



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 01:40 pm BST

PDB ID : 6JUO  
Title : MsDpo4-DNA complex 4  
Authors : Nair, D.T.; Johnson, M.K.  
Deposited on : 2019-04-15  
Resolution : 2.16 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

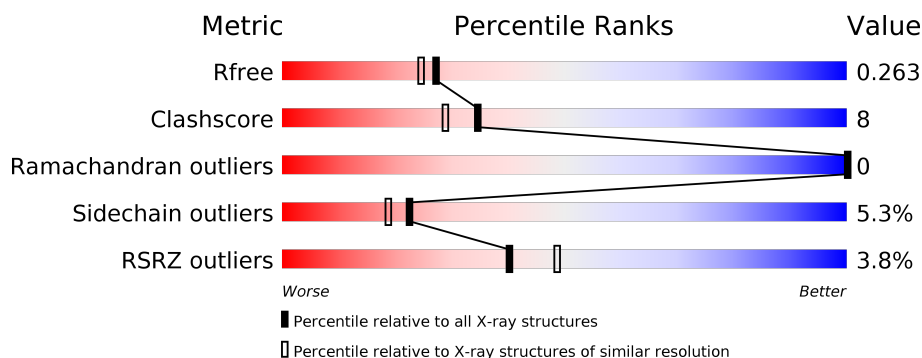
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.16 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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>4%</div> <div> <div></div> <div>79%</div> <div>15%</div> <div>• •</div> </div> </div>
1	F	356	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>17%</div> <div>• •</div> </div> </div>
2	B	18	<div> <div>11%</div> <div> <div></div> <div>28%</div> <div>39%</div> <div>6%</div> <div>28%</div> </div> </div>
2	C	18	<div> <div>17%</div> <div> <div></div> <div>39%</div> <div>11%</div> <div>17%</div> <div>33%</div> </div> </div>
2	G	18	<div> <div>6%</div> <div> <div></div> <div>44%</div> <div>17%</div> <div>39%</div> </div> </div>
2	H	18	<div> <div>6%</div> <div> <div></div> <div>22%</div> <div>22%</div> <div>56%</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6693 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	1	0
			2660	1672	469	508	11			
1	F	347	Total	C	N	O	S	0	0	0
			2649	1666	465	507	11			

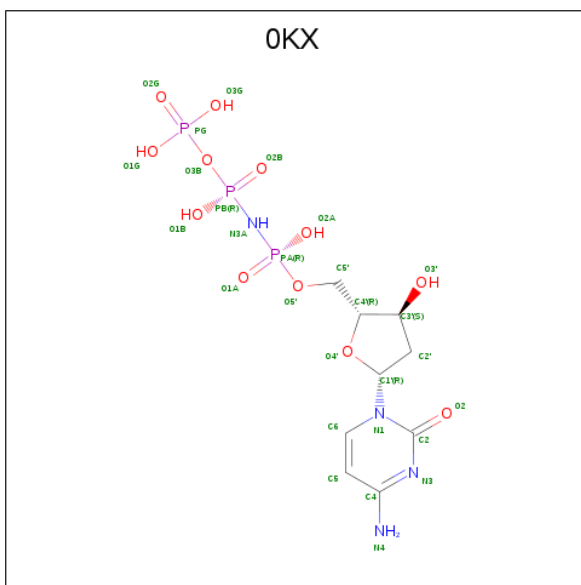
There are 2 discrepancies between the modelled and reference sequences:

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(P\*CP\*TP\*GP\*GP\*GP\*GP\*TP\*CP\*CP\*TP\*AP\*GP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	13	Total	C	N	O	P	0	0	0
			270	127	50	80	13			
2	C	12	Total	C	N	O	P	0	0	0
			243	115	44	72	12			
2	G	11	Total	C	N	O	P	0	0	0
			226	107	40	68	11			
2	H	8	Total	C	N	O	P	0	0	0
			163	77	31	47	8			

