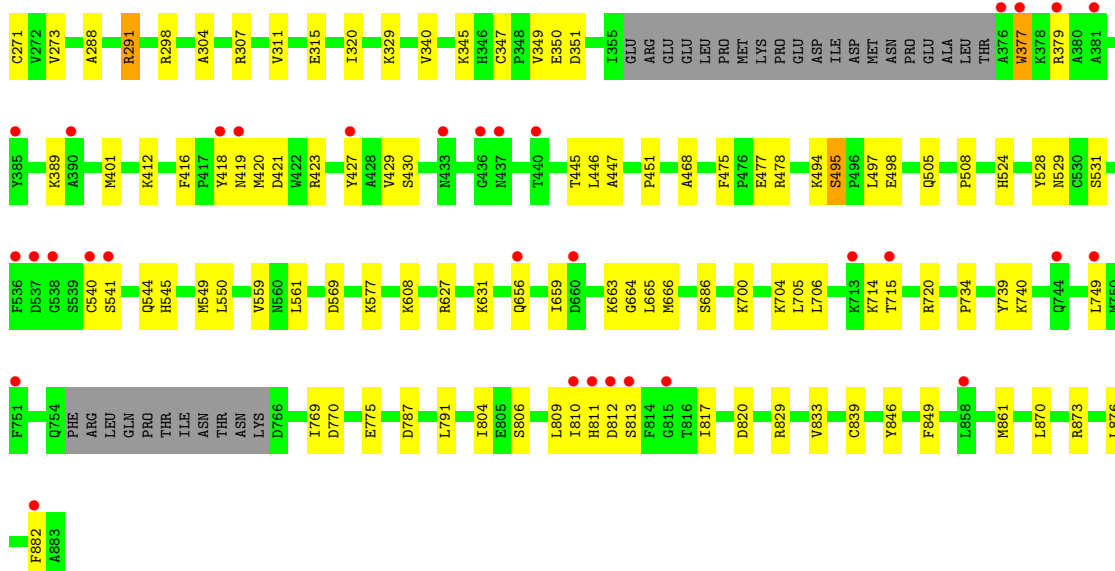
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: T7 RNA polymerase

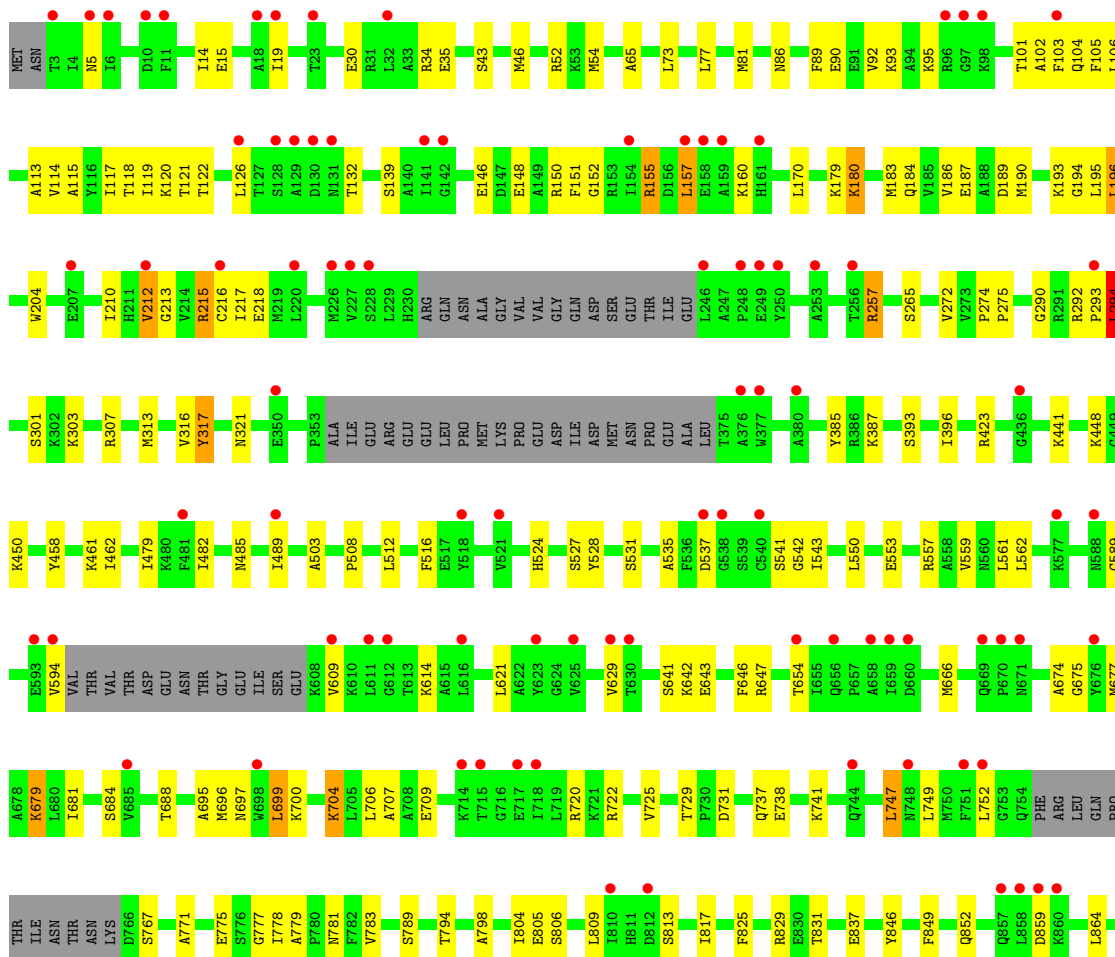


#### • Molecule 1: T7 RNA polymerase



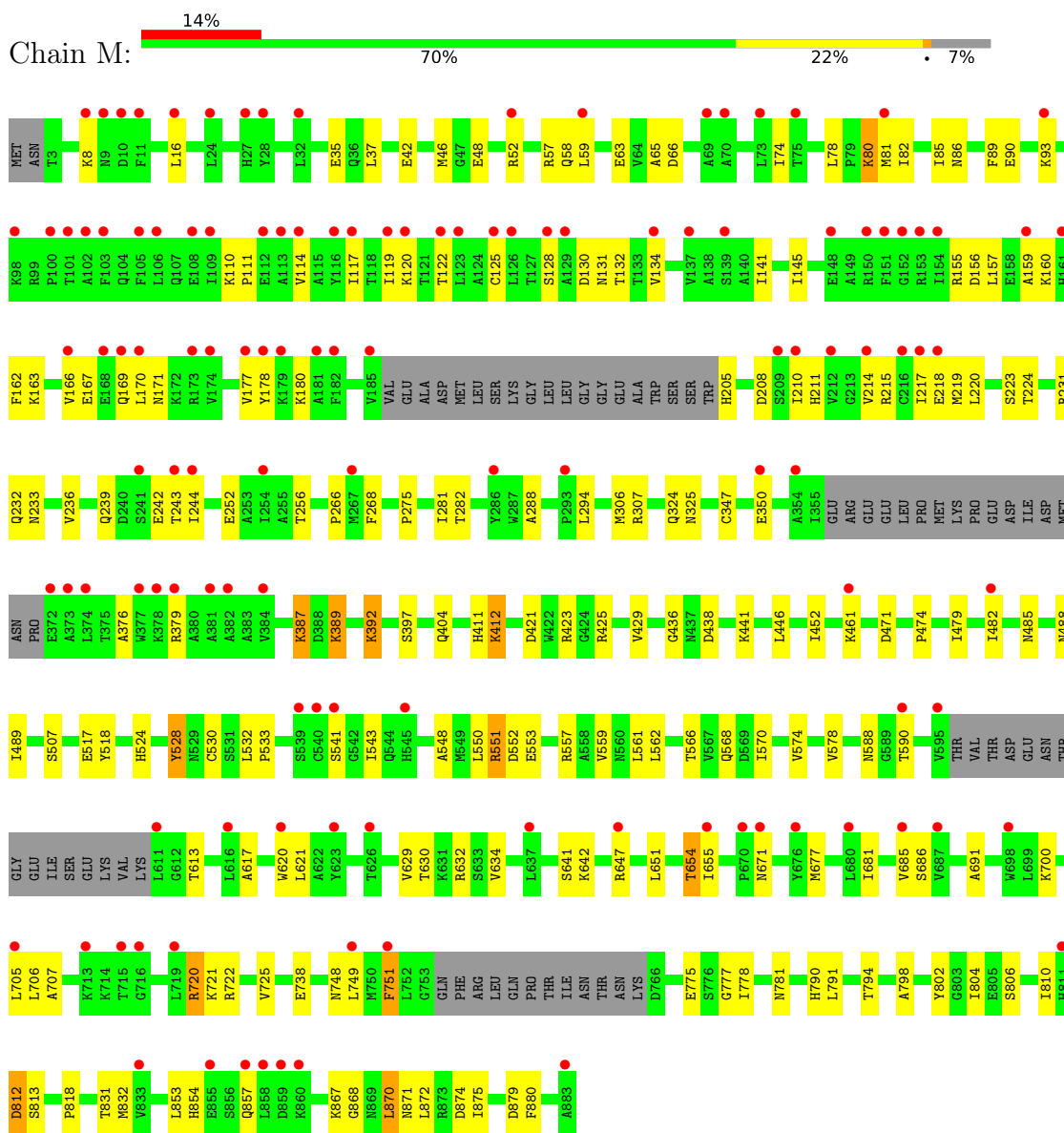


• Molecule 1: T7 RNA polymerase

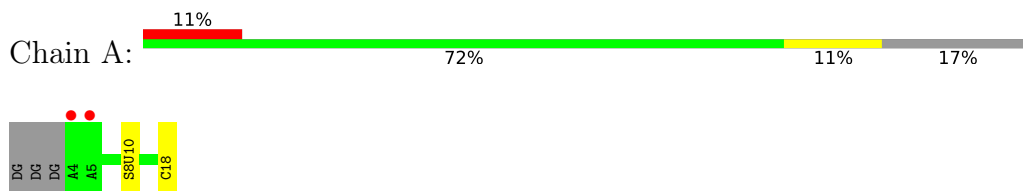




- Molecule 1: T7 RNA polymerase



- Molecule 2: Template strand DNA



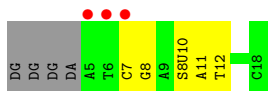
- Molecule 2: Template strand DNA



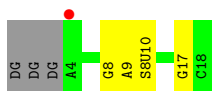




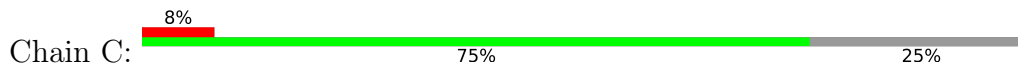
- Molecule 2: Template strand DNA



- Molecule 2: Template strand DNA



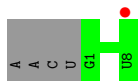
- Molecule 3: RNA



- Molecule 3: RNA



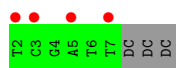
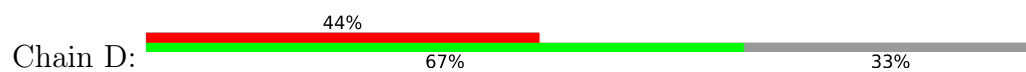
- Molecule 3: RNA



