



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 01:58 am BST

PDB ID : 6JUS  
Title : MsDpo4-DNA complex 6  
Authors : Nair, D.T.; Johnson, M.K.  
Deposited on : 2019-04-15  
Resolution : 2.50 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 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

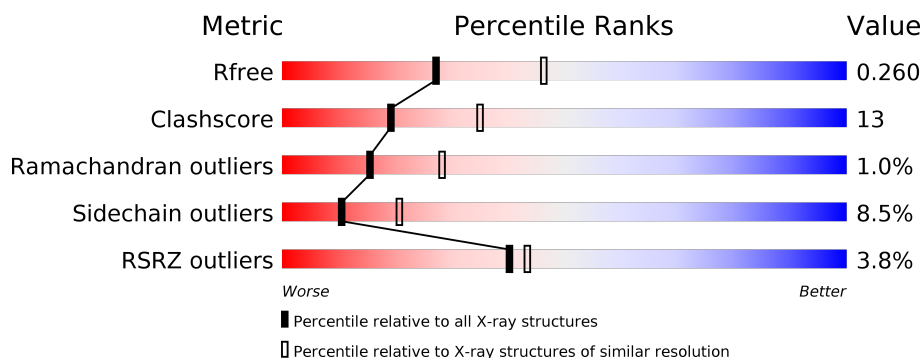
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 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>2%</div> <div> <div></div> <div>71%</div> <div>21%</div> <div>5%</div> <div>• •</div> </div> </div>
1	F	356	<div> <div>3%</div> <div> <div></div> <div>69%</div> <div>24%</div> <div>• • •</div> </div> </div>
2	B	18	<div> <div>22%</div> <div> <div>11%</div> <div>56%</div> <div>6%</div> <div>28%</div> </div> </div>
2	C	18	<div> <div>6%</div> <div> <div>28%</div> <div>22%</div> <div>50%</div> </div> </div>
2	G	18	<div> <div>11%</div> <div> <div>33%</div> <div>33%</div> <div>33%</div> </div> </div>
2	H	18	<div> <div>11%</div> <div> <div>11%</div> <div>33%</div> <div>6%</div> <div>50%</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6318 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.

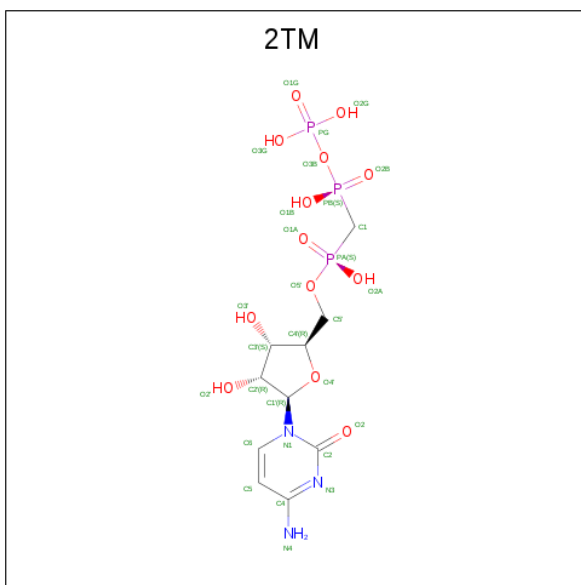
- Molecule 1 is a protein called DNA polymerase IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	347	Total	C	N	O	S	0	0	0
			2645	1663	465	506	11			
1	F	347	Total	C	N	O	S	0	0	0
			2645	1663	465	506	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	13	Total	C	N	O	P	0	0	0
			265	127	47	79	12			
2	C	9	Total	C	N	O	P	0	0	0
			182	86	34	53	9			
2	G	12	Total	C	N	O	P	0	0	0
			248	117	45	74	12			
2	H	9	Total	C	N	O	P	0	0	0
			182	86	34	53	9			

- 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	
			29	10	3	13	3	0
3	F	1	Total	C	N	O	P	
			29	10	3	13	3	0

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

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	26	Total	O		
			26	26	0	0
5	B	4	Total	O		
			4	4	0	0
5	C	4	Total	O		
			4	4	0	0
5	F	47	Total	O		
			47	47	0	0
5	G	5	Total	O		
			5	5	0	0

*Continued on next page...*

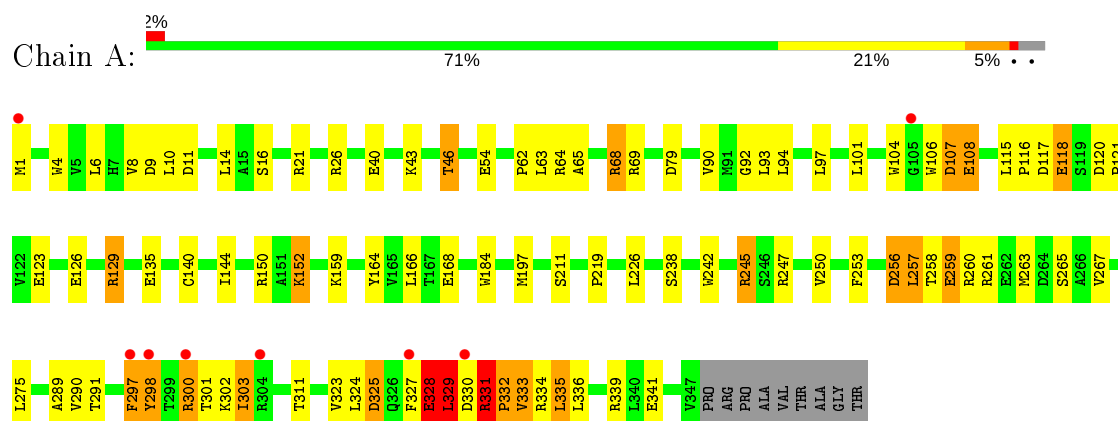
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	3	Total	O	0	0
			3	3		