- Molecule 3 is 2'-deoxy-5'-O-[(R)-hydroxy{[(R)-hydroxy(phosphonooxy)phosphoryl]amino}phosphoryl]cytidine (three-letter code: 0KX) (formula: C<sub>9</sub>H<sub>17</sub>N<sub>4</sub>O<sub>12</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
			28	9	4	12	3		
3	F	1	Total	C	N	O	P	0	0
			28	9	4	12	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	186	Total	O	0	0
			186	186		
5	B	19	Total	O	0	0
			19	19		
5	C	8	Total	O	0	0
			8	8		
5	F	187	Total	O	0	0
			187	187		
5	G	16	Total	O	0	0
			16	16		

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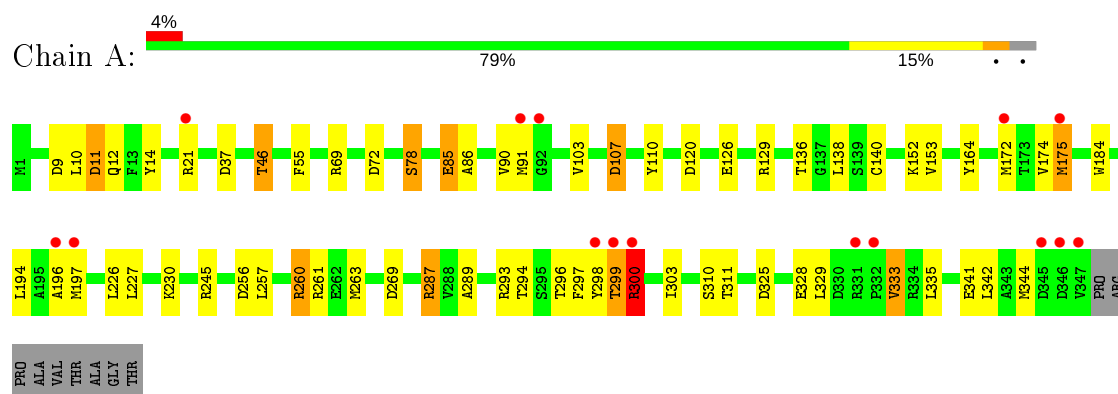
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	6	Total	O	0	0
			6	6		

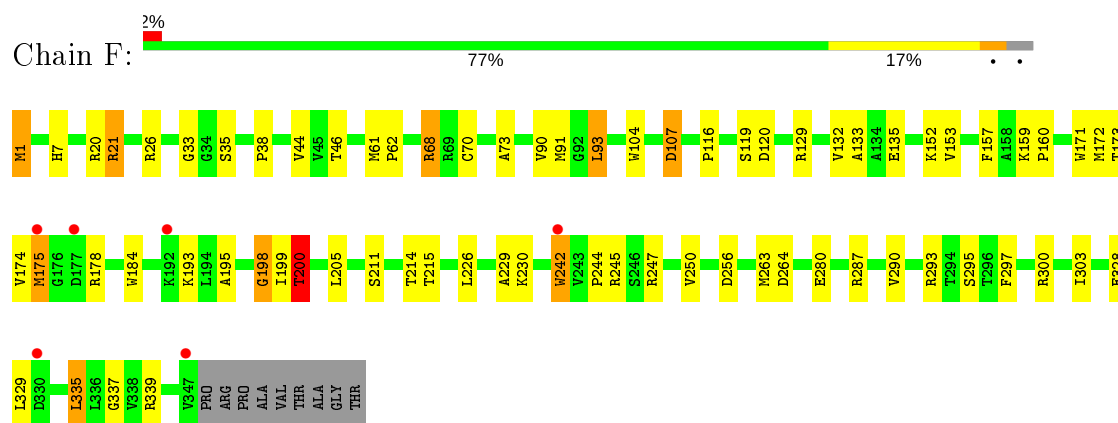
### 3 Residue-property plots [i](#)

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.