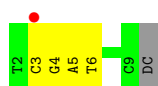
- Molecule 3: RNA



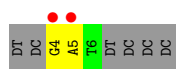
- Molecule 4: Non-template strand DNA



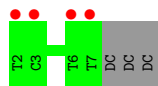
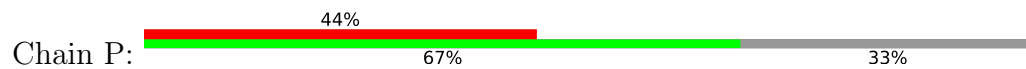
- Molecule 4: Non-template strand DNA



- Molecule 4: Non-template strand DNA



- Molecule 4: Non-template strand DNA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.78Å 86.23Å 201.46Å 89.85° 85.39° 69.59°	Depositor
Resolution (Å)	43.20 – 2.80 43.20 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.7 (43.20-2.80) 97.7 (43.20-2.80)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.25 (at 2.81Å)	Xtrriage
Refinement program	PHENIX 1.19	Depositor
R, $R_{free}$	0.233 , 0.275 0.231 , 0.273	Depositor DCC
$R_{free}$ test set	1905 reflections (1.60%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	82.1	Xtrriage
Anisotropy	0.270	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 69.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	28446	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	116.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, S8U, S96

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	B	0.28	0/6878	0.53	2/9304 (0.0%)
1	E	0.27	0/6542	0.52	1/8859 (0.0%)
1	I	0.30	0/6575	0.56	3/8894 (0.0%)
1	M	0.28	0/6553	0.56	4/8870 (0.0%)
2	A	0.49	0/318	0.85	0/485
2	F	0.48	0/365	0.86	0/559
2	J	0.49	0/294	0.88	0/448
2	N	0.48	0/318	0.93	0/485
3	C	0.19	0/215	0.80	0/333
3	G	0.17	0/193	0.75	0/299
3	K	0.16	0/193	0.72	0/299
3	O	0.19	0/193	0.84	0/299
4	D	0.44	0/135	1.01	0/206
4	H	0.61	0/177	1.07	0/270
4	L	0.45	0/70	0.90	0/106
4	P	0.61	0/135	1.06	0/206
All	All	0.30	0/29154	0.59	10/39922 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	78	LEU	CB-CG-CD2	-12.44	89.86	111.00
1	I	699	LEU	CA-CB-CG	7.48	132.49	115.30
1	E	787	ASP	CB-CG-OD2	7.19	124.77	118.30
1	M	130	ASP	CB-CG-OD1	7.09	124.68	118.30
1	M	870	LEU	CA-CB-CG	6.79	130.91	115.30
1	I	747	LEU	CA-CB-CG	6.03	129.18	115.30
1	I	621	LEU	CA-CB-CG	5.84	128.74	115.30
1	B	246	LEU	CA-CB-CG	5.65	128.29	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	157	LEU	CA-CB-CG	5.52	128.00	115.30
1	M	621	LEU	CA-CB-CG	5.44	127.82	115.30

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	B	6728	0	6694	71	0
1	E	6397	0	6304	68	0
1	I	6429	0	6372	99	0
1	M	6409	0	6347	108	0
2	A	303	0	157	1	0
2	F	344	0	180	4	0
2	J	282	0	146	3	0
2	N	303	0	157	2	0
3	C	193	0	96	0	0
3	G	173	0	86	0	0
3	K	173	0	86	0	0
3	O	173	0	86	2	0
4	D	122	0	70	0	0
4	H	160	0	92	3	0
4	L	63	0	35	2	0
4	P	122	0	70	0	0
5	B	35	0	0	1	0
5	E	35	0	0	2	0
6	B	1	0	0	0	0
6	E	1	0	0	0	0
All	All	28446	0	26978	356	0

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 6.

