



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 01:30 pm BST

PDB ID : 6JUR  
Title : MsDpo4-DNA complex 5  
Authors : Nair, D.T.; Johnson, M.K.  
Deposited on : 2019-04-15  
Resolution : 2.06 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.

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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 : 2.11  
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) : 2.11

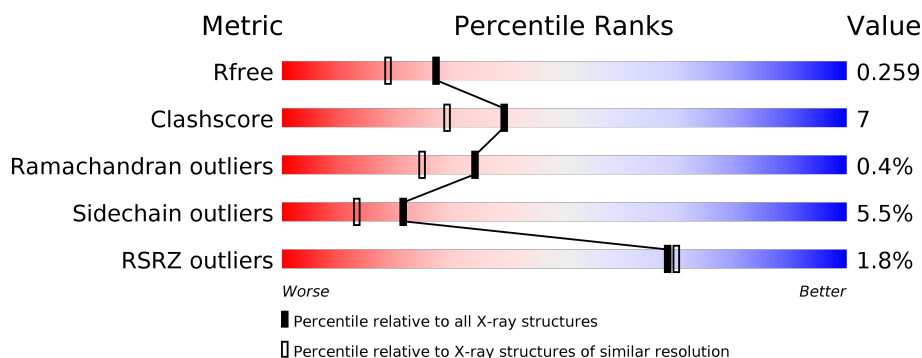
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.06 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	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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 on 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	A	356	<div> <div>72%</div> <div>22%</div> <div>• • •</div> </div>
1	F	356	<div> <div>80%</div> <div>14%</div> <div>• • •</div> </div>
2	B	18	<div> <div>11%</div> <div>33%</div> <div>22%</div> <div>11%</div> <div>33%</div> </div>
2	C	18	<div> <div>28%</div> <div>11%</div> <div>6%</div> <div>56%</div> </div>
2	G	18	<div> <div>17%</div> <div>44%</div> <div>22%</div> <div>33%</div> </div>
2	H	18	<div> <div>28%</div> <div>17%</div> <div>56%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6488 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 DNA polymerase IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	347	Total	C	N	O	S	0	0	0
			2645	1664	465	505	11			
1	F	347	Total	C	N	O	S	0	0	0
			2649	1666	465	507	11			

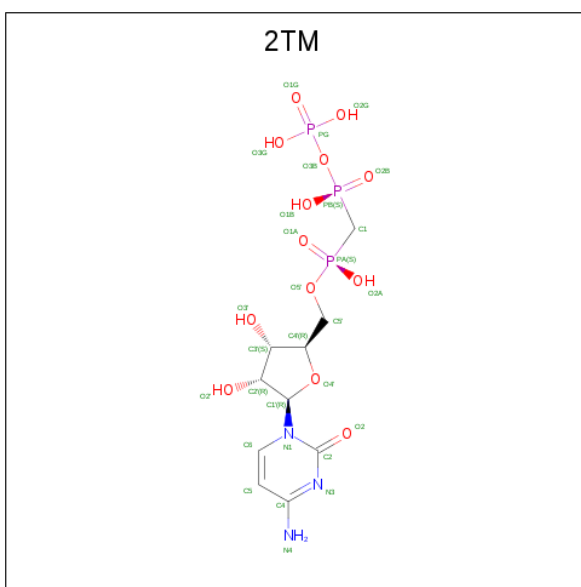
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	TYR	LEU	engineered mutation	UNP A0QR77
F	14	TYR	LEU	engineered mutation	UNP A0QR77

- Molecule 2 is a DNA chain called DNA (5'-D(\*TP\*CP\*TP\*GP\*GP\*GP\*GP\*TP\*CP\*CP\*TP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	12	Total	C	N	O	P	0	0	0
			243	117	42	73	11			
2	C	8	Total	C	N	O	P	0	0	0
			163	77	31	47	8			
2	G	12	Total	C	N	O	P	0	0	0
			243	117	42	73	11			
2	H	8	Total	C	N	O	P	0	0	0
			163	77	31	47	8			

- Molecule 3 is 5'-O-[(S)-hydroxy{[(S)-hydroxy(phosphonooxy)phosphoryl]methyl}phosphoryl]cytidine (three-letter code: 2TM) (formula: C<sub>10</sub>H<sub>18</sub>N<sub>3</sub>O<sub>13</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			29	10	3	13	3		
3	F	1	Total	C	N	O	P	0	0
			29	10	3	13	3		

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mn	0	0
			2	2		
4	F	2	Total	Mn	0	0
			2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	132	Total	O	0	0
			132	132		
5	B	23	Total	O	0	0
			23	23		
5	C	2	Total	O	0	0
			2	2		
5	F	131	Total	O	0	0
			131	131		
5	G	24	Total	O	0	0
			24	24		

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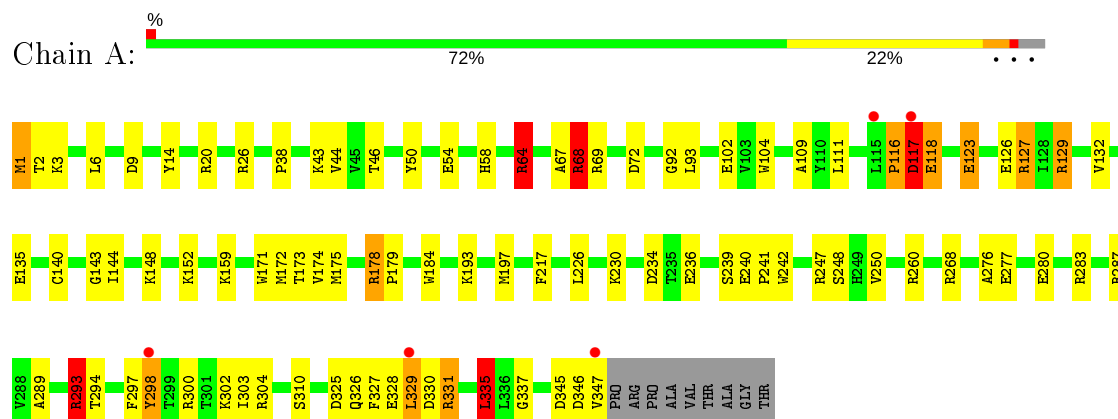
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	8	Total	O	0	0
			8	8		