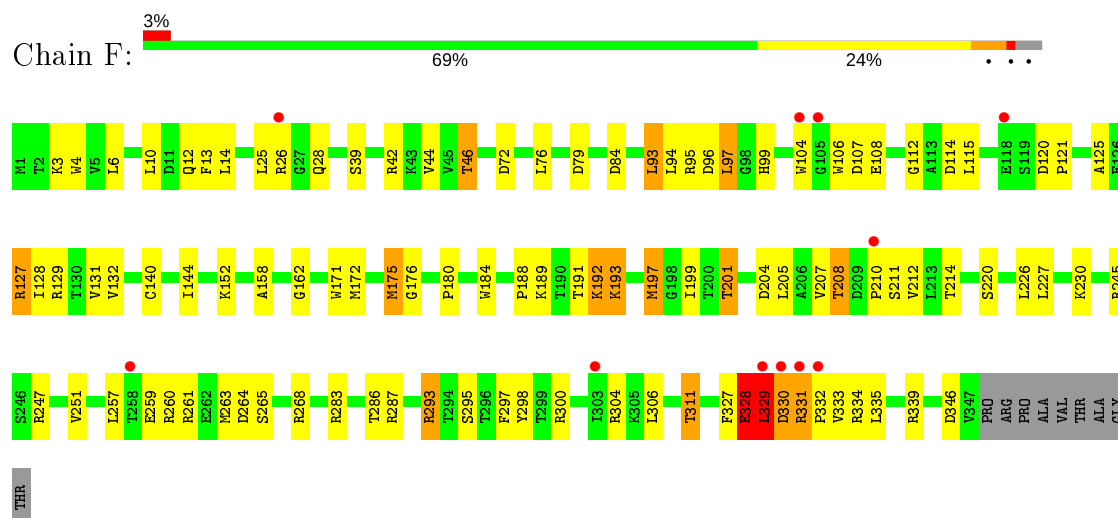
### 3 Residue-property plots [i](#)

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.

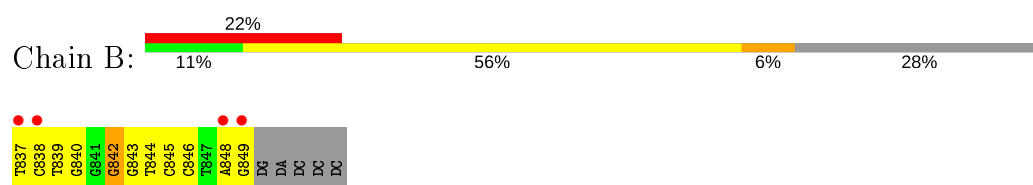
#### • Molecule 1: DNA polymerase IV



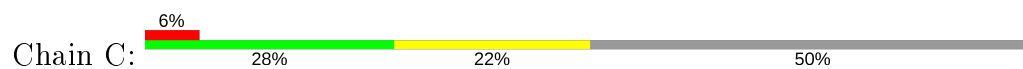
#### • Molecule 1: DNA polymerase IV



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



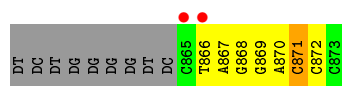
- Molecule 2: DNA (5'-D(\*TP\*CP\*TP\*GP\*GP\*GP\*GP\*TP\*CP\*CP\*TP\*AP\*G)-3')



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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.73 Å 80.34 Å 208.72 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.60 – 2.50 44.66 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.8 (44.60-2.50) 98.9 (44.66-2.50)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.33 (at 2.51 Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, $R_{free}$	0.206 , 0.254 0.209 , 0.260	Depositor DCC
$R_{free}$ test set	1618 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.2	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 40.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6318	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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: 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	1.14	8/2698 (0.3%)	1.18	21/3680 (0.6%)
1	F	1.15	10/2698 (0.4%)	1.25	30/3680 (0.8%)
2	B	0.84	1/296 (0.3%)	1.06	1/456 (0.2%)
2	C	0.70	0/203	0.94	0/310
2	G	0.79	0/277	0.92	0/426
2	H	0.74	1/203 (0.5%)	1.03	1/310 (0.3%)
All	All	1.10	20/6375 (0.3%)	1.18	53/8862 (0.6%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	328	GLU	CG-CD	-10.67	1.35	1.51
1	F	328	GLU	CD-OE1	-9.32	1.15	1.25
1	F	328	GLU	CD-OE2	-8.91	1.15	1.25
1	F	328	GLU	CA-CB	-7.87	1.36	1.53
1	A	331	ARG	C-N	-6.94	1.21	1.34
1	A	328	GLU	C-O	-6.87	1.10	1.23
1	F	333	VAL	C-O	-6.69	1.10	1.23
1	A	332	PRO	N-CA	-6.68	1.35	1.47
1	A	328	GLU	N-CA	-6.60	1.33	1.46
1	A	328	GLU	CA-C	-6.24	1.36	1.52
2	B	842	DG	O3'-P	-6.15	1.53	1.61
1	F	327	PHE	N-CA	-5.96	1.34	1.46
1	A	333	VAL	CA-CB	-5.88	1.42	1.54
1	F	333	VAL	CB-CG2	-5.28	1.41	1.52
1	F	108	GLU	CD-OE2	-5.14	1.20	1.25
1	F	327	PHE	C-O	-5.10	1.13	1.23
1	A	259	GLU	CD-OE1	-5.08	1.20	1.25
1	A	329	LEU	C-O	-5.07	1.13	1.23
2	H	872	DC	O3'-P	5.01	1.67	1.61
1	F	329	LEU	C-O	-5.01	1.13	1.23