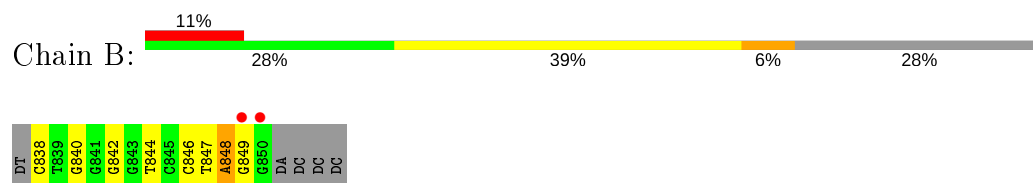
#### • Molecule 1: DNA polymerase IV



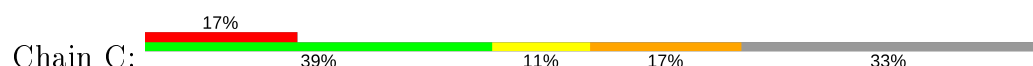
#### • Molecule 1: DNA polymerase IV

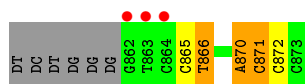


#### • Molecule 2: DNA (5'-D(P\*CP\*TP\*GP\*GP\*GP\*GP\*TP\*CP\*CP\*TP\*AP\*GP\*G)-3')

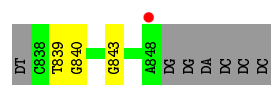


#### • Molecule 2: DNA (5'-D(P\*CP\*TP\*GP\*GP\*GP\*GP\*TP\*CP\*CP\*TP\*AP\*GP\*G)-3')

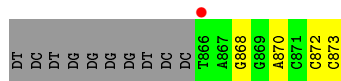




- Molecule 2: DNA (5'-D(P\*CP\*TP\*GP\*GP\*GP\*GP\*TP\*CP\*CP\*TP\*AP\*GP\*G)-3')



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.10 Å 81.03 Å 210.53 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.18 – 2.16 64.21 – 2.16	Depositor EDS
% Data completeness (in resolution range)	99.9 (70.18-2.16) 100.0 (64.21-2.16)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.03 (at 2.16 Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, $R_{free}$	0.200 , 0.255 0.213 , 0.263	Depositor DCC
$R_{free}$ test set	2562 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.8	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 45.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6693	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 4.16% 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: 0KX, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	1.24	6/2714 (0.2%)	1.20	23/3701 (0.6%)
1	F	1.42	24/2703 (0.9%)	1.19	16/3687 (0.4%)
2	B	1.28	4/302 (1.3%)	1.23	3/465 (0.6%)
2	C	0.80	0/271	1.32	4/415 (1.0%)
2	G	0.98	1/252 (0.4%)	1.12	3/387 (0.8%)
2	H	0.91	1/182 (0.5%)	1.24	1/278 (0.4%)
All	All	1.29	36/6424 (0.6%)	1.20	50/8933 (0.6%)

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	171	TRP	CG-CD1	-12.86	1.18	1.36
1	A	342	LEU	C-O	-9.63	1.05	1.23
1	F	172	MET	C-O	-9.50	1.05	1.23
1	F	171	TRP	CD1-NE1	-8.84	1.23	1.38
1	F	199	ILE	C-O	-8.84	1.06	1.23
2	B	846	DC	O3'-P	8.37	1.71	1.61
1	F	171	TRP	C-O	-8.29	1.07	1.23
1	F	171	TRP	CD2-CE2	-8.13	1.31	1.41
1	F	200	THR	C-O	-7.55	1.09	1.23
1	F	195	ALA	C-O	-7.46	1.09	1.23
1	F	280	GLU	CD-OE1	7.02	1.33	1.25
2	B	842	DG	O3'-P	-7.01	1.52	1.61
1	F	90	VAL	C-O	-6.82	1.10	1.23
1	F	91	MET	C-O	-6.80	1.10	1.23
1	F	171	TRP	CG-CD2	-6.64	1.32	1.43
1	F	173	THR	C-O	-6.63	1.10	1.23
1	F	171	TRP	CE3-CZ3	-6.53	1.27	1.38
1	A	85	GLU	CD-OE1	6.50	1.32	1.25
1	F	198	GLY	C-O	-6.32	1.13	1.23
1	F	173	THR	CB-CG2	-6.20	1.31	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	126	GLU	CD-OE2	5.98	1.32	1.25
1	F	90	VAL	CB-CG1	-5.86	1.40	1.52
1	F	171	TRP	CZ3-CH2	-5.86	1.30	1.40
2	G	843	DG	O3'-P	-5.81	1.54	1.61
1	F	171	TRP	NE1-CE2	-5.72	1.30	1.37
1	F	172	MET	CG-SD	-5.69	1.66	1.81
2	B	848	DA	P-OP1	-5.53	1.39	1.49
1	F	33	GLY	C-O	5.48	1.32	1.23
1	A	164	TYR	CE2-CZ	-5.44	1.31	1.38
1	A	126	GLU	CG-CD	5.41	1.60	1.51
2	H	872	DC	O3'-P	-5.31	1.54	1.61
1	F	91	MET	N-CA	-5.27	1.35	1.46
1	F	200	THR	N-CA	-5.22	1.35	1.46
2	B	847	DT	P-OP2	-5.19	1.40	1.49
1	A	110	TYR	CG-CD2	-5.18	1.32	1.39
1	F	242	TRP	CE3-CZ3	5.14	1.47	1.38