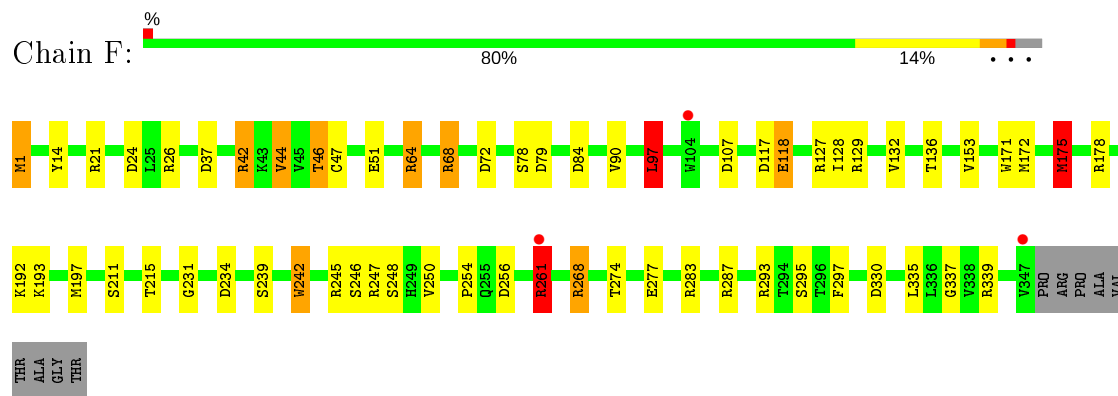
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

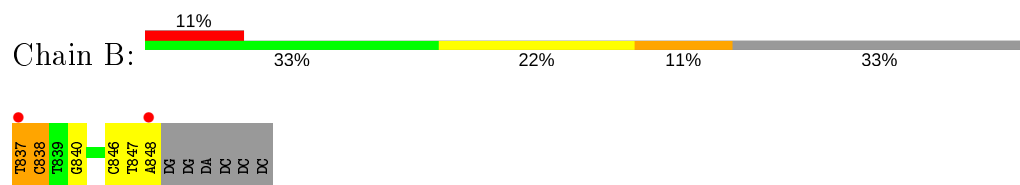
#### • Molecule 1: DNA polymerase IV



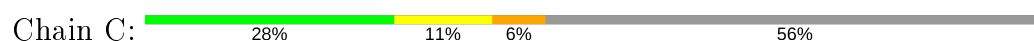
#### • Molecule 1: DNA polymerase IV

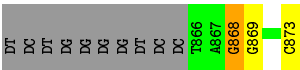


#### • Molecule 2: DNA (5'-D(\*TP\*CP\*TP\*GP\*GP\*GP\*GP\*TP\*CP\*CP\*TP\*A)-3')

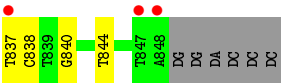


#### • Molecule 2: DNA (5'-D(\*TP\*CP\*TP\*GP\*GP\*GP\*GP\*TP\*CP\*CP\*TP\*A)-3')

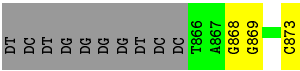
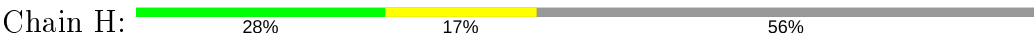




● Molecule 2: DNA (5'-D(\*TP\*CP\*TP\*GP\*GP\*GP\*GP\*TP\*CP\*CP\*TP\*A)-3')