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	328	GLU	N-CA-C	14.46	150.03	111.00
1	F	197	MET	CG-SD-CE	-10.57	83.29	100.20
1	F	328	GLU	CB-CA-C	-10.49	89.42	110.40
1	F	293	ARG	NE-CZ-NH2	-9.30	115.65	120.30
1	F	108	GLU	OE1-CD-OE2	-8.86	112.67	123.30
1	F	247	ARG	NE-CZ-NH1	-8.76	115.92	120.30
1	F	328	GLU	N-CA-CB	-8.70	94.94	110.60
1	A	247	ARG	NE-CZ-NH1	-8.54	116.03	120.30
1	F	264	ASP	CB-CG-OD1	8.21	125.69	118.30
1	A	108	GLU	N-CA-CB	-7.89	96.39	110.60
1	A	245	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	F	26	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	A	332	PRO	N-CA-C	-6.96	94.01	112.10
1	A	108	GLU	N-CA-C	6.76	129.25	111.00
1	A	129	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	A	79	ASP	CB-CG-OD2	-6.66	112.31	118.30
1	F	306	LEU	CB-CG-CD1	-6.65	99.69	111.00
1	F	329	LEU	N-CA-C	6.58	128.76	111.00
1	A	26	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	A	64	ARG	NE-CZ-NH2	-6.45	117.07	120.30
1	F	76	LEU	CB-CG-CD1	-6.37	100.17	111.00
1	F	95	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	A	329	LEU	CB-CG-CD1	-6.35	100.20	111.00
1	F	329	LEU	CB-CG-CD1	6.26	121.64	111.00
1	F	304	ARG	NE-CZ-NH2	-6.23	117.19	120.30
1	F	327	PHE	N-CA-C	6.04	127.31	111.00
1	F	328	GLU	CA-C-O	5.88	132.44	120.10
1	F	339	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	F	334	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	F	95	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	A	64	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	F	328	GLU	O-C-N	-5.68	113.61	122.70
1	F	175	MET	CG-SD-CE	-5.67	91.13	100.20
1	A	63	LEU	CB-CG-CD1	-5.63	101.43	111.00
1	A	263	MET	CG-SD-CE	5.63	109.20	100.20
1	A	226	LEU	CB-CG-CD2	-5.61	101.47	111.00
1	A	152	LYS	CD-CE-NZ	-5.59	98.83	111.70
1	A	257	LEU	CB-CG-CD2	-5.51	101.63	111.00
1	F	263	MET	CG-SD-CE	-5.50	91.40	100.20
1	F	300	ARG	NE-CZ-NH1	5.48	123.04	120.30
2	H	871	DC	O5'-P-OP1	-5.44	100.81	105.70
1	F	268	ARG	NE-CZ-NH1	5.39	123.00	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	283	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	A	197	MET	CA-CB-CG	5.34	122.38	113.30
1	F	79	ASP	CB-CG-OD1	5.33	123.09	118.30
1	A	275	LEU	CB-CG-CD2	-5.28	102.02	111.00
1	A	54	GLU	OE1-CD-OE2	-5.28	116.97	123.30
2	B	844	DT	O5'-P-OP2	-5.23	100.99	105.70
1	F	26	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	A	329	LEU	CA-CB-CG	5.16	127.17	115.30
1	F	93	LEU	CA-CB-CG	5.12	127.08	115.30
1	A	107	ASP	C-N-CA	5.05	134.33	121.70
1	F	268	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2645	0	2659	70	0
1	F	2645	0	2659	62	0
2	B	265	0	149	14	0
2	C	182	0	101	7	0
2	G	248	0	136	6	0
2	H	182	0	101	6	0
3	A	29	0	14	2	0
3	F	29	0	14	1	0
4	A	2	0	0	0	0
4	F	2	0	0	0	0
5	A	26	0	0	2	0
5	B	4	0	0	2	0
5	C	4	0	0	3	0
5	F	47	0	0	6	0
5	G	5	0	0	1	0
5	H	3	0	0	0	0
All	All	6318	0	5833	154	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 13.