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	871	DC	O5'-P-OP1	-11.55	95.30	105.70
1	A	129	ARG	NE-CZ-NH1	10.56	125.58	120.30
2	H	870	DA	O5'-P-OP1	-10.44	96.31	105.70
1	A	129	ARG	NE-CZ-NH2	-9.92	115.34	120.30
2	B	842	DG	O5'-P-OP2	-9.77	96.91	105.70
1	A	11	ASP	CB-CG-OD1	9.64	126.97	118.30
1	F	68	ARG	NE-CZ-NH1	9.42	125.01	120.30
1	F	20	ARG	NE-CZ-NH2	-9.18	115.71	120.30
2	G	839	DT	O5'-P-OP2	-9.16	97.45	105.70
2	C	871	DC	O5'-P-OP2	8.66	121.09	110.70
1	A	245	ARG	NE-CZ-NH1	8.62	124.61	120.30
1	A	37	ASP	CB-CG-OD1	8.60	126.04	118.30
1	F	68	ARG	NE-CZ-NH2	-8.59	116.01	120.30
1	A	245	ARG	NE-CZ-NH2	-8.19	116.20	120.30
1	A	287	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	A	37	ASP	CB-CG-OD2	-7.42	111.63	118.30
1	F	107	ASP	CB-CG-OD2	6.62	124.25	118.30
1	A	120	ASP	CB-CG-OD1	6.51	124.16	118.30
1	A	269	ASP	CB-CG-OD1	6.35	124.02	118.30
1	A	14	TYR	CB-CG-CD2	-6.33	117.20	121.00
1	A	11	ASP	CB-CG-OD2	-6.28	112.65	118.30
1	A	14	TYR	CB-CG-CD1	6.01	124.61	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	200	THR	N-CA-CB	-6.00	98.91	110.30
2	G	839	DT	O5'-P-OP1	5.98	117.88	110.70
1	F	293	ARG	NE-CZ-NH2	-5.95	117.33	120.30
2	B	844	DT	O5'-P-OP2	-5.94	100.35	105.70
1	F	178	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	A	9	ASP	CB-CG-OD2	5.81	123.53	118.30
1	F	245	ARG	NE-CZ-NH1	5.74	123.17	120.30
2	C	866	DT	O5'-P-OP1	-5.72	100.55	105.70
1	A	9	ASP	CB-CG-OD1	-5.62	113.25	118.30
2	C	870	DA	C1'-O4'-C4'	-5.62	104.48	110.10
1	F	120	ASP	CB-CG-OD1	5.61	123.35	118.30
1	A	260	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	F	21	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	F	172	MET	CB-CG-SD	5.46	128.79	112.40
2	B	846	DC	P-O3'-C3'	5.44	126.23	119.70
1	A	107	ASP	CB-CG-OD2	5.39	123.16	118.30
1	A	300	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	F	290	VAL	CG1-CB-CG2	-5.37	102.31	110.90
1	A	256	ASP	CB-CG-OD1	-5.37	113.47	118.30
1	A	261	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	A	300	ARG	NE-CZ-NH2	5.34	122.97	120.30
1	F	264	ASP	CB-CG-OD1	5.27	123.04	118.30
1	A	256	ASP	CB-CG-OD2	5.26	123.03	118.30
1	F	21	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	A	342	LEU	CA-CB-CG	5.14	127.12	115.30
1	F	335	LEU	CB-CG-CD2	5.12	119.70	111.00
1	F	172	MET	CG-SD-CE	5.09	108.34	100.20
2	G	840	DG	O5'-P-OP2	-5.07	101.14	105.70