● Molecule 2: DNA (5'-D(\*TP\*CP\*TP\*GP\*GP\*GP\*GP\*TP\*CP\*CP\*TP\*A)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.67Å 80.24Å 210.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.26 – 2.06 63.84 – 2.06	Depositor EDS
% Data completeness (in resolution range)	99.8 (70.26-2.06) 99.9 (63.84-2.06)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.59 (at 2.07Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, $R_{free}$	0.209 , 0.257 0.211 , 0.259	Depositor DCC
$R_{free}$ test set	2961 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.3	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 46.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6488	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2TM, MN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	1.48	27/2699 (1.0%)	1.34	28/3682 (0.8%)
1	F	1.37	12/2703 (0.4%)	1.27	27/3687 (0.7%)
2	B	1.81	6/271 (2.2%)	1.49	4/417 (1.0%)
2	C	1.06	0/182	1.17	1/278 (0.4%)
2	G	1.31	1/271 (0.4%)	1.10	0/417
2	H	1.08	0/182	1.15	1/278 (0.4%)
All	All	1.42	46/6308 (0.7%)	1.30	61/8759 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	172	MET	C-O	-10.21	1.03	1.23
1	A	173	THR	C-O	-9.93	1.04	1.23
1	F	118	GLU	CD-OE1	9.69	1.36	1.25
2	B	838	DC	N1-C6	9.36	1.42	1.37
1	A	174	VAL	C-O	-8.31	1.07	1.23
1	A	175	MET	C-O	-7.90	1.08	1.23
2	B	837	DT	O3'-P	7.62	1.70	1.61
1	F	84	ASP	CB-CG	7.41	1.67	1.51
1	A	126	GLU	CG-CD	7.27	1.62	1.51
1	A	173	THR	CB-CG2	-6.90	1.29	1.52
1	A	50	TYR	CZ-OH	6.83	1.49	1.37
1	F	175	MET	C-O	-6.75	1.10	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	54	GLU	CD-OE2	6.70	1.33	1.25
1	A	298	TYR	CE1-CZ	6.69	1.47	1.38
2	B	838	DC	N3-C4	6.61	1.38	1.33
1	F	46	THR	CB-CG2	-6.59	1.30	1.52
1	F	44	VAL	CB-CG2	-6.59	1.39	1.52
2	B	847	DT	C4-O4	-6.57	1.17	1.23
1	A	329	LEU	CG-CD2	6.57	1.76	1.51
1	A	104	TRP	CD2-CE2	6.46	1.49	1.41
1	A	72	ASP	CB-CG	6.38	1.65	1.51
2	B	848	DA	C6-N6	-6.35	1.28	1.33
2	B	848	DA	N7-C5	6.21	1.43	1.39
1	A	172	MET	N-CA	-6.12	1.34	1.46
1	A	123	GLU	CD-OE2	6.07	1.32	1.25
1	A	242	TRP	CB-CG	6.00	1.61	1.50
1	F	246	SER	CB-OG	5.88	1.50	1.42
1	A	92	GLY	N-CA	5.81	1.54	1.46
1	F	51	GLU	CD-OE2	5.80	1.32	1.25
1	A	123	GLU	CD-OE1	5.79	1.32	1.25
1	F	51	GLU	CD-OE1	5.75	1.31	1.25
1	F	283	ARG	CZ-NH1	5.74	1.40	1.33
1	F	242	TRP	CE3-CZ3	5.72	1.48	1.38
1	A	298	TYR	CG-CD2	5.65	1.46	1.39
1	A	143	GLY	N-CA	5.57	1.54	1.46
1	F	248	SER	CA-CB	5.53	1.61	1.52
1	F	192	LYS	CE-NZ	5.47	1.62	1.49
1	A	328	GLU	CD-OE2	5.39	1.31	1.25
1	A	283	ARG	CZ-NH1	5.38	1.40	1.33
1	A	109	ALA	CA-CB	5.30	1.63	1.52
1	A	242	TRP	CE3-CZ3	5.29	1.47	1.38
2	G	837	DT	N1-C6	5.29	1.42	1.38
1	A	248	SER	CA-CB	5.25	1.60	1.52
1	A	104	TRP	CZ3-CH2	5.24	1.48	1.40
1	A	173	THR	CB-OG1	-5.19	1.32	1.43
1	A	174	VAL	CB-CG1	-5.12	1.42	1.52

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	ARG	NE-CZ-NH1	11.54	126.07	120.30
1	A	335	LEU	CA-CB-CG	10.36	139.12	115.30
1	A	9	ASP	CB-CG-OD2	10.31	127.58	118.30
1	A	69	ARG	NE-CZ-NH1	9.54	125.07	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	287	ARG	NE-CZ-NH1	9.48	125.04	120.30
1	F	129	ARG	NE-CZ-NH2	-9.22	115.69	120.30
1	A	118	GLU	N-CA-C	-8.84	87.12	111.00
1	A	68	ARG	NE-CZ-NH2	-8.73	115.93	120.30
1	F	64	ARG	NE-CZ-NH1	8.52	124.56	120.30
2	B	848	DA	C8-N9-C4	8.47	109.19	105.80
1	A	287	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	F	245	ARG	NE-CZ-NH1	8.24	124.42	120.30
1	A	64	ARG	NE-CZ-NH2	-8.18	116.21	120.30
1	F	256	ASP	CB-CG-OD1	8.14	125.62	118.30
1	F	287	ARG	NE-CZ-NH2	-8.06	116.27	120.30
1	A	129	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	F	245	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	A	293	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	A	268	ARG	NE-CZ-NH1	7.51	124.05	120.30
1	F	129	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	F	256	ASP	CB-CG-OD2	-7.04	111.97	118.30
1	F	46	THR	N-CA-CB	-7.02	96.96	110.30
1	A	129	ARG	NE-CZ-NH1	6.97	123.79	120.30
1	F	64	ARG	NE-CZ-NH2	-6.89	116.85	120.30
2	B	848	DA	N7-C8-N9	-6.86	110.37	113.80
1	A	26	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	A	69	ARG	NE-CZ-NH2	-6.83	116.89	120.30
2	B	848	DA	C5-N7-C8	6.60	107.20	103.90
1	F	26	ARG	NE-CZ-NH1	-6.54	117.03	120.30
1	A	293	ARG	NE-CZ-NH2	-6.26	117.17	120.30
2	H	868	DG	C1'-O4'-C4'	-6.25	103.84	110.10
1	A	26	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	F	24	ASP	CB-CG-OD1	6.12	123.81	118.30
1	A	331	ARG	NE-CZ-NH1	6.11	123.36	120.30
2	B	838	DC	O5'-P-OP2	-6.06	100.25	105.70
1	A	159	LYS	CD-CE-NZ	-6.03	97.83	111.70
1	A	127	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	F	293	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	F	261	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	F	339	ARG	CG-CD-NE	-5.94	99.32	111.80
1	A	234	ASP	CB-CG-OD2	5.89	123.60	118.30
1	A	283	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	A	335	LEU	CB-CG-CD1	5.82	120.89	111.00
1	A	178	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	A	43	LYS	CD-CE-NZ	-5.78	98.40	111.70
1	F	97	LEU	CB-CG-CD2	-5.76	101.20	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	79	ASP	CB-CG-OD1	5.71	123.44	118.30
1	F	178	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	A	346	ASP	N-CA-C	5.47	125.78	111.00
1	A	111	LEU	CA-CB-CG	5.46	127.86	115.30
1	A	287	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	F	268	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	A	247	ARG	NE-CZ-NH1	-5.40	117.60	120.30
1	F	84	ASP	CB-CG-OD1	5.30	123.07	118.30
1	F	42	ARG	NE-CZ-NH1	5.28	122.94	120.30
2	C	868	DG	C1'-O4'-C4'	-5.17	104.93	110.10
1	F	234	ASP	CB-CG-OD2	5.14	122.92	118.30
1	F	330	ASP	CB-CA-C	-5.13	100.13	110.40
1	F	21	ARG	NE-CZ-NH2	5.07	122.83	120.30
1	F	68	ARG	NE-CZ-NH2	5.04	122.82	120.30
1	F	283	ARG	NE-CZ-NH2	-5.04	117.78	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117	ASP	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2645	0	2653	50	0
1	F	2649	0	2657	23	0
2	B	243	0	136	9	0
2	C	163	0	90	4	0
2	G	243	0	138	5	0
2	H	163	0	90	3	0
3	A	29	0	14	6	0
3	F	29	0	14	8	0
4	A	2	0	0	0	0
4	F	2	0	0	0	0
5	A	132	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	23	0	0	0	0
5	C	2	0	0	0	0
5	F	131	0	0	6	0
5	G	24	0	0	0	0
5	H	8	0	0	1	0
All	All	6488	0	5792	88	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 7.