All (356) 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)
5:E:901:S96:C18	5:E:901:S96:O33	1.66	1.16
5:B:901:S96:C18	5:B:901:S96:O33	1.66	1.15
1:M:80:LYS:NZ	1:M:223:SER:O	1.96	0.99
1:B:78:LEU:HD21	1:B:746:ARG:HH12	1.47	0.78
1:E:700:LYS:HG2	1:E:775:GLU:HB2	1.67	0.76
1:B:226:MET:HG2	1:B:227:VAL:HG23	1.69	0.75
1:M:561:LEU:HD22	1:M:875:ILE:HG12	1.68	0.74
1:M:281:ILE:HD12	1:M:282:THR:HG23	1.72	0.71
1:M:57:ARG:HH12	2:N:17:DG:H5''	1.57	0.70
1:M:548:ALA:O	1:M:551:ARG:NH1	2.25	0.69
1:M:236:VAL:HB	1:M:239:GLN:HG2	1.74	0.69
1:E:421:ASP:OD2	1:E:423:ARG:NH1	2.25	0.69
1:M:86:ASN:HA	1:M:89:PHE:HB2	1.76	0.68
1:M:376:ALA:HA	1:M:379:ARG:HE	1.58	0.68
1:B:715:THR:HG23	1:B:717:GLU:H	1.59	0.68
1:I:184:GLN:HA	1:I:187:GLU:HB3	1.77	0.67
1:M:85:ILE:HD13	1:M:111:PRO:HB2	1.77	0.67
1:M:436:GLY:O	1:M:441:LYS:NZ	2.28	0.66
1:E:36:GLN:HG3	1:E:273:VAL:HG12	1.79	0.65
1:B:46:MET:SD	1:B:269:GLN:NE2	2.71	0.64
1:I:706:LEU:HD12	1:I:725:VAL:HG12	1.79	0.64
1:I:825:PHE:O	1:I:829:ARG:NH1	2.30	0.63
1:B:126:LEU:HD13	1:B:246:LEU:HB2	1.80	0.63
1:M:700:LYS:HG3	1:M:775:GLU:HB2	1.81	0.62
1:B:798:ALA:HB1	1:B:804:ILE:HD12	1.82	0.62
1:B:310:ASP:OD2	1:I:307:ARG:NE	2.33	0.61
1:M:171:ASN:HB3	3:O:3:G:H5'	1.82	0.61
1:E:705:LEU:HD12	1:E:861:MET:HG2	1.82	0.61
1:M:163:LYS:HA	1:M:166:VAL:HB	1.82	0.61
1:I:629:VAL:HG13	1:I:654:THR:HG21	1.83	0.60
1:I:707:ALA:O	1:I:722:ARG:NH1	2.32	0.60
1:I:14:ILE:HG22	1:I:290:GLY:HA2	1.84	0.60
1:I:542:GLY:HA2	1:I:783:VAL:HG21	1.82	0.60
1:M:721:LYS:HE3	1:M:722:ARG:H	1.68	0.59
1:I:316:VAL:HG12	1:I:731:ASP:OD2	2.02	0.59
1:I:448:LYS:NZ	1:I:805:GLU:OE2	2.36	0.58
1:I:461:LYS:HE2	1:I:479:ILE:HG23	1.86	0.58
1:I:696:MET:HG2	1:I:779:ALA:HB1	1.86	0.58
1:M:812:ASP:N	1:M:812:ASP:OD1	2.37	0.58
1:B:227:VAL:HG13	1:B:244:ILE:HD11	1.86	0.58
1:E:544:GLN:HG2	1:E:561:LEU:HD21	1.86	0.57
1:B:163:LYS:HA	1:B:166:VAL:HG22	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:317:TYR:O	1:I:321:ASN:ND2	2.37	0.57
1:B:159:ALA:O	1:B:163:LYS:N	2.33	0.57
1:E:791:LEU:HD21	1:E:809:LEU:HD13	1.86	0.57
2:F:5:DA:H61	4:H:6:DT:H3	1.51	0.57
1:E:345:LYS:NZ	1:E:351:ASP:O	2.36	0.57
1:M:232:GLN:O	1:M:233:ASN:ND2	2.38	0.57
1:M:307:ARG:NH1	1:M:738:GLU:OE1	2.35	0.57
1:E:36:GLN:NE2	1:E:271:CYS:SG	2.78	0.56
1:B:57:ARG:NH1	2:A:18:DC:OP2	2.39	0.56
1:B:334:VAL:HG23	1:B:443:LEU:HD23	1.88	0.55
1:B:663:LYS:HA	1:B:663:LYS:HE2	1.88	0.55
1:B:298:ARG:NH1	1:B:419:ASN:OD1	2.39	0.55
1:E:740:LYS:HA	1:E:769:ILE:HA	1.87	0.55
1:B:24:LEU:HD21	1:B:273:VAL:HG21	1.87	0.55
1:I:709:GLU:HG3	1:I:722:ARG:HG3	1.88	0.55
1:B:541:SER:HA	1:B:544:GLN:HB2	1.88	0.55
1:I:677:MET:HG3	1:I:681:ILE:HD11	1.89	0.55
1:E:706:LEU:HD11	1:E:849:PHE:HB2	1.88	0.55
1:I:543:ILE:HB	1:I:559:VAL:HG11	1.88	0.55
1:M:425:ARG:NH2	3:O:8:U:O2'	2.40	0.55
1:M:798:ALA:HB1	1:M:804:ILE:HD12	1.88	0.55
1:B:85:ILE:HD11	1:B:111:PRO:HB3	1.89	0.55
1:B:226:MET:CG	1:B:227:VAL:HG23	2.37	0.54
1:E:804:ILE:HG12	1:E:820:ASP:HB3	1.88	0.54
1:I:35:GLU:HG2	1:I:272:VAL:HG21	1.89	0.54
1:M:471:ASP:N	1:M:471:ASP:OD1	2.40	0.54
1:E:347:CYS:HB3	1:E:350:GLU:HB2	1.89	0.54
1:M:590:THR:HG22	1:M:613:THR:HG23	1.90	0.54
1:I:180:LYS:HE3	1:I:184:GLN:HE22	1.73	0.54
1:B:78:LEU:HD21	1:B:746:ARG:NH1	2.21	0.54
1:I:594:VAL:HA	1:I:609:VAL:HA	1.89	0.54
1:M:421:ASP:OD2	1:M:423:ARG:NH1	2.40	0.54
1:B:78:LEU:HD23	1:B:79:PRO:HD3	1.90	0.53
1:I:503:ALA:HA	1:I:508:PRO:HB3	1.90	0.53
1:B:466:ASN:OD1	1:B:478:ARG:NH1	2.41	0.53
1:I:157:LEU:N	1:I:160:LYS:HZ1	2.07	0.53
1:M:530:CYS:HB3	1:M:818:PRO:HG2	1.89	0.53
1:M:217:ILE:HA	1:M:220:LEU:HD12	1.90	0.53
1:E:118:THR:HG22	1:E:141:ILE:HD13	1.91	0.53
1:M:707:ALA:O	1:M:722:ARG:NH1	2.42	0.53
1:B:810:ILE:O	1:B:812:ASP:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:461:LYS:HB3	1:I:482:ILE:HG13	1.91	0.53
1:M:651:LEU:HA	1:M:655:ILE:HB	1.91	0.53
1:B:73:LEU:HD11	1:B:250:TYR:HD1	1.74	0.53
1:I:160:LYS:HE2	1:I:160:LYS:N	2.23	0.53
1:I:152:GLY:O	1:I:155:ARG:N	2.41	0.53
1:M:205:HIS:HB3	1:M:208:ASP:HB2	1.91	0.53
1:I:115:ALA:O	1:I:118:THR:OG1	2.24	0.52
1:I:794:THR:HA	1:I:831:THR:HG21	1.92	0.52
1:E:329:LYS:HG2	1:E:447:ALA:HA	1.91	0.52
1:I:557:ARG:HG2	1:I:562:LEU:HD13	1.90	0.52
1:M:231:ARG:HB3	1:M:242:GLU:HA	1.90	0.52
1:B:446:LEU:HD13	1:B:806:SER:HB3	1.92	0.52
1:E:349:VAL:HG11	1:E:508:PRO:HG3	1.91	0.52
1:E:475:PHE:HA	1:E:478:ARG:HG3	1.90	0.52
1:M:85:ILE:HA	1:M:219:MET:HE1	1.92	0.52
1:E:569:ASP:OD2	1:E:627:ARG:NH1	2.43	0.52
1:B:859:ASP:HB2	1:B:860:LYS:HE2	1.92	0.52
1:I:561:LEU:HD22	1:I:875:ILE:HD13	1.92	0.52
1:M:524:HIS:HB2	1:M:528:TYR:HB2	1.91	0.52
1:M:275:PRO:HG2	1:M:324:GLN:HB3	1.92	0.52
1:M:59:LEU:O	1:M:128:SER:OG	2.28	0.51
1:E:524:HIS:HB2	1:E:528:TYR:HB2	1.92	0.51
1:M:790:HIS:O	1:M:794:THR:OG1	2.25	0.51
1:B:109:ILE:HD12	1:B:145:ILE:HG23	1.92	0.51
1:M:376:ALA:HA	1:M:379:ARG:NE	2.24	0.51
1:E:304:ALA:HA	1:E:307:ARG:HD2	1.92	0.51
1:E:150:ARG:HH21	1:E:187:GLU:HG2	1.76	0.51
1:B:93:LYS:HA	1:B:99:ARG:HH21	1.76	0.51
1:B:468:ALA:HA	1:B:505:GLN:HG3	1.92	0.50
1:M:553:GLU:HG3	1:M:870:LEU:HA	1.93	0.50
1:B:3:THR:OG1	1:B:52:ARG:NH1	2.44	0.50
1:E:810:ILE:HB	1:E:813:SER:HB2	1.92	0.50
1:I:155:ARG:HG2	1:I:749:LEU:HD11	1.92	0.50
1:E:419:ASN:N	1:E:427:TYR:O	2.42	0.50
1:I:148:GLU:OE2	1:I:155:ARG:NH2	2.43	0.50
1:E:311:VAL:HG11	1:E:734:PRO:HG3	1.94	0.50
1:M:65:ALA:HB3	1:M:120:LYS:HE3	1.92	0.50
1:M:74:ILE:HD12	1:M:119:ILE:HD12	1.94	0.50
1:M:446:LEU:HG	1:M:533:PRO:HG3	1.93	0.50
1:M:557:ARG:HD3	1:M:562:LEU:HD12	1.93	0.50
1:B:42:GLU:O	1:B:46:MET:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:170:LEU:HD11	1:I:179:LYS:HB3	1.94	0.50
1:B:227:VAL:CG1	1:B:244:ILE:HD11	2.41	0.49
1:E:531:SER:HA	1:E:817:ILE:HD12	1.94	0.49
1:I:695:ALA:O	1:I:699:LEU:HD12	2.12	0.49
1:B:10:ASP:HB3	1:B:291:ARG:NH1	2.27	0.49
1:B:551:ARG:HA	1:B:870:LEU:HD23	1.94	0.49
1:I:19:ILE:HD12	1:I:19:ILE:H	1.77	0.49
1:I:151:PHE:HE1	1:I:184:GLN:HB3	1.76	0.49
1:M:617:ALA:O	1:M:620:TRP:N	2.45	0.49
1:M:588:ASN:OD1	1:M:588:ASN:N	2.46	0.49
1:M:160:LYS:HG3	1:M:163:LYS:HZ3	1.77	0.49
1:B:692:ALA:O	1:B:696:MET:HG3	2.11	0.49
1:E:495:SER:OG	1:E:498:GLU:OE1	2.28	0.49
1:E:163:LYS:O	1:E:167:GLU:N	2.45	0.49
1:I:798:ALA:HB1	1:I:804:ILE:HD12	1.94	0.49
1:M:461:LYS:HD3	1:M:479:ILE:HD12	1.95	0.49
1:B:226:MET:HG2	1:B:227:VAL:CG2	2.41	0.48
1:E:219:MET:SD	1:E:219:MET:N	2.83	0.48
1:I:139:SER:HB3	1:I:210:ILE:HG13	1.95	0.48
1:I:643:GLU:HA	1:I:646:PHE:CD2	2.48	0.48
1:I:778:ILE:HD12	1:I:779:ALA:N	2.27	0.48
1:I:190:MET:O	1:I:194:GLY:N	2.46	0.48
1:I:537:ASP:OD1	1:I:813:SER:OG	2.22	0.48
1:E:151:PHE:HB3	1:E:749:LEU:HD11	1.96	0.48
1:E:714:LYS:HA	1:E:714:LYS:HD3	1.64	0.48
1:E:631:LYS:NZ	5:E:901:S96:O11	2.46	0.48
1:B:7:ALA:HA	1:B:11:PHE:HB2	1.95	0.48
1:I:186:VAL:O	1:I:190:MET:HG2	2.13	0.48
1:I:115:ALA:O	1:I:119:ILE:HG13	2.14	0.48
1:I:393:SER:HA	1:I:396:ILE:HD12	1.96	0.48
1:M:706:LEU:HD12	1:M:725:VAL:HG22	1.96	0.48
1:E:419:ASN:HB2	1:E:429:VAL:HG22	1.96	0.47
1:B:247:ALA:HB3	1:B:250:TYR:HD2	1.80	0.47
1:B:350:GLU:OE1	1:B:391:ARG:NH2	2.46	0.47
1:I:675:GLY:O	1:I:679:LYS:N	2.36	0.47
2:J:7:DC:H42	4:L:4:DG:H1	1.60	0.47
1:I:771:ALA:O	1:I:775:GLU:HG3	2.14	0.47
1:M:122:THR:HG23	1:M:141:ILE:HD11	1.96	0.47
1:M:613:THR:O	1:M:617:ALA:N	2.41	0.47
1:M:810:ILE:HB	1:M:813:SER:HB3	1.95	0.47
1:E:739:TYR:O	1:E:770:ASP:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:65:ALA:HB3	1:E:120:LYS:HG3	1.97	0.47
1:E:541:SER:HA	1:E:544:GLN:HB2	1.96	0.47
1:I:92:VAL:HA	1:I:95:LYS:HB3	1.97	0.47
1:E:160:LYS:O	1:E:164:LYS:N	2.47	0.47
1:I:829:ARG:HB3	1:I:876:LEU:HD13	1.97	0.47
1:M:854:HIS:HB3	1:M:857:GLN:HG3	1.97	0.47
1:I:152:GLY:O	1:I:155:ARG:HG3	2.15	0.46
1:I:589:GLY:HA3	1:I:614:LYS:HB3	1.96	0.46
1:M:452:ILE:HG13	1:M:818:PRO:HB2	1.97	0.46
1:E:468:ALA:HA	1:E:505:GLN:HB3	1.96	0.46
1:I:65:ALA:HB3	1:I:120:LYS:HG3	1.97	0.46
1:I:215:ARG:HD2	1:I:215:ARG:HA	1.65	0.46
1:M:78:LEU:O	1:M:82:ILE:HG12	2.15	0.46
1:M:629:VAL:HG12	1:M:654:THR:HG21	1.97	0.46
1:I:512:LEU:HG	1:I:516:PHE:HE1	1.80	0.46
1:I:837:GLU:HG3	1:I:872:LEU:HD22	1.97	0.46