All (154) 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:F:331:ARG:HB3	5:F:537:HOH:O	1.17	1.32
1:A:331:ARG:CG	1:A:332:PRO:HD3	1.66	1.25
1:A:331:ARG:CG	1:A:332:PRO:CD	2.16	1.23
1:A:331:ARG:HG3	1:A:332:PRO:HD3	1.21	1.15
1:A:9:ASP:OD1	1:A:159:LYS:NZ	1.80	1.14
1:A:331:ARG:HG2	1:A:332:PRO:HD2	1.31	1.11
1:A:334:ARG:NH2	2:B:840:DG:OP1	1.88	1.06
1:A:331:ARG:CG	1:A:332:PRO:HD2	1.88	0.98
1:A:331:ARG:CB	1:A:332:PRO:CD	2.34	0.98
1:F:3:LYS:HG2	1:F:114:ASP:OD1	1.62	0.97
1:A:329:LEU:HD22	1:A:331:ARG:HD3	1.48	0.94
1:A:14:LEU:HD12	1:A:46:THR:CG2	2.02	0.89
1:A:14:LEU:HD12	1:A:46:THR:HG22	1.56	0.84
1:F:295:SER:HB2	1:F:332:PRO:HB2	1.60	0.83
1:F:201:THR:HG22	1:F:204:ASP:H	1.45	0.81
1:A:331:ARG:HG2	1:A:332:PRO:CD	1.95	0.80
1:A:4:TRP:CE2	1:A:121:PRO:HG3	2.17	0.79
2:B:840:DG:OP2	5:B:901:HOH:O	2.01	0.78
1:A:11:ASP:OD1	1:A:159:LYS:HE2	1.83	0.77
1:A:257:LEU:HB3	1:A:333:VAL:CG2	2.13	0.77
1:F:93:LEU:HD21	1:F:131:VAL:HG12	1.66	0.77
2:C:867:DA:OP1	5:C:901:HOH:O	2.03	0.77
1:A:302:LYS:HG2	5:C:901:HOH:O	1.84	0.77
1:A:258:THR:O	1:A:330:ASP:OD2	2.04	0.76
1:F:329:LEU:O	1:F:330:ASP:C	2.22	0.75
1:A:14:LEU:CD1	1:A:46:THR:CG2	2.64	0.75
1:A:289:ALA:HB2	1:A:303:ILE:HG22	1.72	0.72
2:B:845:DC:OP1	5:B:902:HOH:O	2.08	0.71
1:A:14:LEU:CD1	1:A:46:THR:HG21	2.21	0.71
2:C:867:DA:P	5:C:901:HOH:O	2.49	0.69
1:A:257:LEU:CB	1:A:333:VAL:HG23	2.22	0.69
2:B:848:DA:H61	2:C:866:DT:H3	1.40	0.68
1:F:211:SER:O	1:F:212:VAL:C	2.29	0.68
2:G:846:DC:OP2	5:G:901:HOH:O	2.10	0.68
1:A:219:PRO:HD2	5:A:506:HOH:O	1.93	0.67
1:A:238:SER:OG	5:A:501:HOH:O	2.14	0.66
1:A:6:LEU:HD22	1:A:144:ILE:HG12	1.79	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:LEU:HB3	1:A:333:VAL:HG23	1.78	0.65
1:F:127:ARG:NH2	5:F:503:HOH:O	2.27	0.65
1:A:120:ASP:HB3	1:A:123:GLU:HB2	1.81	0.63
1:A:10:LEU:HD11	1:A:90:VAL:HG11	1.79	0.63
1:A:331:ARG:HB3	1:A:332:PRO:CD	2.27	0.61
1:A:123:GLU:O	1:A:126:GLU:HG2	2.01	0.60
2:G:843:DG:H2''	2:G:844:DT:H5'	1.84	0.59
1:A:331:ARG:CB	1:A:332:PRO:HD2	2.21	0.59
1:F:176:GLY:O	1:F:201:THR:HG23	2.02	0.58
1:A:253:PHE:CZ	1:A:336:LEU:HD12	2.39	0.58
2:H:870:DA:H1'	2:H:871:DC:H5''	1.86	0.58
1:A:289:ALA:HB2	1:A:303:ILE:CG2	2.34	0.56
1:A:260:ARG:HH22	1:A:325:ASP:HA	1.70	0.56
1:F:46:THR:HG21	5:F:511:HOH:O	2.06	0.56
1:A:257:LEU:HB2	1:A:333:VAL:HG23	1.86	0.55
2:C:866:DT:H2''	2:C:867:DA:C8	2.41	0.55
2:B:848:DA:N6	2:C:866:DT:H3	2.04	0.55
1:F:295:SER:HB2	1:F:332:PRO:CB	2.35	0.55
1:A:327:PHE:O	1:A:328:GLU:O	2.25	0.54
1:A:14:LEU:HD12	1:A:46:THR:HG21	1.83	0.54
1:F:25:LEU:O	1:F:28:GLN:HB2	2.07	0.54
1:F:129:ARG:HD2	1:F:140:CYS:O	2.08	0.54
2:H:866:DT:H2''	2:H:867:DA:C8	2.42	0.54
1:A:65:ALA:HA	2:B:837:DT:H1'	1.91	0.53
1:A:115:LEU:O	1:A:117:ASP:N	2.42	0.53
1:F:3:LYS:CG	1:F:114:ASP:OD1	2.48	0.53
2:G:842:DG:H2''	2:G:843:DG:H5''	1.91	0.53
2:H:868:DG:H4'	2:H:869:DG:H5'	1.89	0.53
1:F:188:PRO:O	1:F:192:LYS:HD2	2.10	0.52
1:A:107:ASP:OD2	3:A:401:2TM:H1	2.10	0.52
1:A:297:PHE:HD2	2:B:839:DT:N3	2.07	0.52
1:F:311:THR:CG2	1:F:311:THR:O	2.58	0.52
1:F:205:LEU:HA	1:F:208:THR:HG23	1.93	0.51
1:F:331:ARG:CB	5:F:537:HOH:O	2.00	0.51
1:F:286:THR:HG22	1:F:287:ARG:HG3	1.93	0.50
1:F:6:LEU:HD22	1:F:144:ILE:HG12	1.93	0.50
1:A:257:LEU:O	1:A:332:PRO:HA	2.12	0.50
1:F:72:ASP:HB2	5:F:513:HOH:O	2.12	0.50
1:A:69:ARG:NH1	1:F:204:ASP:OD2	2.43	0.50
2:H:866:DT:H2''	2:H:867:DA:H8	1.77	0.49
1:F:328:GLU:O	1:F:328:GLU:CG	2.57	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:39:SER:OG	1:F:39:SER:O	2.20	0.49