All (88) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:LEU:CG	1:A:329:LEU:CD2	1.76	1.56
3:F:401:2TM:C1	5:F:512:HOH:O	2.12	0.96
3:A:401:2TM:H2	2:C:873:DC:H2"	1.61	0.82
1:F:261:ARG:HH11	1:F:261:ARG:HG3	1.43	0.81
3:A:401:2TM:C1	3:A:401:2TM:O3G	2.30	0.79
3:A:401:2TM:H1	3:A:401:2TM:H10	1.64	0.78
3:F:401:2TM:H1	2:H:873:DC:H2"	1.65	0.78
3:F:401:2TM:H17	5:F:512:HOH:O	1.79	0.77
1:A:277:GLU:OE2	5:A:501:HOH:O	2.03	0.77
1:A:329:LEU:HG	1:A:329:LEU:O	1.88	0.74
1:A:117:ASP:N	1:A:118:GLU:O	2.21	0.72
3:A:401:2TM:H18	3:A:401:2TM:O3G	1.90	0.72
1:A:2:THR:HG22	1:A:116:PRO:O	1.90	0.72
3:F:401:2TM:H18	5:F:512:HOH:O	1.81	0.71
3:F:401:2TM:H1	3:F:401:2TM:H10	1.72	0.71
1:A:68:ARG:HD3	2:B:837:DT:H3	1.59	0.67
1:A:276:ALA:O	1:A:280:GLU:HG3	1.96	0.65
1:A:329:LEU:HG	1:A:329:LEU:CD2	2.14	0.64
3:F:401:2TM:C5'	2:H:873:DC:H2"	2.26	0.64
1:F:1:MET:HG2	1:F:117:ASP:OD1	1.98	0.63
1:F:153:VAL:HG11	1:F:175:MET:SD	2.39	0.63
1:F:261:ARG:NH1	1:F:261:ARG:HG3	2.13	0.61
1:F:268:ARG:NH2	5:F:502:HOH:O	2.22	0.61
2:H:869:DG:H2'	5:H:907:HOH:O	2.02	0.60
1:A:123:GLU:O	1:A:127:ARG:HG3	2.03	0.59
3:A:401:2TM:H17	3:A:401:2TM:O3G	2.02	0.59
1:F:193:LYS:O	1:F:197:MET:HE3	2.05	0.57
1:A:58:HIS:NE2	5:A:505:HOH:O	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:64:ARG:NH2	5:F:506:HOH:O	2.40	0.55
1:F:44:VAL:HG11	2:G:840:DG:C4	2.41	0.55
1:A:129:ARG:HD2	1:A:140:CYS:O	2.07	0.54
1:A:240:GLU:OE1	1:A:241:PRO:HD2	2.08	0.54
1:A:289:ALA:HB2	1:A:303:ILE:HD12	1.89	0.54
1:A:64:ARG:CB	2:B:837:DT:H5''	2.38	0.53
1:A:302:LYS:HD2	1:A:327:PHE:CE1	2.44	0.52
1:F:37:ASP:OD2	5:F:501:HOH:O	2.18	0.52
1:F:247:ARG:HG2	1:F:274:THR:HG23	1.93	0.51
1:A:44:VAL:HG21	2:B:840:DG:C4	2.45	0.51
2:B:838:DC:C4	1:F:193:LYS:HD3	2.45	0.51
1:A:193:LYS:HD2	1:A:217:PHE:CE1	2.46	0.50
1:A:293:ARG:HA	1:A:298:TYR:O	2.12	0.49
1:A:68:ARG:CD	2:B:837:DT:H3	2.23	0.49
1:F:242:TRP:HZ2	2:G:844:DT:H5''	1.76	0.49
1:A:102:GLU:OE2	1:A:148:LYS:NZ	2.45	0.49
1:F:242:TRP:CZ2	2:G:844:DT:H5''	2.47	0.49
1:F:250:VAL:HG12	1:F:337:GLY:HA3	1.94	0.48
1:A:1:MET:HB2	1:A:116:PRO:HA	1.96	0.48
1:A:329:LEU:CG	1:A:329:LEU:O	2.57	0.48
1:A:93:LEU:HD21	1:A:135:GLU:HB2	1.94	0.48
1:F:261:ARG:NH2	1:F:268:ARG:HH12	2.13	0.47
1:A:250:VAL:HG12	1:A:337:GLY:HA3	1.97	0.47
3:A:401:2TM:C5'	2:C:873:DC:H2''	2.39	0.46
1:A:293:ARG:HG2	1:A:335:LEU:HB3	1.97	0.46
1:A:64:ARG:HB2	2:B:837:DT:C5'	2.45	0.46
1:F:247:ARG:NE	1:F:277:GLU:OE1	2.42	0.46
1:A:304:ARG:NH2	1:A:326:GLN:OE1	2.49	0.46
1:A:14:TYR:HD2	1:A:46:THR:HG23	1.81	0.46
1:A:64:ARG:HB3	2:B:837:DT:H5''	1.97	0.46
1:A:260:ARG:HH22	1:A:325:ASP:HA	1.82	0.45
1:A:329:LEU:CD1	1:A:329:LEU:CD2	2.85	0.45
1:A:193:LYS:HG3	2:G:838:DC:C2	2.53	0.44
1:A:178:ARG:NH2	5:A:513:HOH:O	2.48	0.44
1:F:90:VAL:HG22	1:F:136:THR:HG21	2.00	0.44
1:F:14:TYR:HB2	1:F:47:CYS:HB3	2.00	0.44
1:A:38:PRO:HB2	1:A:67:ALA:HB2	2.00	0.44
3:F:401:2TM:O3G	3:F:401:2TM:H17	2.17	0.44
3:F:401:2TM:O3'	3:F:401:2TM:O1B	2.31	0.44
1:F:211:SER:O	1:F:215:THR:HG23	2.18	0.43
1:A:127:ARG:HB3	1:A:127:ARG:CZ	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:ASP:OD2	1:A:331:ARG:NH2	2.51	0.43
1:A:193:LYS:HE2	2:G:838:DC:C4	2.53	0.43
1:A:193:LYS:HB2	1:A:193:LYS:HE3	1.59	0.43
1:A:197:MET:O	1:F:68:ARG:HD2	2.18	0.43
1:A:294:THR:OG1	1:A:298:TYR:HB3	2.19	0.43
1:A:226:LEU:HA	1:A:226:LEU:HD23	1.85	0.43
1:F:128:ILE:O	1:F:132:VAL:HG23	2.19	0.42
1:A:2:THR:CG2	1:A:116:PRO:O	2.64	0.42
1:A:6:LEU:HG	1:A:144:ILE:HG12	2.00	0.42
1:F:97:LEU:HA	1:F:97:LEU:HD12	1.86	0.42
1:A:64:ARG:HB2	2:B:837:DT:H5"	2.00	0.42
1:A:329:LEU:CB	1:A:329:LEU:CD2	2.85	0.41
2:B:846:DC:O2	2:C:869:DG:N2	2.54	0.41
1:A:132:VAL:HG21	1:A:140:CYS:SG	2.61	0.41
1:F:171:TRP:CE2	1:F:231:GLY:HA2	2.56	0.41
1:A:178:ARG:HB3	1:A:179:PRO:HD2	2.04	0.40
1:A:300:ARG:HD2	2:C:868:DG:OP2	2.21	0.40
1:A:152:LYS:HG2	1:A:184:TRP:CD1	2.56	0.40
1:A:226:LEU:HD22	1:A:230:LYS:HE2	2.03	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	A	345/356 (97%)	335 (97%)	7 (2%)	3 (1%)	17	8
1	F	345/356 (97%)	337 (98%)	8 (2%)	0	100	100
All	All	690/712 (97%)	672 (97%)	15 (2%)	3 (0%)	34	25