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	2660	0	2669	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2649	0	2657	51	0
2	B	270	0	147	15	0
2	C	243	0	135	7	0
2	G	226	0	125	0	0
2	H	163	0	90	2	0
3	A	28	0	14	0	0
3	F	28	0	16	1	0
4	A	2	0	0	0	0
4	F	2	0	0	0	0
5	A	186	0	0	1	0
5	B	19	0	0	1	0
5	C	8	0	0	0	0
5	F	187	0	0	8	0
5	G	16	0	0	0	0
5	H	6	0	0	0	0
All	All	6693	0	5853	98	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 8.

All (98) 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:196:ALA:O	1:F:62:PRO:HG2	1.52	1.08
1:F:129:ARG:O	5:F:501:HOH:O	1.79	0.99
2:B:849:DG:N2	2:C:865:DC:O2	1.98	0.96
1:F:263:MET:CE	1:F:329:LEU:HD13	1.98	0.93
1:F:152:LYS:NZ	2:H:873:DC:OP1	2.06	0.88
1:F:174:VAL:HG12	1:F:175:MET:HG2	1.56	0.85
1:A:293:ARG:HE	1:A:299:THR:HG21	1.42	0.83
1:A:174:VAL:HG12	1:A:175:MET:HG2	1.62	0.82
2:C:870:DA:H2"	2:C:871:DC:H5"	1.63	0.81
1:F:263:MET:HE2	1:F:329:LEU:HD13	1.61	0.81
1:F:153:VAL:CG1	1:F:175:MET:SD	2.72	0.78
1:F:153:VAL:HG11	1:F:175:MET:SD	2.26	0.75
1:A:91:MET:SD	1:A:103:VAL:HG22	2.26	0.74
1:F:152:LYS:HG2	1:F:184:TRP:CD1	2.22	0.73
1:A:293:ARG:HE	1:A:299:THR:CG2	2.01	0.73
1:F:263:MET:CE	1:F:329:LEU:HD22	2.20	0.72
1:F:157:PHE:HE2	1:F:175:MET:SD	2.14	0.70
1:F:1:MET:N	5:F:506:HOH:O	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:838:DC:H5	1:F:193:LYS:HZ1	1.43	0.67
1:F:132:VAL:N	5:F:501:HOH:O	2.27	0.67
1:A:46:THR:HG21	1:A:78:SER:OG	1.96	0.66
2:B:838:DC:H5	1:F:193:LYS:NZ	1.94	0.64
1:F:263:MET:HE3	1:F:329:LEU:HD22	1.79	0.64
1:F:157:PHE:CE2	1:F:175:MET:SD	2.92	0.62
1:F:263:MET:HE1	1:F:329:LEU:HB3	1.80	0.62
1:A:196:ALA:O	1:F:62:PRO:CG	2.39	0.61
1:F:263:MET:HE1	1:F:329:LEU:HD13	1.78	0.61
1:F:300:ARG:HD2	2:H:868:DG:OP2	2.01	0.61
1:A:153:VAL:HG11	1:A:175:MET:SD	2.41	0.60
1:F:263:MET:HE1	1:F:329:LEU:HD22	1.84	0.59
2:B:848:DA:H2''	2:B:849:DG:H5'	1.85	0.58
1:A:289:ALA:HB2	1:A:303:ILE:HD12	1.86	0.57
1:A:263:MET:HE1	1:A:329:LEU:HB3	1.86	0.57
1:A:69:ARG:HD2	1:F:198:GLY:O	2.05	0.57
1:A:194:LEU:HA	1:A:197:MET:HE3	1.87	0.57
1:A:153:VAL:CG1	1:A:175:MET:SD	2.93	0.56
1:F:93:LEU:HD21	1:F:135:GLU:HB2	1.86	0.56
1:F:7:HIS:CE1	1:F:152:LYS:HE3	2.42	0.55
2:B:848:DA:C6	2:B:849:DG:C6	2.94	0.55
2:B:849:DG:N2	2:C:865:DC:C2	2.64	0.54
2:B:848:DA:N6	2:B:849:DG:C6	2.76	0.54
2:B:840:DG:OP2	5:B:901:HOH:O	2.17	0.54
1:A:152:LYS:HE2	1:A:184:TRP:NE1	2.22	0.54
1:A:86:ALA:O	1:A:90:VAL:HG23	2.07	0.54
1:A:91:MET:HE2	1:A:91:MET:HA	1.90	0.54
1:A:293:ARG:HG3	1:A:299:THR:HG22	1.89	0.53
1:A:55:PHE:HB3	1:A:69:ARG:O	2.08	0.53