1:M:550:LEU:O	1:M:868:GLY:N	2.48	0.46
1:B:550:LEU:HD21	1:B:842:LEU:HD12	1.96	0.46
1:E:67:ASN:OD1	1:E:68:ALA:N	2.48	0.46
1:E:8:LYS:HE3	1:E:8:LYS:HB3	1.48	0.46
1:I:113:ALA:O	1:I:117:ILE:HG13	2.15	0.46
1:M:63:GLU:O	1:M:66:ASP:N	2.46	0.46
1:M:705:LEU:O	1:M:720:ARG:NH2	2.48	0.46
1:B:550:LEU:HB2	1:B:691:ALA:HB1	1.98	0.46
1:I:105:PHE:CD2	1:I:212:VAL:HB	2.50	0.46
1:I:190:MET:HB3	1:I:196:LEU:HD23	1.98	0.46
1:B:118:THR:O	1:B:122:THR:OG1	2.23	0.46
1:E:416:PHE:HB2	1:E:418:TYR:HE1	1.78	0.46
1:I:102:ALA:HA	1:I:105:PHE:CE2	2.50	0.46
1:I:151:PHE:CD1	1:I:183:MET:HB3	2.50	0.46
1:I:313:MET:HE2	1:I:316:VAL:HG21	1.97	0.46
1:E:298:ARG:HH21	1:E:419:ASN:HB3	1.80	0.46
1:I:684:SER:O	1:I:688:THR:OG1	2.28	0.46
1:M:412:LYS:H	1:M:412:LYS:HD2	1.79	0.46
1:E:36:GLN:HA	1:E:39:LEU:HG	1.97	0.45
1:M:134:VAL:HA	1:M:244:ILE:HD11	1.98	0.45
1:I:704:LYS:HZ3	4:L:5:DA:H4'	1.81	0.45
1:M:871:ASN:ND2	1:M:874:ASP:OD1	2.48	0.45
1:I:146:GLU:HG3	1:I:204:TRP:CD2	2.52	0.45
1:I:777:GLY:O	1:I:781:ASN:ND2	2.49	0.45
1:B:688:THR:HG22	1:B:689:VAL:HG13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:700:LYS:HE2	1:I:775:GLU:HB3	1.98	0.45
1:M:387:LYS:HA	1:M:387:LYS:HD3	1.77	0.45
1:M:777:GLY:O	1:M:781:ASN:ND2	2.50	0.45
1:E:141:ILE:O	1:E:145:ILE:HG12	2.17	0.45
1:B:349:VAL:HG11	1:B:508:PRO:HG3	1.98	0.45
2:F:16:DC:H2'	2:F:17:DG:C8	2.52	0.45
1:I:93:LYS:HD2	1:I:93:LYS:HA	1.76	0.45
1:I:118:THR:HG21	1:I:216:CYS:HB3	1.98	0.45
1:M:35:GLU:OE2	1:M:411:HIS:NE2	2.43	0.45
1:M:85:ILE:HD12	1:M:86:ASN:N	2.31	0.45
1:M:214:VAL:HA	1:M:217:ILE:HD12	1.98	0.45
1:M:294:LEU:HD11	1:M:429:VAL:HG11	1.99	0.45
1:B:10:ASP:HB3	1:B:291:ARG:HH12	1.82	0.45
1:B:78:LEU:HD21	1:B:746:ARG:HH22	1.82	0.45
1:E:446:LEU:HD22	1:E:806:SER:HB3	1.99	0.45
1:M:543:ILE:HB	1:M:559:VAL:HG11	1.99	0.45
1:B:551:ARG:NE	1:B:872:LEU:HD11	2.32	0.45
1:I:43:SER:HA	1:I:46:MET:HE2	1.98	0.45
1:M:132:THR:HG23	1:M:243:THR:HB	1.99	0.45
1:B:186:VAL:O	1:B:190:MET:HG3	2.18	0.44
1:I:89:PHE:HA	1:I:103:PHE:HE1	1.82	0.44
1:I:293:PRO:O	1:I:294:LEU:HB2	2.16	0.44
1:M:268:PHE:CD1	1:M:429:VAL:HG12	2.52	0.44
1:E:51:PHE:HE2	1:E:261:LEU:HB3	1.82	0.44
1:I:120:LYS:HZ2	1:I:752:LEU:H	1.64	0.44
1:E:55:PHE:HA	1:E:58:GLN:HE21	1.82	0.44
1:B:19:ILE:HD12	1:B:19:ILE:H	1.81	0.44
1:B:611:LEU:HD11	1:B:669:GLN:HB2	1.99	0.44
1:I:30:GLU:OE2	1:I:34:ARG:NH2	2.51	0.44
1:M:132:THR:OG1	1:M:244:ILE:O	2.34	0.44
1:M:552:ASP:HB2	1:M:691:ALA:HB2	1.99	0.44
1:M:775:GLU:HA	1:M:778:ILE:HG22	2.00	0.44
1:B:73:LEU:HD11	1:B:250:TYR:CD1	2.52	0.44
1:I:180:LYS:HE3	1:I:184:GLN:NE2	2.31	0.44
1:I:213:GLY:O	1:I:217:ILE:HG13	2.18	0.44
4:H:5:DA:H2'	4:H:6:DT:C6	2.53	0.43
1:B:226:MET:HA	1:B:250:TYR:CD2	2.52	0.43
1:E:10:ASP:CG	1:E:291:ARG:HE	2.21	0.43
1:E:24:LEU:HD12	1:E:24:LEU:HA	1.82	0.43
1:E:545:HIS:O	1:E:549:MET:HG3	2.18	0.43
1:B:707:ALA:O	1:B:722:ARG:HD3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:118:THR:O	1:I:122:THR:HG23	2.18	0.43
2:N:8:DG:H2''	2:N:9:DA:N7	2.33	0.43
1:I:257:ARG:HD3	1:I:257:ARG:HA	1.74	0.43
1:M:790:HIS:CE1	1:M:832:MET:HB2	2.53	0.43
1:M:177:VAL:HA	1:M:180:LYS:HE3	2.00	0.43
1:B:69:ALA:HA	1:B:257:ARG:HG2	2.00	0.43
1:I:647:ARG:HB2	1:I:674:ALA:HB1	2.00	0.43
1:M:252:GLU:O	1:M:256:THR:HG23	2.18	0.43
1:M:266:PRO:HG2	1:M:268:PHE:HE2	1.84	0.43
1:B:378:LYS:HE3	1:E:377:TRP:CE2	2.54	0.43
1:E:704:LYS:HB3	1:E:704:LYS:HE2	1.70	0.43
1:I:809:LEU:HD13	1:I:809:LEU:HA	1.74	0.43
1:M:389:LYS:HD3	1:M:389:LYS:HA	1.79	0.43
1:I:215:ARG:NE	1:I:218:GLU:OE1	2.52	0.43
1:B:766:ASP:OD1	1:B:766:ASP:N	2.52	0.43
1:M:208:ASP:HA	1:M:211:HIS:ND1	2.34	0.43
1:B:112:GLU:OE2	1:B:112:GLU:N	2.51	0.42
1:E:106:LEU:HD23	1:E:106:LEU:HA	1.90	0.42
2:F:12:DT:H2'	2:F:13:DC:C6	2.54	0.42
1:I:535:ALA:HB1	1:I:813:SER:HB3	2.01	0.42
2:J:7:DC:H2''	2:J:8:DG:C8	2.54	0.42
1:M:681:ILE:O	1:M:685:VAL:HG13	2.18	0.42
1:B:463:HIS:CD2	1:B:535:ALA:H	2.38	0.42
1:E:44:TYR:HA	1:E:266:PRO:HB3	2.01	0.42
1:I:105:PHE:HB2	1:I:106:LEU:HD23	2.00	0.42
1:M:42:GLU:O	1:M:46:MET:HG3	2.19	0.42
1:M:446:LEU:HD13	1:M:806:SER:HB3	2.01	0.42
1:M:485:ASN:O	1:M:489:ILE:HG13	2.19	0.42
1:M:748:ASN:OD1	1:M:749:LEU:N	2.53	0.42
1:I:313:MET:HG3	1:I:316:VAL:HG22	2.01	0.42
1:I:725:VAL:HG22	1:I:737:GLN:HB3	2.01	0.42
1:M:132:THR:OG1	1:M:132:THR:O	2.37	0.42
1:M:159:ALA:HB1	1:M:162:PHE:HD2	1.83	0.42
1:M:215:ARG:O	1:M:219:MET:HG3	2.19	0.42
1:I:553:GLU:HG3	1:I:870:LEU:HA	2.01	0.42
1:M:461:LYS:HG2	1:M:482:ILE:HG21	2.02	0.42
1:E:663:LYS:HE2	1:E:663:LYS:HB3	1.76	0.42
1:I:450:LYS:HE2	1:I:817:ILE:HD11	2.01	0.42
1:I:741:LYS:HB3	1:I:741:LYS:HE2	1.86	0.42
1:M:517:GLU:HG3	1:M:532:LEU:HB2	2.02	0.42
1:M:566:THR:O	1:M:568:GLN:NE2	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:829:ARG:NH2	1:B:882:PHE:H	2.17	0.42
1:E:329:LYS:HG3	1:E:445:THR:HG23	2.02	0.42
1:E:559:VAL:HG23	1:E:561:LEU:HG	2.01	0.42
1:M:474:PRO:HA	1:M:880:PHE:CZ	2.54	0.42
1:B:230:HIS:HB2	1:B:243:THR:HG22	2.00	0.42
1:B:402:LEU:HD12	1:B:402:LEU:HA	1.89	0.42
1:B:650:VAL:HG21	1:B:677:MET:HB3	2.01	0.42
1:I:852:GLN:OE1	1:I:852:GLN:N	2.53	0.42
1:M:392:LYS:H	1:M:392:LYS:HG2	1.57	0.42
1:M:474:PRO:HA	1:M:880:PHE:HZ	1.85	0.42
1:B:153:ARG:O	1:B:157:LEU:HB2	2.20	0.42
1:B:345:LYS:NZ	1:B:351:ASP:O	2.37	0.42
1:E:109:ILE:HD11	1:E:149:ALA:HA	2.01	0.42
1:E:659:ILE:HD13	1:E:664:GLY:HA3	2.02	0.42
1:I:485:ASN:O	1:I:489:ILE:HG13	2.19	0.42
1:M:114:VAL:HG13	1:M:145:ILE:HD12	2.00	0.42
1:M:798:ALA:HA	1:M:802:TYR:HD2	1.83	0.42
1:M:802:TYR:HB2	1:M:804:ILE:HG13	2.02	0.42
1:E:494:LYS:HB3	1:E:494:LYS:HE2	1.72	0.41
1:I:189:ASP:O	1:I:193:LYS:HG2	2.19	0.41
1:M:266:PRO:HG2	1:M:268:PHE:CE2	2.55	0.41
1:I:120:LYS:NZ	1:I:752:LEU:H	2.18	0.41
1:M:214:VAL:O	1:M:218:GLU:HG3	2.20	0.41
1:M:570:ILE:O	1:M:574:VAL:HG12	2.20	0.41
1:B:545:HIS:O	1:B:549:MET:HG3	2.20	0.41
1:M:163:LYS:O	1:M:167:GLU:N	2.52	0.41
1:E:549:MET:HB2	1:E:550:LEU:HD22	2.02	0.41
1:E:700:LYS:HE3	1:E:775:GLU:HG3	2.02	0.41
1:M:794:THR:HA	1:M:831:THR:HG21	2.02	0.41
1:I:479:ILE:HD12	1:I:479:ILE:H	1.86	0.41
1:E:340:VAL:HG11	1:E:497:LEU:HD11	2.01	0.41
1:E:833:VAL:HG21	1:E:876:LEU:HG	2.02	0.41
2:F:4:DA:H2''	2:F:5:DA:H5'	2.02	0.41
1:E:6:ILE:H	1:E:6:ILE:HG13	1.32	0.41
1:E:846:TYR:HA	1:E:849:PHE:CE2	2.56	0.41
1:I:458:TYR:O	1:I:462:ILE:HG12	2.21	0.41
1:I:642:LYS:HA	1:I:642:LYS:HD3	1.83	0.41
1:M:90:GLU:HA	1:M:93:LYS:HD2	2.03	0.41
1:B:113:ALA:O	1:B:117:ILE:HD12	2.21	0.41
1:E:829:ARG:NH2	1:E:882:PHE:H	2.18	0.41
1:I:274:PRO:HA	1:I:275:PRO:HD3	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:846:TYR:HA	1:I:849:PHE:CE2	2.56	0.41
1:M:574:VAL:O	1:M:578:VAL:HG23	2.21	0.41
1:B:329:LYS:HG2	1:B:447:ALA:HA	2.03	0.41
1:E:37:LEU:HD13	1:E:288:ALA:HB2	2.03	0.41
1:I:14:ILE:HD12	1:I:15:GLU:N	2.36	0.41
1:M:37:LEU:HD22	1:M:288:ALA:HB2	2.02	0.41
1:M:48:GLU:O	1:M:52:ARG:HG2	2.21	0.41
1:B:189:ASP:O	1:B:192:SER:OG	2.31	0.40
1:I:550:LEU:O	1:I:868:GLY:N	2.54	0.40
1:I:729:THR:HB	1:I:789:SER:HB2	2.03	0.40
2:J:11:DA:H2'	2:J:12:DT:C6	2.56	0.40
1:M:117:ILE:HG23	1:M:751:PHE:HE2	1.86	0.40
1:M:677:MET:O	1:M:681:ILE:HG13	2.21	0.40
1:B:791:LEU:HA	1:B:814:PHE:HE1	1.86	0.40
1:E:451:PRO:HA	1:E:529:ASN:HA	2.03	0.40
1:I:524:HIS:HB2	1:I:528:TYR:HB2	2.02	0.40
1:M:155:ARG:HG2	1:M:163:LYS:HD2	2.03	0.40
1:M:347:CYS:HB2	1:M:350:GLU:HB2	2.04	0.40
1:B:574:VAL:HG13	1:B:684:SER:HB2	2.03	0.40
1:B:302:LYS:O	1:B:306:MET:HG2	2.21	0.40
1:B:461:LYS:HE3	1:B:479:ILE:HD12	2.02	0.40
1:E:161:HIS:HA	1:E:164:LYS:HD2	2.03	0.40
4:H:3:DC:H2''	4:H:4:DG:H5''	2.04	0.40
1:I:73:LEU:O	1:I:77:LEU:HG	2.21	0.40
1:M:110:LYS:HE3	1:M:156:ASP:OD2	2.22	0.40
1:M:629:VAL:HG23	1:M:630:THR:HG23	2.03	0.40
1:M:630:THR:O	1:M:634:VAL:HG23	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	850/883 (96%)	828 (97%)	21 (2%)	1 (0%)	51	81
1	E	809/883 (92%)	798 (99%)	11 (1%)	0	100	100
1	I	811/883 (92%)	796 (98%)	14 (2%)	1 (0%)	51	81
1	M	809/883 (92%)	797 (98%)	12 (2%)	0	100	100
All	All	3279/3532 (93%)	3219 (98%)	58 (2%)	2 (0%)	51	81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	811	HIS
1	I	294	LEU