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	116	PRO
1	A	117	ASP
1	A	171	TRP

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	283/290 (98%)	269 (95%)	14 (5%)	25	17
1	F	284/290 (98%)	267 (94%)	17 (6%)	19	11
All	All	567/580 (98%)	536 (94%)	31 (6%)	21	13

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	3	LYS
1	A	20	ARG
1	A	64	ARG
1	A	68	ARG
1	A	117	ASP
1	A	236	GLU
1	A	239	SER
1	A	293	ARG
1	A	297	PHE
1	A	310	SER
1	A	335	LEU
1	A	345	ASP
1	A	347	VAL
1	F	1	MET
1	F	42	ARG
1	F	46	THR
1	F	72	ASP
1	F	78	SER
1	F	97	LEU
1	F	107	ASP

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Mol	Chain	Res	Type
1	F	118	GLU
1	F	127	ARG
1	F	172	MET
1	F	175	MET
1	F	239	SER
1	F	254	PRO
1	F	261	ARG
1	F	295	SER
1	F	297	PHE
1	F	335	LEU

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 4 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	$\# Z  > 2$
3	2TM	A	401	4	24,30,30	3.92	8 (33%)	30,47,47	3.15	13 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	2TM	F	401	4	24,30,30	3.85	10 (41%)	30,47,47	2.51	13 (43%)