1:A:267:VAL:HG21	1:A:324:LEU:HD22	1.95	0.49
1:F:44:VAL:HG13	2:G:840:DG:H5'	1.94	0.49
2:B:838:DC:H1'	1:F:197:MET:CE	2.43	0.49
1:F:199:ILE:HG12	1:F:208:THR:HG21	1.94	0.49
1:F:4:TRP:CE2	1:F:121:PRO:HG3	2.48	0.49
1:A:257:LEU:O	1:A:331:ARG:O	2.30	0.49
1:F:14:LEU:HD12	1:F:46:THR:HG23	1.96	0.48
1:A:242:TRP:CH2	1:A:245:ARG:NH1	2.82	0.48
2:B:838:DC:H1'	1:F:197:MET:HE2	1.94	0.48
1:F:189:LYS:HB2	2:H:870:DA:H3'	1.96	0.47
1:F:193:LYS:O	1:F:197:MET:HG3	2.14	0.47
2:G:838:DC:O4'	2:G:838:DC:O2	2.31	0.47
2:B:848:DA:N1	2:C:866:DT:O2	2.48	0.47
1:F:210:PRO:O	1:F:214:THR:HG23	2.15	0.46
1:A:257:LEU:CB	1:A:333:VAL:CG2	2.84	0.46
1:F:295:SER:CB	1:F:332:PRO:HG2	2.46	0.46
1:F:295:SER:HB3	1:F:332:PRO:HG2	1.98	0.46
1:A:94:LEU:HA	1:A:97:LEU:HD13	1.97	0.46
1:A:331:ARG:HB3	1:A:332:PRO:HD2	1.94	0.45
1:A:14:LEU:HD11	1:A:46:THR:CG2	2.47	0.45
1:F:94:LEU:HA	1:F:97:LEU:HD12	1.98	0.45
1:A:257:LEU:HB3	1:A:333:VAL:HG22	1.97	0.45
1:A:164:TYR:HE2	1:A:166:LEU:HD13	1.82	0.45
1:F:10:LEU:HD12	1:F:107:ASP:HA	1.97	0.45
1:F:180:PRO:HD2	1:F:191:THR:HG23	1.98	0.45
1:F:211:SER:HA	1:F:214:THR:OG1	2.17	0.45
1:A:40:GLU:OE2	1:A:43:LYS:HE3	2.17	0.45
1:A:129:ARG:HD2	1:A:140:CYS:O	2.17	0.44
1:F:128:ILE:O	1:F:132:VAL:HG23	2.17	0.44
1:F:201:THR:O	1:F:204:ASP:HB2	2.17	0.44
1:A:8:VAL:O	1:A:108:GLU:HA	2.18	0.44
1:A:150:ARG:NH1	1:A:168:GLU:OE2	2.45	0.44
1:F:205:LEU:HA	1:F:208:THR:CG2	2.48	0.44
2:B:845:DC:H2''	2:B:846:DC:C6	2.53	0.44
1:F:99:HIS:HB3	1:F:112:GLY:O	2.18	0.44
1:F:14:LEU:HD12	1:F:46:THR:CG2	2.47	0.43
1:A:300:ARG:HH22	1:A:328:GLU:H	1.65	0.43
1:F:158:ALA:O	1:F:162:GLY:HA3	2.18	0.43
1:F:204:ASP:O	1:F:208:THR:HG22	2.17	0.43
2:B:842:DG:H2''	2:B:843:DG:H5''	2.00	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:VAL:HB	1:A:323:VAL:HG12	2.00	0.43
1:F:331:ARG:CG	5:F:537:HOH:O	2.54	0.43
1:A:115:LEU:C	1:A:117:ASP:H	2.22	0.43
1:A:116:PRO:HG2	1:A:118:GLU:H	1.83	0.43
1:A:11:ASP:OD1	1:A:159:LYS:CE	2.62	0.43
2:B:848:DA:H2'	2:B:849:DG:C8	2.53	0.43
1:F:226:LEU:HD23	1:F:226:LEU:HA	1.72	0.43
1:F:171:TRP:CZ3	1:F:175:MET:HG3	2.54	0.42
1:A:68:ARG:HD3	1:A:68:ARG:HA	1.79	0.42
1:A:14:LEU:HD11	1:A:46:THR:HG21	1.99	0.42
1:F:199:ILE:HG23	1:F:204:ASP:HB3	2.01	0.42
1:F:260:ARG:HA	1:F:260:ARG:HD2	1.87	0.42
1:F:121:PRO:HB2	1:F:144:ILE:HD13	2.01	0.42
1:F:210:PRO:O	1:F:214:THR:N	2.50	0.42
1:F:42:ARG:O	2:G:840:DG:H4'	2.19	0.42
1:F:261:ARG:O	1:F:265:SER:HB2	2.19	0.42
1:F:12:GLN:O	1:F:13:PHE:C	2.58	0.42
1:F:251:VAL:O	1:F:335:LEU:HA	2.20	0.42
1:A:152:LYS:HG2	1:A:184:TRP:CD1	2.55	0.42
3:F:401:2TM:O5'	3:F:401:2TM:H10	2.20	0.41
1:A:291:THR:OG1	1:A:301:THR:HG22	2.19	0.41
3:A:401:2TM:PB	3:A:401:2TM:H2	2.60	0.41
1:F:125:ALA:HB2	1:F:144:ILE:HD11	2.02	0.41
1:F:152:LYS:HG2	1:F:184:TRP:CD1	2.55	0.41
1:F:293:ARG:HB3	1:F:335:LEU:HB3	2.03	0.41
1:A:93:LEU:HD11	1:A:135:GLU:HB2	2.01	0.41
1:A:250:VAL:HB	1:A:335:LEU:HD11	2.03	0.41
2:C:870:DA:H1'	2:C:871:DC:H5''	2.02	0.41
1:A:253:PHE:HD1	1:A:334:ARG:O	2.04	0.40
1:A:256:ASP:N	1:A:256:ASP:OD1	2.35	0.40
1:A:339:ARG:NH1	1:A:341:GLU:OE1	2.51	0.40
1:F:293:ARG:HA	1:F:298:TYR:O	2.22	0.40
1:A:62:PRO:HG3	2:B:839:DT:H4'	2.04	0.40
2:H:869:DG:H2''	2:H:870:DA:H5'	2.03	0.40
1:F:227:LEU:HA	1:F:227:LEU:HD23	1.92	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%)	324 (94%)	17 (5%)	4 (1%)	13	24
1	F	345/356 (97%)	324 (94%)	18 (5%)	3 (1%)	17	31
All	All	690/712 (97%)	648 (94%)	35 (5%)	7 (1%)	15	28