### 5.3.2 Protein 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	Percentiles	
1	B	701/729 (96%)	661 (94%)	40 (6%)	20	50
1	E	660/729 (90%)	622 (94%)	38 (6%)	20	50
1	I	664/729 (91%)	618 (93%)	46 (7%)	15	41
1	M	662/729 (91%)	620 (94%)	42 (6%)	18	46
All	All	2687/2916 (92%)	2521 (94%)	166 (6%)	18	47

All (166) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	13	ASP
1	B	50	ARG
1	B	99	ARG
1	B	133	THR
1	B	202	SER
1	B	203	SER
1	B	206	LYS
1	B	219	MET
1	B	229	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	243	THR
1	B	267	MET
1	B	291	ARG
1	B	292	ARG
1	B	301	SER
1	B	303	LYS
1	B	310	ASP
1	B	375	THR
1	B	401	MET
1	B	423	ARG
1	B	430	SER
1	B	471	ASP
1	B	477	GLU
1	B	505	GLN
1	B	507	SER
1	B	514	PHE
1	B	539	SER
1	B	540	CYS
1	B	609	VAL
1	B	648	GLN
1	B	666	MET
1	B	712	ASP
1	B	735	VAL
1	B	738	GLU
1	B	744	GLN
1	B	746	ARG
1	B	750	MET
1	B	791	LEU
1	B	812	ASP
1	B	813	SER
1	B	859	ASP
1	E	6	ILE
1	E	8	LYS
1	E	13	ASP
1	E	21	PHE
1	E	51	PHE
1	E	78	LEU
1	E	90	GLU
1	E	123	LEU
1	E	155	ARG
1	E	186	VAL
1	E	219	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	E	220	LEU
1	E	291	ARG
1	E	315	GLU
1	E	320	ILE
1	E	377	TRP
1	E	379	ARG
1	E	389	LYS
1	E	401	MET
1	E	412	LYS
1	E	420	MET
1	E	430	SER
1	E	477	GLU
1	E	495	SER
1	E	540	CYS
1	E	577	LYS
1	E	608	LYS
1	E	656	GLN
1	E	665	LEU
1	E	666	MET
1	E	686	SER
1	E	715	THR
1	E	720	ARG
1	E	811	HIS
1	E	812	ASP
1	E	839	CYS
1	E	870	LEU
1	E	873	ARG
1	I	5	ASN
1	I	52	ARG
1	I	54	MET
1	I	81	MET
1	I	86	ASN
1	I	90	GLU
1	I	101	THR
1	I	104	GLN
1	I	114	VAL
1	I	121	THR
1	I	126	LEU
1	I	132	THR
1	I	150	ARG
1	I	155	ARG
1	I	157	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	I	180	LYS
1	I	195	LEU
1	I	196	LEU
1	I	212	VAL
1	I	215	ARG
1	I	257	ARG
1	I	265	SER
1	I	292	ARG
1	I	294	LEU
1	I	301	SER
1	I	303	LYS
1	I	317	TYR
1	I	385	TYR
1	I	387	LYS
1	I	423	ARG
1	I	441	LYS
1	I	527	SER
1	I	531	SER
1	I	541	SER
1	I	641	SER
1	I	666	MET
1	I	679	LYS
1	I	697	ASN
1	I	704	LYS
1	I	720	ARG
1	I	738	GLU
1	I	747	LEU
1	I	767	SER
1	I	806	SER
1	I	859	ASP
1	I	864	LEU
1	M	8	LYS
1	M	16	LEU
1	M	58	GLN
1	M	80	LYS
1	M	81	MET
1	M	125	CYS
1	M	131	ASN
1	M	169	GLN
1	M	170	LEU
1	M	178	TYR
1	M	210	ILE

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Mol	Chain	Res	Type
1	M	224	THR
1	M	306	MET
1	M	325	ASN
1	M	387	LYS
1	M	389	LYS
1	M	392	LYS
1	M	397	SER
1	M	404	GLN
1	M	412	LYS
1	M	438	ASP
1	M	488	ASN
1	M	507	SER
1	M	518	TYR
1	M	528	TYR
1	M	541	SER
1	M	551	ARG
1	M	632	ARG
1	M	641	SER
1	M	642	LYS
1	M	647	ARG
1	M	654	THR
1	M	671	ASN
1	M	686	SER
1	M	720	ARG
1	M	751	PHE
1	M	791	LEU
1	M	812	ASP
1	M	853	LEU
1	M	867	LYS
1	M	872	LEU
1	M	879	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	22	ASN
1	B	463	HIS
1	E	36	GLN
1	E	58	GLN
1	E	781	ASN
1	E	869	ASN
1	I	672	GLN

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Mol	Chain	Res	Type
1	M	869	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	C	7/12 (58%)	0	0
3	G	6/12 (50%)	0	0
3	K	6/12 (50%)	0	0
3	O	6/12 (50%)	2 (33%)	0
All	All	25/48 (52%)	2 (8%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	O	2	C
3	O	4	G

There are no RNA pucker outliers to report.