5:A:641:HOH:O	1:F:200:THR:HG21	2.08	0.52
1:F:129:ARG:C	5:F:501:HOH:O	2.37	0.51
1:A:257:LEU:HB2	1:A:333:VAL:HG12	1.93	0.50
2:B:848:DA:C2'	2:B:849:DG:H5'	2.42	0.50
2:B:849:DG:N1	2:C:865:DC:N3	2.52	0.49
1:F:250:VAL:HG12	1:F:337:GLY:HA3	1.93	0.49
2:B:838:DC:O2	2:B:838:DC:O4'	2.31	0.49
1:F:339:ARG:HD2	5:F:585:HOH:O	2.12	0.49
1:F:211:SER:O	1:F:215:THR:HG23	2.13	0.48
1:F:247:ARG:NH1	5:F:512:HOH:O	2.40	0.48
1:F:256:ASP:OD2	1:F:295:SER:HB3	2.13	0.47
3:F:401:OKX:H15	3:F:401:OKX:O5'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:ARG:HD3	1:A:341:GLU:OE2	2.15	0.47
1:A:184:TRP:CZ2	2:C:872:DC:H4'	2.50	0.47
2:B:838:DC:H5	1:F:193:LYS:CE	2.28	0.46
1:A:197:MET:HB3	1:F:68:ARG:NH2	2.30	0.46
2:B:848:DA:H1'	2:B:849:DG:H5'	1.97	0.46
1:A:11:ASP:O	1:A:12:GLN:C	2.53	0.46
1:F:205:LEU:HD23	1:F:229:ALA:HB2	1.98	0.46
1:A:10:LEU:HD23	1:A:140:CYS:HB3	1.97	0.46
2:B:838:DC:C5'	2:B:838:DC:O2	2.65	0.45
1:F:61:MET:HG2	1:F:62:PRO:HD2	1.99	0.45
1:A:136:THR:O	1:A:138:LEU:HD13	2.17	0.45
1:F:328:GLU:CD	1:F:328:GLU:H	2.20	0.45
1:F:263:MET:CE	1:F:329:LEU:CD1	2.83	0.44
2:B:848:DA:C5	2:B:849:DG:C5	3.05	0.44
1:F:226:LEU:HD22	1:F:230:LYS:HE2	1.99	0.44
1:A:296:THR:HG22	1:A:296:THR:O	2.18	0.44
1:A:298:TYR:CZ	1:A:300:ARG:HD3	2.52	0.44
2:C:865:DC:H2'	2:C:866:DT:C6	2.53	0.44
1:F:26:ARG:NH2	5:F:502:HOH:O	2.14	0.44
1:A:260:ARG:NH1	1:A:329:LEU:HD12	2.32	0.43
1:F:242:TRP:CZ3	1:F:244:PRO:HG3	2.54	0.43
1:A:263:MET:HE2	1:A:329:LEU:HD13	2.00	0.43
1:F:263:MET:HE1	1:F:329:LEU:CD1	2.49	0.42
1:A:293:ARG:NE	1:A:299:THR:HG21	2.21	0.42
1:F:152:LYS:HZ2	1:F:184:TRP:HE1	1.66	0.42
1:A:91:MET:SD	1:A:103:VAL:CG2	3.04	0.42
1:F:104:TRP:CE3	1:F:104:TRP:HA	2.54	0.42
1:A:263:MET:HE1	1:A:329:LEU:HD22	2.02	0.41
1:A:260:ARG:HH22	1:A:325:ASP:HA	1.85	0.41
1:F:70:CYS:SG	1:F:73:ALA:HB2	2.60	0.41
2:C:871:DC:H2''	2:C:872:DC:O4'	2.21	0.41
1:F:287:ARG:NH2	1:F:303:ILE:HD13	2.36	0.41
1:F:159:LYS:HA	1:F:160:PRO:HA	1.85	0.41
1:F:44:VAL:HA	1:F:61:MET:O	2.21	0.41
1:F:116:PRO:HG2	1:F:119:SER:HB2	2.02	0.40
1:A:294:THR:OG1	1:A:298:TYR:HB3	2.21	0.40
1:F:175:MET:HB3	1:F:175:MET:HE3	1.89	0.40
1:A:226:LEU:HD22	1:A:230:LYS:HE2	2.04	0.40
1:F:133:ALA:N	5:F:501:HOH:O	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	346/356 (97%)	339 (98%)	7 (2%)	0	100	100
1	F	345/356 (97%)	339 (98%)	6 (2%)	0	100	100
All	All	691/712 (97%)	678 (98%)	13 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	285/290 (98%)	267 (94%)	18 (6%)	18	13
1	F	284/290 (98%)	272 (96%)	12 (4%)	30	28
All	All	569/580 (98%)	539 (95%)	30 (5%)	22	19