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	346	ASP
1	A	328	GLU
1	F	259	GLU
1	F	257	LEU
1	A	92	GLY
1	A	331	ARG
1	A	298	TYR

### 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	A	284/290 (98%)	260 (92%)	24 (8%)	10	21
1	F	284/290 (98%)	260 (92%)	24 (8%)	10	21
All	All	568/580 (98%)	520 (92%)	48 (8%)	10	21

All (48) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	1	MET
1	A	16	SER
1	A	21	ARG
1	A	46	THR
1	A	68	ARG
1	A	101	LEU
1	A	104	TRP
1	A	106	TRP
1	A	118	GLU
1	A	211	SER
1	A	256	ASP
1	A	259	GLU
1	A	261	ARG
1	A	265	SER
1	A	297	PHE
1	A	298	TYR
1	A	300	ARG
1	A	303	ILE
1	A	311	THR
1	A	325	ASP
1	A	328	GLU
1	A	329	LEU
1	A	331	ARG
1	A	335	LEU
1	F	46	THR
1	F	84	ASP
1	F	96	ASP
1	F	97	LEU
1	F	104	TRP
1	F	106	TRP
1	F	115	LEU
1	F	120	ASP
1	F	127	ARG
1	F	172	MET
1	F	192	LYS
1	F	193	LYS
1	F	201	THR
1	F	207	VAL
1	F	208	THR
1	F	220	SER
1	F	230	LYS
1	F	245	ARG
1	F	297	PHE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	311	THR
1	F	328	GLU
1	F	329	LEU
1	F	330	ASP
1	F	331	ARG

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	1.87	5 (20%)	30,47,47	1.99	12 (40%)
3	2TM	F	401	4	24,30,30	1.54	2 (8%)	30,47,47	1.80	9 (30%)

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	-	6/17/38/38	0/2/2/2
3	2TM	F	401	4	-	4/17/38/38	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	2TM	PB-O2B	5.63	1.65	1.51
3	F	401	2TM	PB-O1B	-5.07	1.44	1.56
3	F	401	2TM	PB-O3B	3.99	1.62	1.58
3	A	401	2TM	PA-O5'	3.24	1.62	1.57
3	A	401	2TM	PB-O3B	3.09	1.61	1.58
3	A	401	2TM	O4'-C1'	2.81	1.45	1.41
3	A	401	2TM	PA-O2A	-2.35	1.50	1.56

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	401	2TM	C2-N3-C4	3.96	120.35	116.34
3	A	401	2TM	O3G-PG-O1G	3.90	125.95	110.68
3	A	401	2TM	C2-N3-C4	3.83	120.22	116.34
3	F	401	2TM	C3'-C2'-C1'	3.76	106.64	100.98
3	F	401	2TM	O3G-PG-O3B	3.48	116.30	104.64
3	A	401	2TM	PG-O3B-PB	-3.25	121.19	132.62
3	A	401	2TM	C3'-C2'-C1'	3.21	105.81	100.98
3	F	401	2TM	PG-O3B-PB	-3.06	121.86	132.62
3	A	401	2TM	O1A-PA-C1	-2.86	101.51	109.07
3	F	401	2TM	O2A-PA-C1	2.82	118.10	106.58
3	A	401	2TM	O2G-PG-O3G	-2.75	97.12	107.64
3	A	401	2TM	O2A-PA-C1	2.48	116.73	106.58
3	A	401	2TM	O5'-C5'-C4'	2.47	117.48	108.99
3	A	401	2TM	O1B-PB-O2B	2.47	118.30	110.07
3	F	401	2TM	O1B-PB-O2B	2.29	117.71	110.07
3	A	401	2TM	O2B-PB-C1	2.27	115.07	109.07
3	F	401	2TM	C5'-C4'-C3'	-2.18	107.02	115.18
3	A	401	2TM	O2G-PG-O3B	2.17	111.91	104.64
3	F	401	2TM	O2G-PG-O3G	2.14	115.80	107.64
3	F	401	2TM	O3'-C3'-C4'	2.08	117.06	111.05
3	A	401	2TM	C5'-C4'-C3'	-2.04	107.55	115.18

There are no chirality outliers.