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
3	2TM	A	401	4	-	4/17/38/38	0/2/2/2
3	2TM	F	401	4	-	3/17/38/38	0/2/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	401	2TM	PA-O2A	14.81	1.91	1.56
3	A	401	2TM	PA-O2A	13.29	1.87	1.56
3	A	401	2TM	PB-O3B	8.75	1.68	1.58
3	F	401	2TM	PA-O1A	-7.52	1.33	1.51
3	A	401	2TM	PB-O2B	7.12	1.68	1.51
3	A	401	2TM	C2-N3	-4.23	1.29	1.38
3	F	401	2TM	C2-N3	-3.43	1.31	1.38
3	F	401	2TM	PG-O2G	-3.41	1.41	1.54
3	F	401	2TM	PA-O5'	3.35	1.62	1.57
3	A	401	2TM	PA-O5'	-3.08	1.52	1.57
3	F	401	2TM	O4'-C1'	-2.92	1.37	1.41
3	F	401	2TM	PB-O3B	2.65	1.61	1.58
3	A	401	2TM	C5-C4	-2.60	1.35	1.41
3	A	401	2TM	O5'-C5'	-2.51	1.35	1.44
3	F	401	2TM	C6-C5	-2.28	1.33	1.38
3	F	401	2TM	PG-O3G	-2.14	1.46	1.54
3	A	401	2TM	PA-O1A	2.10	1.56	1.51
3	F	401	2TM	C5-C4	-2.03	1.36	1.41

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	2TM	O1A-PA-C1	12.59	142.34	109.07
3	F	401	2TM	O2A-PA-C1	6.97	135.11	106.58
3	F	401	2TM	O2G-PG-O3G	5.00	126.74	107.64
3	A	401	2TM	PG-O3B-PB	-4.66	116.21	132.62
3	F	401	2TM	C2-N3-C4	4.21	120.61	116.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	2TM	O2A-PA-C1	-3.96	90.37	106.58
3	F	401	2TM	O1B-PB-C1	3.81	122.15	106.58
3	A	401	2TM	O1B-PB-O2B	3.42	121.49	110.07
3	F	401	2TM	C5'-C4'-C3'	-3.40	102.43	115.18
3	A	401	2TM	C5-C4-N4	-3.36	115.31	121.14
3	A	401	2TM	C5'-C4'-C3'	-3.34	102.67	115.18
3	F	401	2TM	O1B-PB-O2B	-3.28	99.13	110.07
3	F	401	2TM	N4-C4-N3	3.07	121.34	116.49
3	A	401	2TM	O4'-C4'-C5'	-3.02	99.45	109.37
3	A	401	2TM	O2G-PG-O3G	3.00	119.10	107.64
3	A	401	2TM	C2-N3-C4	2.79	119.17	116.34
3	A	401	2TM	O3'-C3'-C4'	2.74	118.98	111.05
3	A	401	2TM	N4-C4-N3	2.74	120.82	116.49
3	F	401	2TM	O4'-C4'-C5'	-2.56	100.94	109.37
3	F	401	2TM	O2B-PB-C1	2.49	115.65	109.07
3	F	401	2TM	O3G-PG-O1G	-2.42	101.19	110.68
3	A	401	2TM	O2A-PA-O1A	-2.41	102.03	110.07
3	F	401	2TM	O1A-PA-C1	-2.40	102.74	109.07
3	A	401	2TM	O2B-PB-C1	2.30	115.16	109.07
3	F	401	2TM	PG-O3B-PB	-2.23	124.75	132.62
3	F	401	2TM	O2G-PG-O3B	-2.20	97.25	104.64

There are no chirality outliers.

All (7) torsion outliers are listed below:

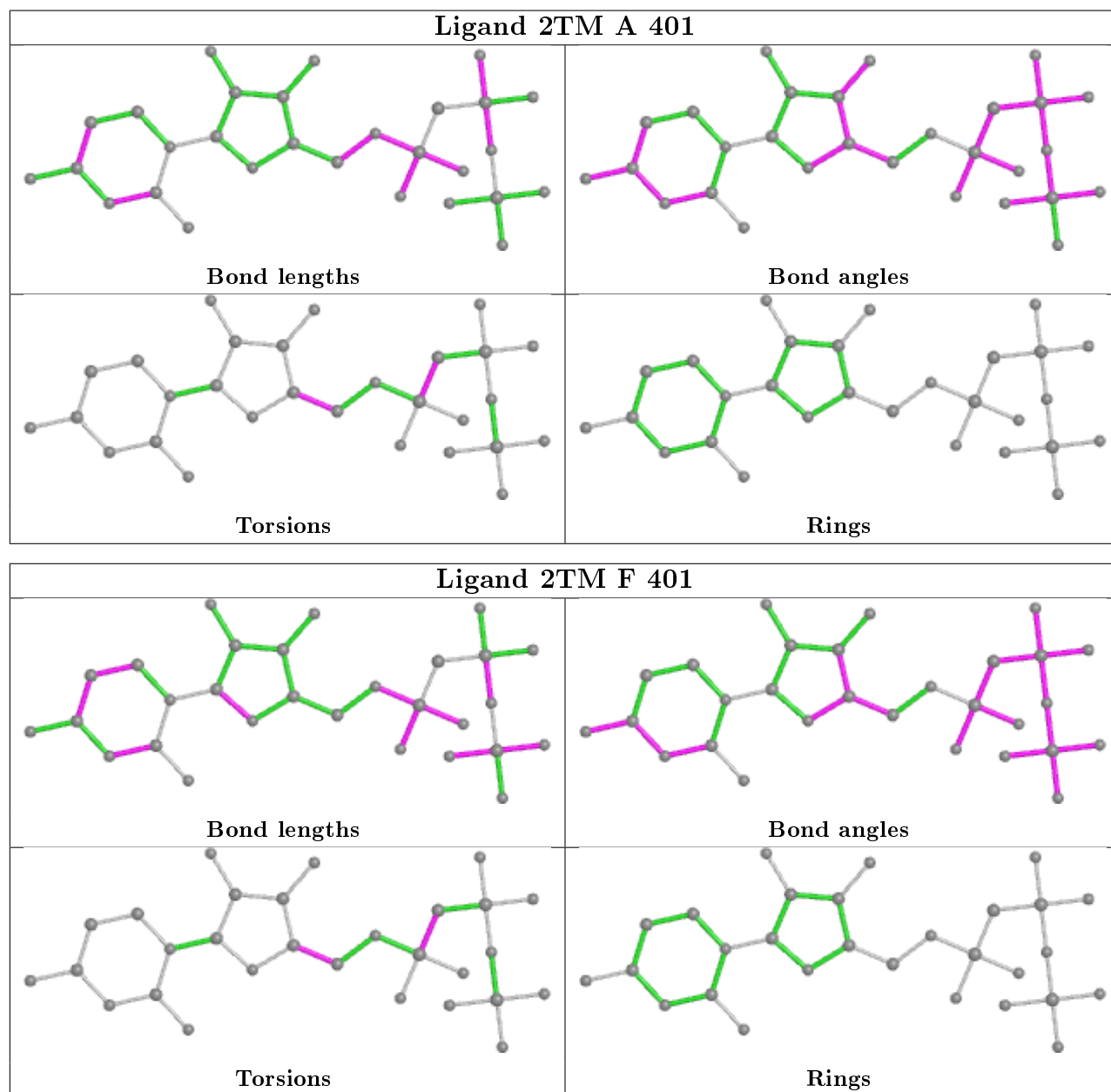
Mol	Chain	Res	Type	Atoms
3	A	401	2TM	PB-C1-PA-O1A
3	A	401	2TM	PB-C1-PA-O2A
3	F	401	2TM	PB-C1-PA-O5'
3	F	401	2TM	PB-C1-PA-O1A
3	F	401	2TM	O4'-C4'-C5'-O5'
3	A	401	2TM	PB-C1-PA-O5'
3	A	401	2TM	O4'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	2TM	6	0
3	F	401	2TM	8	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

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	A	347/356 (97%)	0.12	5 (1%) 75 76	21, 38, 68, 102	0
1	F	347/356 (97%)	0.08	3 (0%) 84 85	23, 37, 61, 90	0
2	B	12/18 (66%)	0.73	2 (16%) 1 1	35, 45, 106, 115	0
2	C	8/18 (44%)	0.28	0 100 100	45, 60, 78, 85	0
2	G	12/18 (66%)	0.91	3 (25%) 0 0	29, 42, 110, 124	0
2	H	8/18 (44%)	0.43	0 100 100	42, 54, 71, 75	0
All	All	734/784 (93%)	0.13	13 (1%) 68 70	21, 38, 71, 124	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	837	DT	7.2
2	B	837	DT	3.7
1	A	347	VAL	3.7
1	F	104	TRP	3.6
2	G	848	DA	3.3
1	F	347	VAL	3.3
1	A	117	ASP	2.8
1	A	298	TYR	2.8
1	A	115	LEU	2.7
1	F	261	ARG	2.4
2	B	848	DA	2.4
1	A	329	LEU	2.2
2	G	847	DT	2.1

### 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 ⓘ

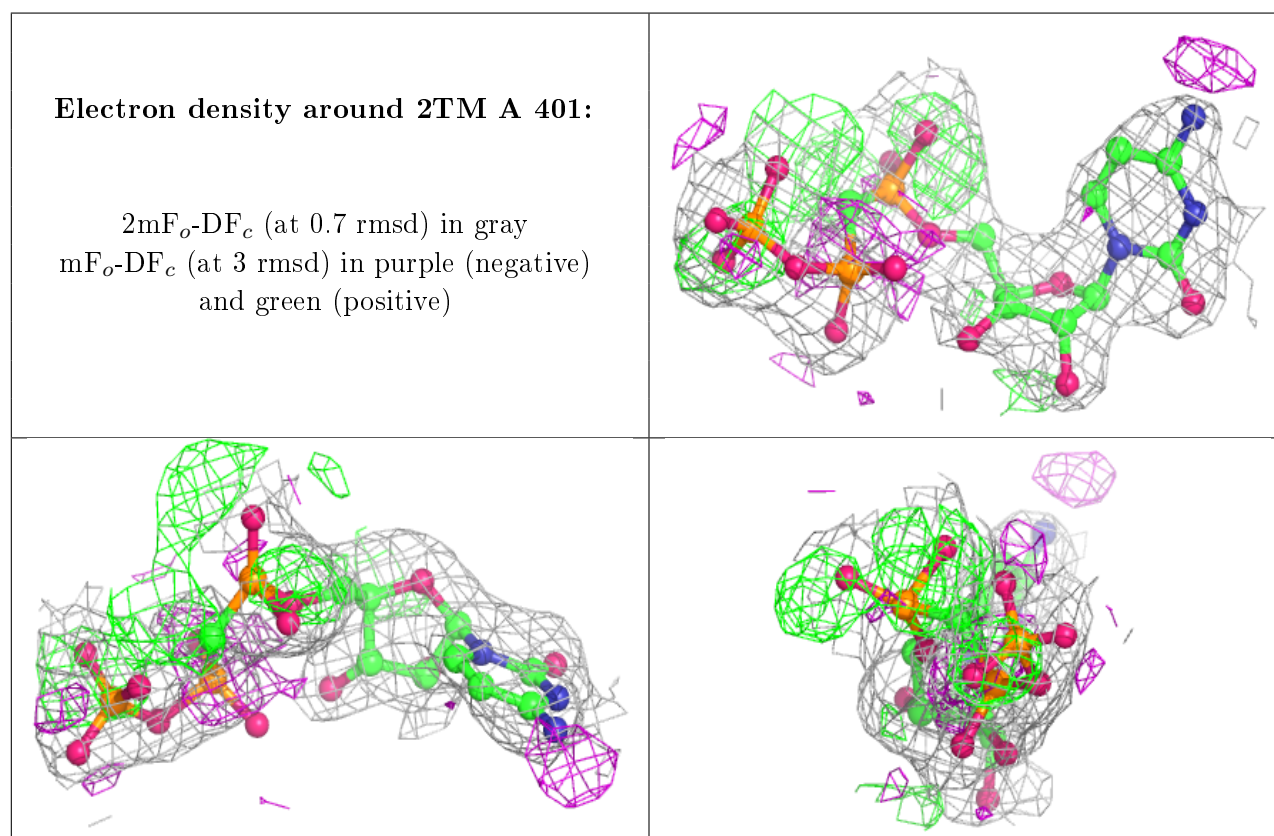
There are no carbohydrates in this entry.