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

4 non-standard protein/DNA/RNA residues 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
2	S8U	A	10	2	15,19,20	4.37	7 (46%)	16,26,29	1.27	2 (12%)
2	S8U	N	10	2	15,19,20	4.36	7 (46%)	16,26,29	1.37	2 (12%)
2	S8U	J	10	2	15,19,20	4.36	7 (46%)	16,26,29	1.39	2 (12%)
2	S8U	F	10	2	15,19,20	4.37	7 (46%)	16,26,29	1.40	2 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	S8U	A	10	2	-	0/3/23/24	0/2/2/2
2	S8U	N	10	2	-	0/3/23/24	0/2/2/2
2	S8U	J	10	2	-	0/3/23/24	0/2/2/2
2	S8U	F	10	2	-	0/3/23/24	0/2/2/2

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	10	S8U	C2'-C3'	-11.29	1.23	1.52
2	A	10	S8U	C2'-C3'	-11.28	1.23	1.52
2	N	10	S8U	C2'-C3'	-11.27	1.23	1.52
2	F	10	S8U	C2'-C3'	-11.25	1.23	1.52
2	F	10	S8U	O4'-C4'	-8.10	1.26	1.45
2	J	10	S8U	O4'-C4'	-8.08	1.26	1.45
2	N	10	S8U	O4'-C4'	-8.05	1.27	1.45
2	A	10	S8U	O4'-C4'	-8.05	1.27	1.45
2	A	10	S8U	C1'-N11	-5.24	1.33	1.49
2	F	10	S8U	C1'-N11	-5.23	1.33	1.49
2	N	10	S8U	C1'-N11	-5.22	1.33	1.49
2	J	10	S8U	C1'-N11	-5.21	1.33	1.49
2	A	10	S8U	C3'-C4'	5.10	1.67	1.53
2	N	10	S8U	C3'-C4'	5.07	1.66	1.53
2	F	10	S8U	C3'-C4'	5.07	1.66	1.53
2	J	10	S8U	C3'-C4'	5.00	1.66	1.53
2	N	10	S8U	O4'-C1'	4.12	1.51	1.42
2	F	10	S8U	O4'-C1'	4.12	1.51	1.42
2	J	10	S8U	O4'-C1'	4.11	1.51	1.42
2	A	10	S8U	O4'-C1'	4.09	1.51	1.42
2	A	10	S8U	O3'-C3'	3.23	1.50	1.43
2	F	10	S8U	O3'-C3'	3.23	1.50	1.43
2	N	10	S8U	O3'-C3'	3.20	1.50	1.43
2	J	10	S8U	O3'-C3'	3.14	1.50	1.43
2	F	10	S8U	O5'-C5'	-2.20	1.39	1.44
2	A	10	S8U	O5'-C5'	-2.18	1.39	1.44
2	J	10	S8U	O5'-C5'	-2.18	1.39	1.44
2	N	10	S8U	O5'-C5'	-2.11	1.39	1.44

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	10	S8U	O14-C13-C12	-2.96	119.98	124.17
2	N	10	S8U	O14-C13-C12	-2.94	120.01	124.17
2	A	10	S8U	O14-C13-C12	-2.89	120.07	124.17
2	F	10	S8U	O14-C13-C12	-2.88	120.09	124.17
2	J	10	S8U	C2'-C3'-C4'	2.68	108.35	102.76
2	F	10	S8U	C2'-C3'-C4'	2.65	108.27	102.76
2	N	10	S8U	C2'-C3'-C4'	2.64	108.27	102.76
2	A	10	S8U	C2'-C3'-C4'	2.22	107.39	102.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	S96	E	901	6	31,38,38	6.95	16 (51%)	35,59,59	1.68	7 (20%)
5	S96	B	901	6	31,38,38	6.94	16 (51%)	35,59,59	1.67	6 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	S96	E	901	6	-	6/20/42/42	0/4/4/4
5	S96	B	901	6	-	4/20/42/42	0/4/4/4

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	901	S96	O33-C18	18.34	1.66	1.41
5	B	901	S96	O33-C18	18.29	1.66	1.41
5	B	901	S96	C24-S25	-16.82	1.56	1.72
5	E	901	S96	C24-S25	-16.72	1.56	1.72
5	E	901	S96	C17-C18	-16.27	1.29	1.53
5	B	901	S96	C17-C18	-16.16	1.29	1.53
5	E	901	S96	C32-N31	15.16	1.56	1.35
5	B	901	S96	C32-N31	15.12	1.56	1.35
5	E	901	S96	C23-C22	9.75	1.58	1.43
5	B	901	S96	C23-C22	9.55	1.58	1.43
5	B	901	S96	C30-N31	8.09	1.48	1.32
5	E	901	S96	C30-N31	8.04	1.48	1.32
5	E	901	S96	C27-C28	6.77	1.61	1.39
5	B	901	S96	C27-C28	6.72	1.61	1.39
5	B	901	S96	O33-C15	-6.16	1.31	1.45
5	E	901	S96	O33-C15	-5.99	1.31	1.45
5	E	901	S96	C29-C30	5.75	1.50	1.38
5	B	901	S96	C29-C30	5.75	1.50	1.38
5	B	901	S96	C29-C23	5.48	1.48	1.38
5	E	901	S96	C29-C23	5.48	1.48	1.38
5	E	901	S96	O35-C16	-3.94	1.33	1.43
5	B	901	S96	O35-C16	-3.93	1.33	1.43
5	B	901	S96	C26-S25	-3.34	1.54	1.71
5	E	901	S96	C26-S25	-3.33	1.55	1.71
5	E	901	S96	C20-N21	3.31	1.40	1.34
5	B	901	S96	C20-N21	3.21	1.40	1.34
5	B	901	S96	C27-C26	3.18	1.44	1.34
5	E	901	S96	C27-C26	3.14	1.44	1.34
5	B	901	S96	C23-C24	3.07	1.51	1.48
5	E	901	S96	C23-C24	3.04	1.51	1.48
5	E	901	S96	O34-C17	2.98	1.50	1.43
5	B	901	S96	O34-C17	2.96	1.49	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	901	S96	C27-C26-S25	-6.24	107.92	112.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	901	S96	C27-C26-S25	-6.07	108.05	112.98
5	E	901	S96	C29-C30-N31	-3.19	119.64	124.58
5	B	901	S96	C29-C30-N31	-3.07	119.83	124.58
5	E	901	S96	C30-N31-C32	2.96	120.44	116.77
5	B	901	S96	C23-C24-S25	2.80	126.06	117.13
5	B	901	S96	C30-N31-C32	2.69	120.11	116.77
5	E	901	S96	C23-C24-S25	2.68	125.67	117.13
5	B	901	S96	P05-O08-P09	-2.60	123.90	132.83
5	E	901	S96	C16-C17-C18	2.40	104.60	100.98
5	E	901	S96	P05-O08-P09	-2.38	124.64	132.83
5	B	901	S96	C28-C27-C26	-2.03	108.11	113.74
5	E	901	S96	P05-O04-P01	-2.03	125.88	132.83

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	901	S96	C14-O13-P01-O03
5	B	901	S96	C14-O13-P01-O04
5	E	901	S96	O13-C14-C15-O33
5	E	901	S96	C14-O13-P01-O04
5	E	901	S96	O13-C14-C15-C16
5	E	901	S96	P05-O04-P01-O02
5	B	901	S96	C14-O13-P01-O02
5	E	901	S96	C14-O13-P01-O03
5	E	901	S96	C15-C14-O13-P01
5	B	901	S96	C29-C23-C24-C28

There are no ring outliers.

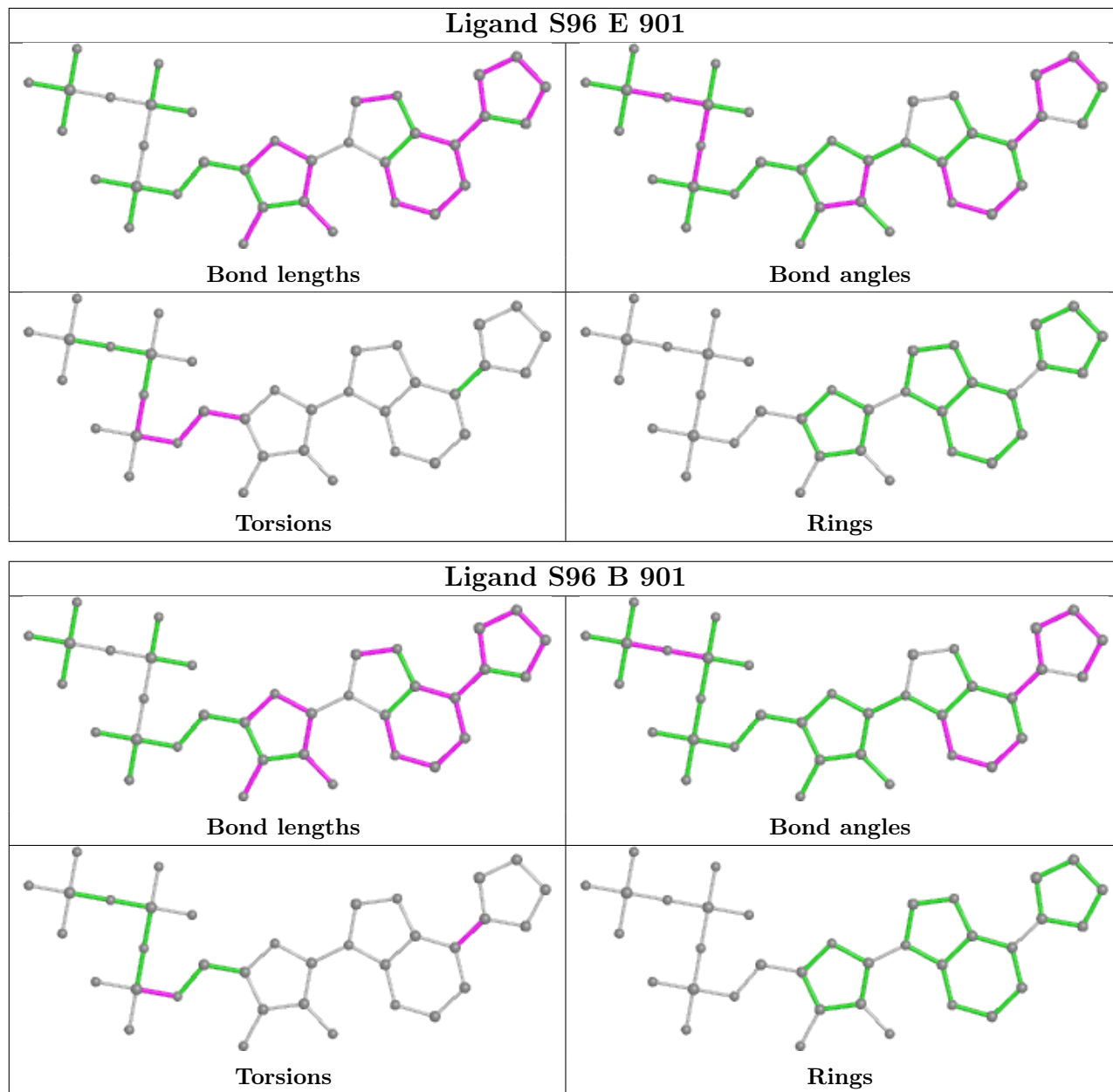
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	901	S96	2	0
5	B	901	S96	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring



in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	B	856/883 (96%)	0.32	36 (4%) 36 26	46, 79, 149, 207	0
1	E	819/883 (92%)	0.66	101 (12%) 4 2	51, 91, 194, 254	0
1	I	821/883 (92%)	0.60	89 (10%) 5 3	65, 116, 181, 226	0
1	M	819/883 (92%)	0.83	125 (15%) 2 1	79, 130, 209, 268	0
2	A	14/18 (77%)	0.76	2 (14%) 2 1	57, 83, 257, 270	0
2	F	16/18 (88%)	0.27	0 100 100	74, 128, 257, 274	0
2	J	13/18 (72%)	1.00	3 (23%) 0 0	82, 92, 293, 308	0
2	N	14/18 (77%)	0.53	1 (7%) 16 9	102, 150, 228, 260	0
3	C	9/12 (75%)	0.94	1 (11%) 5 3	65, 75, 116, 168	0
3	G	8/12 (66%)	0.93	2 (25%) 0 0	77, 92, 140, 155	0
3	K	8/12 (66%)	0.60	1 (12%) 3 2	96, 100, 125, 152	0
3	O	8/12 (66%)	0.61	1 (12%) 3 2	114, 124, 185, 194	0
4	D	6/9 (66%)	2.30	4 (66%) 0 0	217, 228, 252, 264	0
4	H	8/9 (88%)	1.38	1 (12%) 3 2	224, 231, 239, 254	0
4	L	3/9 (33%)	2.40	2 (66%) 0 0	251, 251, 273, 277	0
4	P	6/9 (66%)	2.37	4 (66%) 0 0	244, 258, 263, 277	0
All	All	3428/3688 (92%)	0.61	373 (10%) 5 3	46, 106, 197, 308	0

All (373) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	174	VAL	6.9
1	I	377	TRP	6.5
1	E	106	LEU	6.4
1	M	159	ALA	6.1
1	M	620	TRP	5.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	9	ASN	5.8
1	M	670	PRO	5.5
1	I	593	GLU	5.5
1	M	177	VAL	5.5
1	I	131	ASN	5.5
1	M	377	TRP	5.3
1	M	129	ALA	5.3
2	N	4	DA	5.3
1	E	142	GLY	5.2
1	M	182	PHE	5.2
1	M	11	PHE	5.2
1	E	379	ARG	5.1
1	I	714	LYS	5.1
1	M	24	LEU	5.0
1	E	6	ILE	4.9
1	E	221	ILE	4.9
1	B	605	ILE	4.9
1	E	246	LEU	4.9
1	E	52	ARG	4.9
1	M	857	GLN	4.8
1	M	181	ALA	4.8
1	I	228	SER	4.8
1	E	178	TYR	4.8
1	I	671	ASN	4.7
1	M	106	LEU	4.6
1	I	161	HIS	4.6
1	E	220	LEU	4.6
1	M	108	GLU	4.5
1	E	216	CYS	4.5
1	M	241	SER	4.5
1	M	623	TYR	4.5
1	I	253	ALA	4.5
1	I	11	PHE	4.4
1	M	168	GLU	4.4
1	E	173	ARG	4.4
1	M	102	ALA	4.4
1	M	595	VAL	4.4
1	I	130	ASP	4.3
1	M	166	VAL	4.3
1	M	126	LEU	4.2
1	M	32	LEU	4.2
1	M	216	CYS	4.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	M	616	LEU	4.2
1	M	98	LYS	4.2
1	E	5	ASN	4.2
1	E	8	LYS	4.2
1	E	16	LEU	4.1
1	M	676	TYR	4.1
1	B	754	GLN	4.1
1	E	105	PHE	4.1
1	I	23	THR	4.1
1	M	626	THR	4.1
1	I	226	MET	4.1
1	E	135	GLN	4.1
1	E	104	GLN	4.0
1	B	9	ASN	4.0
1	E	751	PHE	4.0
1	I	98	LYS	4.0
1	M	751	PHE	4.0
1	B	540	CYS	4.0
1	E	14	ILE	4.0
1	E	131	ASN	3.9
1	M	883	ALA	3.9
1	I	752	LEU	3.9
1	E	13	ASP	3.8
1	M	119	ILE	3.8
1	M	117	ILE	3.8
1	M	116	TYR	3.8
1	M	112	GLU	3.8
1	E	182	PHE	3.8
1	M	655	ILE	3.8
1	B	746	ARG	3.8
2	J	6	DT	3.7
1	M	374	LEU	3.7
1	E	197	GLY	3.7
1	B	135	GLN	3.7
1	E	82	ILE	3.7
1	E	107	GLN	3.7
1	I	860	LYS	3.7
1	E	129	ALA	3.7
1	B	134	VAL	3.7
1	M	185	VAL	3.6
1	M	123	LEU	3.6
1	I	157	LEU	3.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	186	VAL	3.6
4	P	6	DT	3.6
1	I	660	ASP	3.6
2	A	4	DA	3.5
1	M	173	ARG	3.5
1	E	376	ALA	3.5
1	M	9	ASN	3.5
1	I	212	VAL	3.5
1	M	93	LYS	3.5
1	B	857	GLN	3.5
1	E	130	ASP	3.5
1	M	178	TYR	3.5
1	M	100	PRO	3.5
1	I	3	THR	3.5
1	E	11	PHE	3.5
1	E	251	ALA	3.4
1	I	594	VAL	3.4
1	E	168	GLU	3.4
1	M	148	GLU	3.4
4	D	2	DT	3.4
1	E	10	ASP	3.3
1	E	813	SER	3.3
4	P	2	DT	3.3
1	I	537	ASP	3.3
1	I	126	LEU	3.3
1	M	286	TYR	3.3
1	I	5	ASN	3.3
1	M	109	ILE	3.3
4	H	3	DC	3.3
1	E	137	VAL	3.3
1	E	212	VAL	3.3
1	E	17	ALA	3.3
1	I	616	LEU	3.2
1	I	859	ASP	3.2
1	I	97	GLY	3.2
1	M	647	ARG	3.2
1	E	713	LYS	3.2
1	E	385	TYR	3.2
1	I	376	ALA	3.2
1	I	609	VAL	3.2
1	B	129	ALA	3.2
1	I	717	GLU	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	749	LEU	3.2
1	I	629	VAL	3.2
1	E	179	LYS	3.1
1	M	382	ALA	3.1
1	I	630	THR	3.1
1	M	161	HIS	3.1
1	M	545	HIS	3.1
2	J	5	DA	3.1
1	M	174	VAL	3.1
1	M	378	LYS	3.1
1	M	716	GLY	3.1
1	M	719	LEU	3.0
1	I	540	CYS	3.0
1	M	8	LYS	3.0
1	I	489	ILE	3.0
1	M	137	VAL	3.0
1	M	384	VAL	3.0
1	I	577	LYS	3.0
1	E	660	ASP	3.0
4	L	5	DA	3.0
1	E	91	GLU	3.0
1	B	355	ILE	3.0
1	M	715	THR	3.0
1	B	714	LYS	3.0
1	M	81	MET	3.0
1	M	120	LYS	2.9
1	E	201	TRP	2.9
1	E	811	HIS	2.9
1	M	611	LEU	2.9
1	B	8	LYS	2.9
1	E	214	VAL	2.9
1	I	698	TRP	2.9
1	I	880	PHE	2.9
3	G	8	U	2.9
1	M	540	CYS	2.9
1	E	63	GLU	2.9
1	E	114	VAL	2.9
1	E	858	LEU	2.9
1	M	105	PHE	2.9
1	B	719	LEU	2.9
1	M	698	TRP	2.8
1	I	350	GLU	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	M	855	GLU	2.8
1	I	656	GLN	2.8
1	I	6	ILE	2.8
1	B	607	GLU	2.8
1	E	111	PRO	2.8
1	I	538	GLY	2.8
1	I	623	TYR	2.8
1	I	216	CYS	2.8
1	M	16	LEU	2.8
1	I	293	PRO	2.8
1	E	161	HIS	2.8
1	E	656	GLN	2.8
1	I	518	TYR	2.8
1	E	536	PHE	2.8
4	L	4	DG	2.8
1	I	744	GLN	2.8
1	E	103	PHE	2.7
1	I	103	PHE	2.7
1	E	812	ASP	2.7
1	I	227	VAL	2.7
1	M	153	ARG	2.7
1	E	169	GLN	2.7
1	M	69	ALA	2.7
1	M	713	LYS	2.7
1	I	142	GLY	2.7
1	M	244	ILE	2.7
1	E	437	ASN	2.7
1	I	481	PHE	2.7
1	M	671	ASN	2.7
1	E	390	ALA	2.7
1	E	810	ILE	2.7
1	M	590	THR	2.7
4	D	3	DC	2.7
1	I	748	ASN	2.7
1	M	749	LEU	2.7
4	D	7	DT	2.6
1	I	521	VAL	2.6
1	I	436	GLY	2.6
1	E	815	GLY	2.6
1	M	637	LEU	2.6
1	B	720	ARG	2.6
1	I	611	LEU	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	M	114	VAL	2.6
1	B	769	ILE	2.6
1	B	752	LEU	2.6
1	B	158	GLU	2.6
1	M	218	GLU	2.6
1	M	539	SER	2.6
1	B	126	LEU	2.5
1	M	75	THR	2.5
2	A	5	DA	2.5
4	D	5	DA	2.5
1	M	293	PRO	2.5
1	I	207	GLU	2.5
1	I	96	ARG	2.5
1	E	183	MET	2.5
1	E	381	ALA	2.5
1	M	354	ALA	2.5
1	E	418	TYR	2.5
1	M	254	ILE	2.5
1	I	246	LEU	2.5
1	M	267	MET	2.5
1	E	30	GLU	2.5
1	E	538	GLY	2.5
1	B	859	ASP	2.5
1	I	10	ASP	2.5
1	I	812	ASP	2.5
1	E	377	TRP	2.5
1	M	687	VAL	2.4
1	I	669	GLN	2.4
1	I	250	TYR	2.4
1	I	857	GLN	2.4
1	E	715	THR	2.4
1	E	540	CYS	2.4
1	M	379	ARG	2.4
1	M	811	HIS	2.4
3	G	7	A	2.4
1	E	51	PHE	2.4
1	M	134	VAL	2.4
3	C	8	U	2.4
1	B	510	CYS	2.4
1	I	588	ASN	2.4
1	I	18	ALA	2.4
1	E	744	GLN	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	I	715	THR	2.4
1	M	212	VAL	2.4
1	E	541	SER	2.4
1	I	810	ILE	2.4
1	M	151	PHE	2.4
1	E	108	GLU	2.4
1	E	37	LEU	2.4
1	I	129	ALA	2.3
1	E	128	SER	2.3
1	M	209	SER	2.3
1	M	217	ILE	2.3
1	M	860	LYS	2.3
1	E	436	GLY	2.3
1	M	179	LYS	2.3
1	E	419	ASN	2.3
1	M	350	GLU	2.3
1	B	860	LYS	2.3
1	M	541	SER	2.3
1	E	15	GLU	2.3
1	M	10	ASP	2.3
1	E	191	LEU	2.3
1	I	32	LEU	2.3
1	E	198	GLY	2.3
1	M	128	SER	2.3
1	B	377	TRP	2.3
1	B	709	GLU	2.3
1	M	59	LEU	2.3
1	I	19	ILE	2.3
1	E	252	GLU	2.3
1	E	120	LYS	2.2
1	M	381	ALA	2.2
1	M	858	LEU	2.2
1	I	159	ALA	2.2
1	I	658	ALA	2.2
1	I	141	ILE	2.2
1	M	103	PHE	2.2
1	E	433	ASN	2.2
1	B	374	LEU	2.2
1	I	249	GLU	2.2
1	I	380	ALA	2.2
1	M	154	ILE	2.2
1	E	116	TYR	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	M	461	LYS	2.2
1	E	537	ASP	2.2
1	I	158	GLU	2.2
1	I	256	THR	2.2
2	J	7	DC	2.2
1	E	90	GLU	2.2
1	M	859	ASP	2.2
1	B	379	ARG	2.2
1	M	122	THR	2.2
1	B	705	LEU	2.2
1	M	52	ARG	2.2
1	E	882	PHE	2.2
3	K	8	U	2.2
1	I	654	THR	2.2
1	B	391	ARG	2.2
1	B	808	ALA	2.2
1	E	109	ILE	2.2
1	I	625	VAL	2.2
1	M	150	ARG	2.2
1	B	118	THR	2.2
1	E	250	TYR	2.2
1	M	152	GLY	2.1
1	M	73	LEU	2.1
1	I	154	ILE	2.1
1	I	676	TYR	2.1
1	E	24	LEU	2.1
1	E	196	LEU	2.1
4	P	7	DT	2.1
1	B	611	LEU	2.1
1	M	113	ALA	2.1
1	M	373	ALA	2.1
3	O	8	U	2.1
1	B	434	PRO	2.1
1	M	210	ILE	2.1
1	B	137	VAL	2.1
1	M	139	SER	2.1
1	E	217	ILE	2.1
1	M	70	ALA	2.1
1	I	670	PRO	2.1
1	E	211	HIS	2.1
1	I	128	SER	2.1
1	M	27	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	M	169	GLN	2.1
1	I	718	ILE	2.1
1	I	685	VAL	2.1
1	M	214	VAL	2.1
1	M	482	ILE	2.1
1	I	220	LEU	2.1
1	I	751	PHE	2.1
1	E	177	VAL	2.1
1	I	248	PRO	2.1
1	M	833	VAL	2.1
1	E	123	LEU	2.0
1	E	427	TYR	2.0
1	I	659	ILE	2.0
1	I	612	GLY	2.0
1	B	712	ASP	2.0
1	E	440	THR	2.0
1	M	372	GLU	2.0
1	M	125	CYS	2.0
1	M	685	VAL	2.0
4	P	3	DC	2.0
1	M	28	TYR	2.0
1	M	243	THR	2.0
1	E	20	PRO	2.0
1	M	170	LEU	2.0
1	M	705	LEU	2.0
1	E	74	ILE	2.0
1	B	633	SER	2.0
1	B	64	VAL	2.0
1	M	101	THR	2.0
1	E	55	PHE	2.0
1	I	858	LEU	2.0
1	M	680	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	S8U	N	10	18/19	0.90	0.23	133,140,152,158	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	S8U	J	10	18/19	0.94	0.22	102,109,130,139	0
2	S8U	F	10	18/19	0.95	0.20	78,87,103,108	0
2	S8U	A	10	18/19	0.97	0.21	62,75,87,89	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