All (10) torsion outliers are listed below:

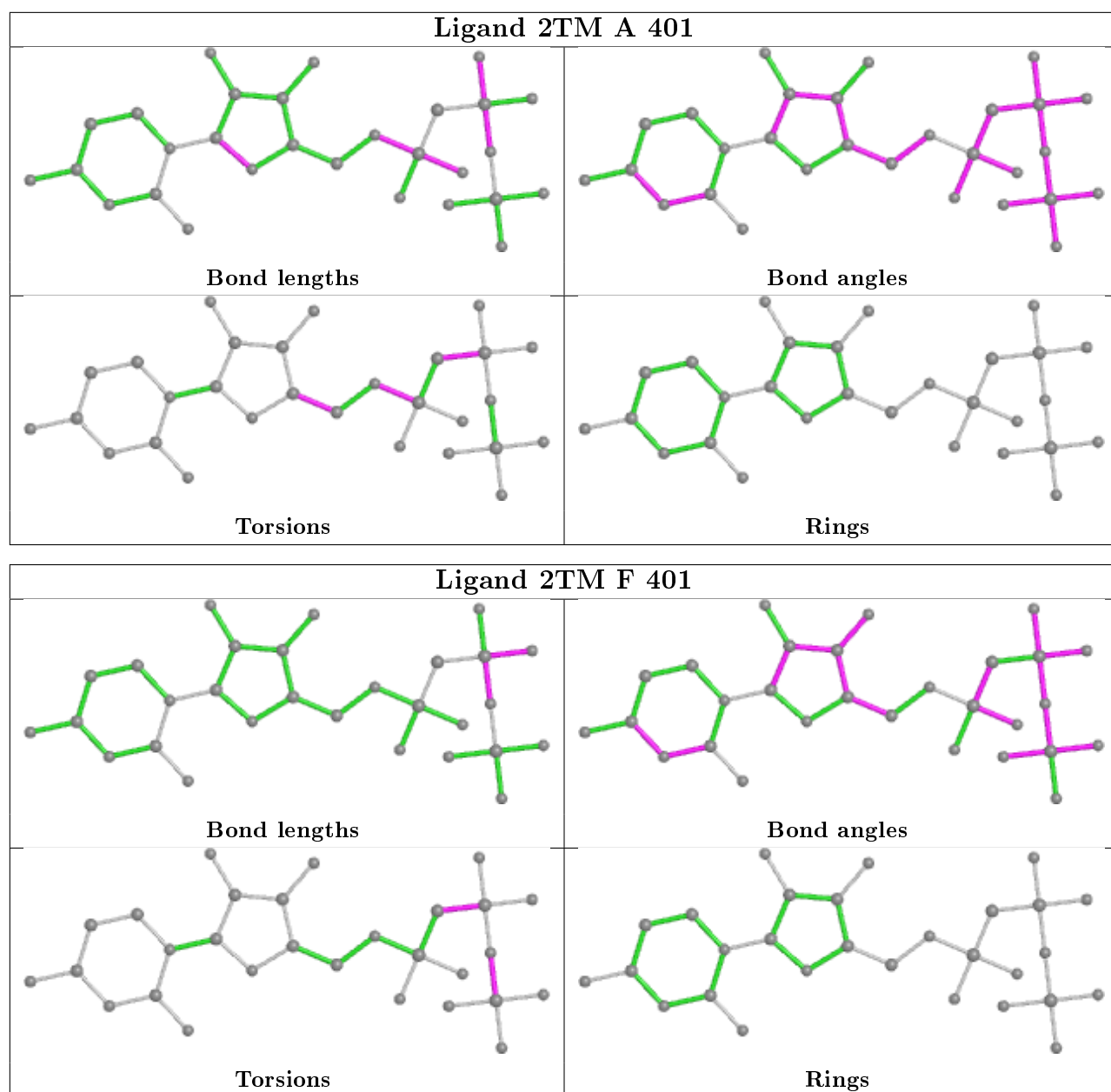
Mol	Chain	Res	Type	Atoms
3	A	401	2TM	O4'-C4'-C5'-O5'
3	A	401	2TM	PA-C1-PB-O3B
3	A	401	2TM	PA-C1-PB-O1B
3	A	401	2TM	PA-C1-PB-O2B
3	F	401	2TM	PA-C1-PB-O3B
3	F	401	2TM	PA-C1-PB-O1B
3	F	401	2TM	PA-C1-PB-O2B
3	A	401	2TM	C3'-C4'-C5'-O5'
3	A	401	2TM	C5'-O5'-PA-C1
3	F	401	2TM	PB-O3B-PG-O2G