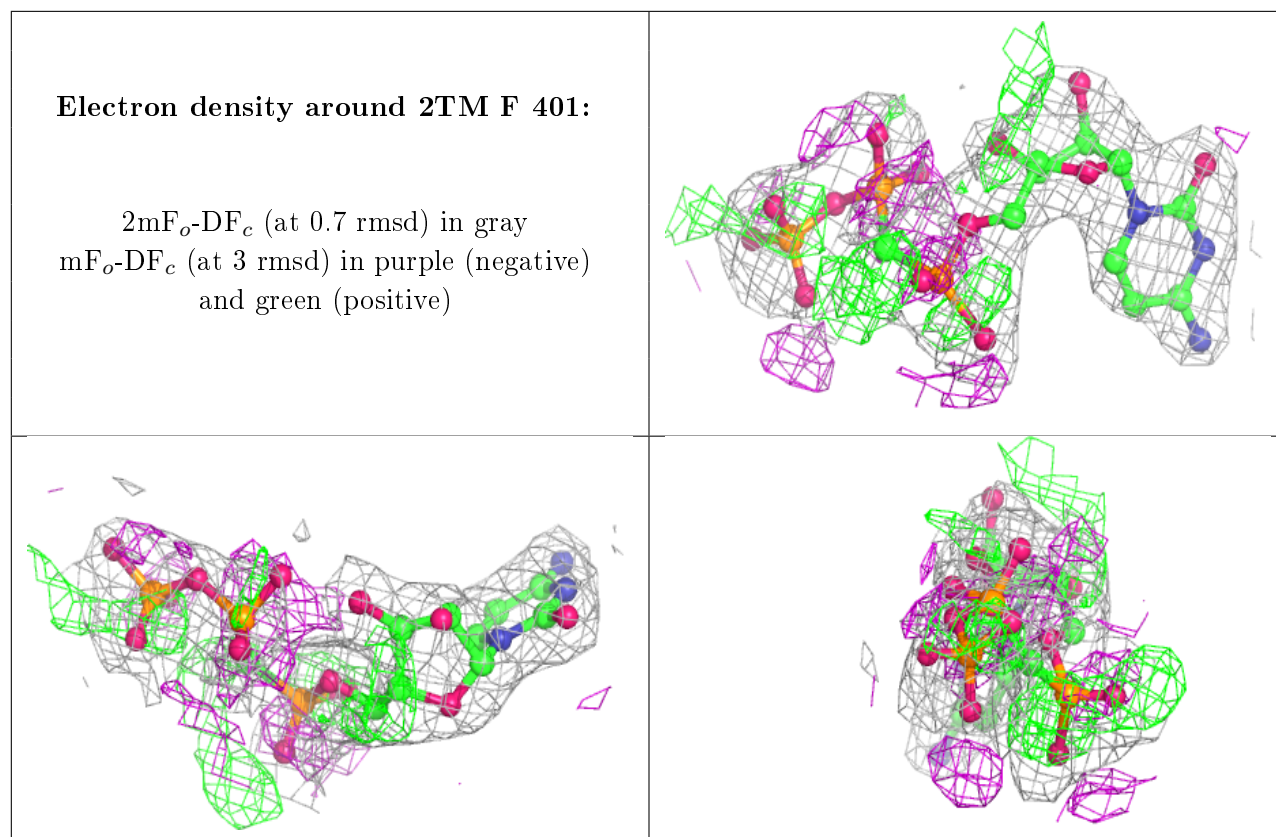
## 6.4 Ligands ⓘ

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
3	2TM	A	401	29/29	0.86	0.21	44,52,79,87	0
3	2TM	F	401	29/29	0.88	0.20	41,48,68,85	0
4	MN	F	402	1/1	0.89	0.16	63,63,63,63	0
4	MN	A	402	1/1	0.90	0.23	73,73,73,73	0
4	MN	A	403	1/1	0.97	0.07	52,52,52,52	0
4	MN	F	403	1/1	0.99	0.08	44,44,44,44	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.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.