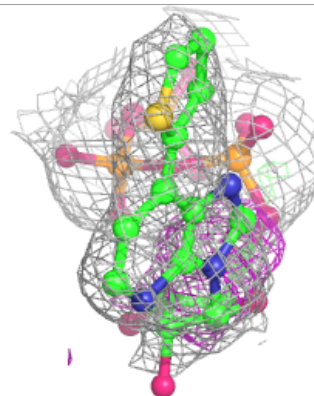
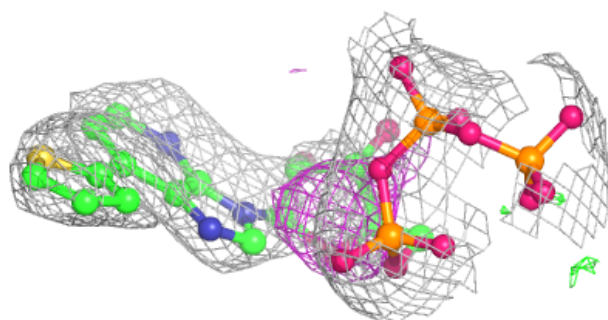
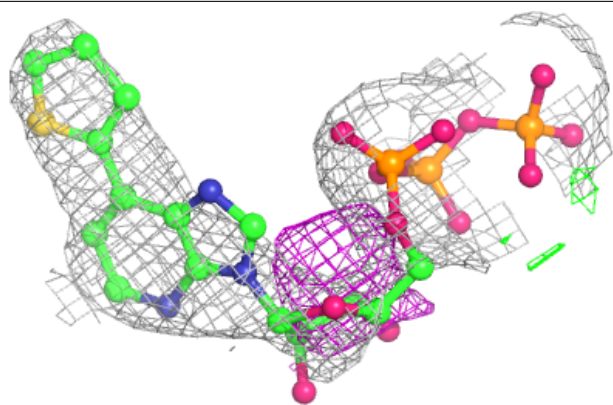
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

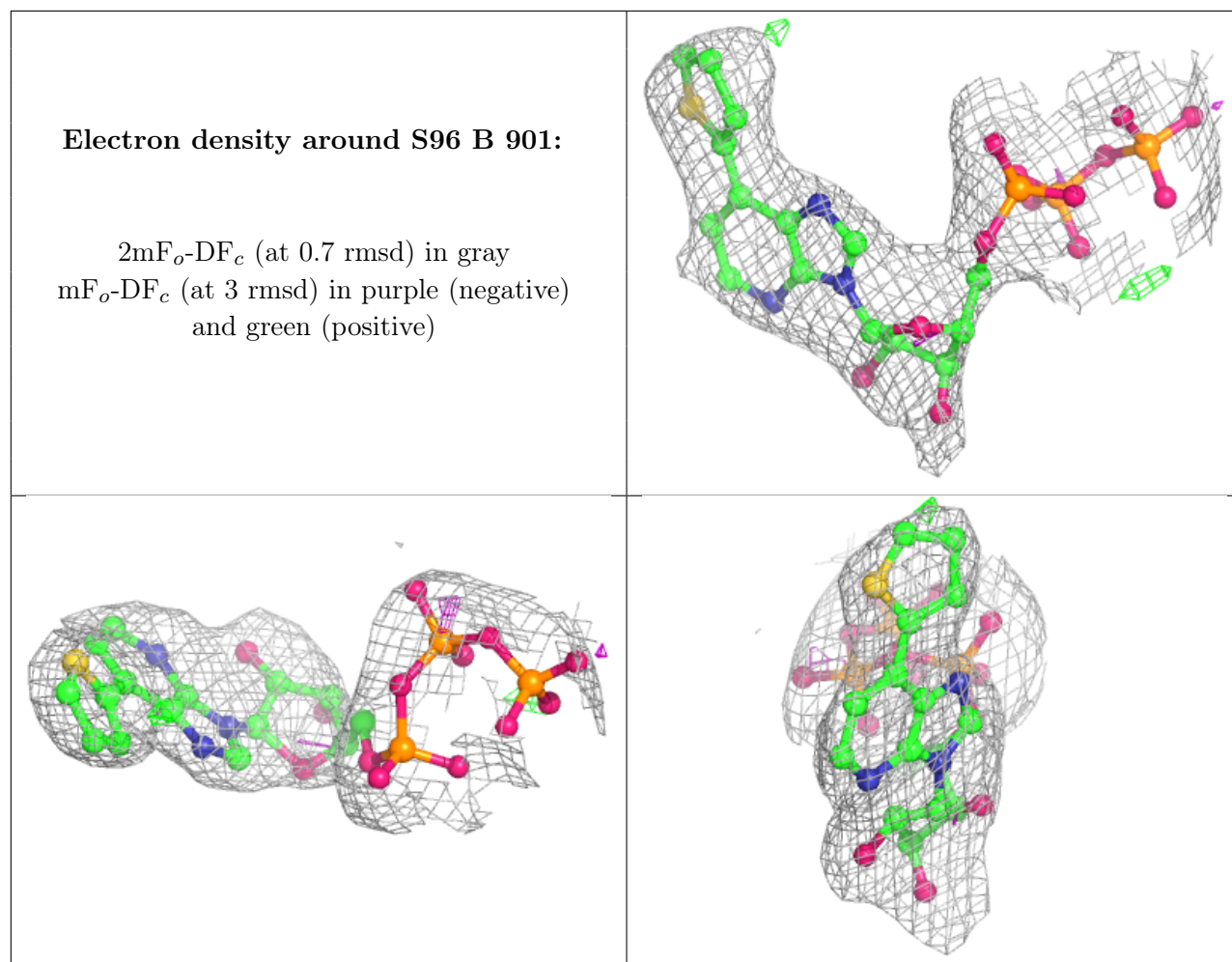
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	E	902	1/1	0.80	0.61	103,103,103,103	0
5	S96	E	901	35/35	0.90	0.22	76,122,135,140	0
5	S96	B	901	35/35	0.92	0.21	68,102,129,134	0
6	MG	B	902	1/1	0.94	0.40	79,79,79,79	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around S96 E 901:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.