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	2TM	2	0
3	F	401	2TM	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 [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.17	8 (2%) 60 63	27, 49, 94, 141	0
1	F	347/356 (97%)	0.26	11 (3%) 47 51	30, 48, 74, 104	0
2	B	13/18 (72%)	1.01	4 (30%) 0 0	54, 68, 139, 146	0
2	C	9/18 (50%)	0.61	1 (11%) 5 5	59, 72, 108, 131	0
2	G	12/18 (66%)	0.34	2 (16%) 1 1	43, 58, 117, 135	0
2	H	9/18 (50%)	0.95	2 (22%) 0 0	49, 64, 98, 124	0
All	All	737/784 (94%)	0.25	28 (3%) 40 43	27, 49, 96, 146	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	331	ARG	8.3
1	F	329	LEU	5.0
1	A	297	PHE	4.7
1	F	330	ASP	4.2
1	F	332	PRO	4.1
2	B	848	DA	4.1
1	A	330	ASP	3.9
1	A	105	GLY	3.9
2	H	865	DC	3.7
2	G	849	DG	3.4
2	B	849	DG	3.4
1	A	327	PHE	3.0
1	F	26	ARG	3.0
1	F	104	TRP	2.9
1	F	105	GLY	2.7
1	A	1	MET	2.7
1	F	118	GLU	2.6
1	A	298	TYR	2.5
1	A	300	ARG	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	F	303	ILE	2.5
1	F	210	PRO	2.3
2	G	848	DA	2.3
2	B	837	DT	2.3
1	F	258	THR	2.2
2	B	838	DC	2.1
1	A	304	ARG	2.1
2	C	865	DC	2.1
2	H	866	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 [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

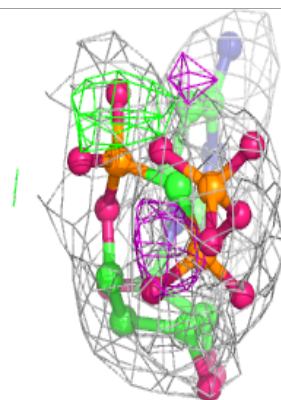
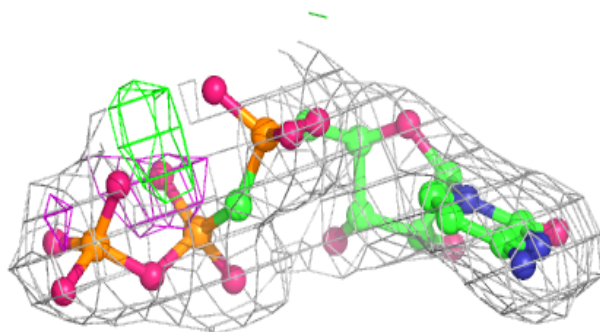
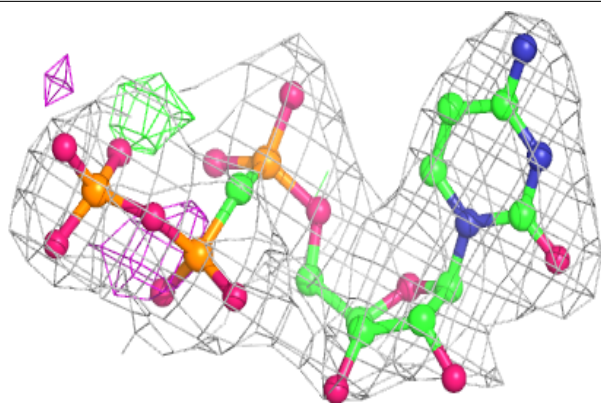
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	MN	A	403	1/1	0.84	0.12	100,100,100,100	0
3	2TM	A	401	29/29	0.92	0.17	53,62,73,77	0
4	MN	A	402	1/1	0.92	0.14	89,89,89,89	0
4	MN	F	403	1/1	0.96	0.12	55,55,55,55	0
3	2TM	F	401	29/29	0.97	0.14	40,53,57,59	0
4	MN	F	402	1/1	0.98	0.12	47,47,47,47	0

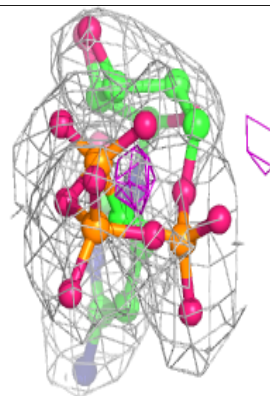
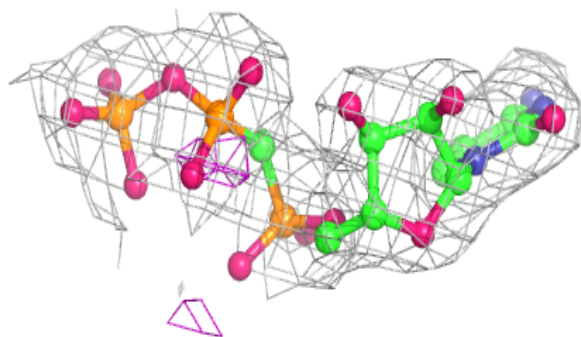
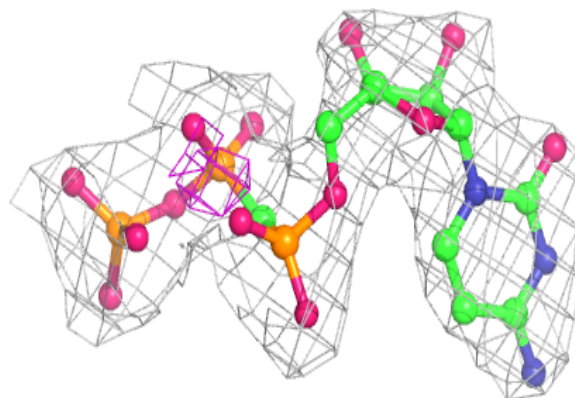
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 2TM A 401:**

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

**Electron density around 2TM F 401:**

$2mF_o-DF_c$  (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.