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ARG
1	A	46	THR
1	A	72	ASP
1	A	78	SER
1	A	85	GLU
1	A	107	ASP
1	A	172	MET
1	A	175	MET

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Mol	Chain	Res	Type
1	A	227	LEU
1	A	297	PHE
1	A	299	THR
1	A	300	ARG
1	A	310	SER
1	A	311	THR
1	A	328	GLU
1	A	333	VAL
1	A	335	LEU
1	A	344	MET
1	F	1	MET
1	F	21	ARG
1	F	35	SER
1	F	38	PRO
1	F	46	THR
1	F	93	LEU
1	F	107	ASP
1	F	175	MET
1	F	200	THR
1	F	214	THR
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	0KX	A	401	4	26,29,29	5.25	19 (73%)	33,45,45	2.44	9 (27%)
3	0KX	F	401	4	26,29,29	3.79	14 (53%)	33,45,45	2.27	12 (36%)

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	0KX	A	401	4	-	4/16/34/34	0/2/2/2
3	0KX	F	401	4	-	5/16/34/34	0/2/2/2

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	0KX	PB-O3B	14.60	1.77	1.59
3	F	401	0KX	C6-N1	10.73	1.49	1.35
3	A	401	0KX	C6-N1	8.75	1.46	1.35
3	A	401	0KX	PA-O1A	8.75	1.60	1.46
3	A	401	0KX	PB-O2B	-8.61	1.32	1.46
3	F	401	0KX	O4'-C4'	-7.41	1.28	1.45
3	A	401	0KX	O4'-C1'	7.09	1.58	1.42
3	F	401	0KX	O4'-C1'	6.70	1.57	1.42
3	F	401	0KX	C4-N3	6.56	1.46	1.35
3	A	401	0KX	C4-N3	6.08	1.45	1.35
3	A	401	0KX	PG-O3G	-5.72	1.32	1.54
3	A	401	0KX	C2'-C1'	-5.47	1.37	1.52
3	F	401	0KX	C6-C5	4.64	1.48	1.38
3	A	401	0KX	O4'-C4'	-4.38	1.35	1.45
3	F	401	0KX	C2'-C1'	-4.28	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	0KX	PG-O1G	4.15	1.70	1.54
3	A	401	0KX	C2-N3	3.92	1.45	1.38
3	A	401	0KX	PB-O1B	3.46	1.66	1.56
3	A	401	0KX	C5'-C4'	3.43	1.62	1.51
3	A	401	0KX	PA-O2A	-3.36	1.47	1.56
3	A	401	0KX	C6-C5	3.23	1.45	1.38
3	F	401	0KX	C2-N3	3.08	1.44	1.38
3	F	401	0KX	PB-O3B	-3.06	1.55	1.59
3	A	401	0KX	PB-N3A	2.87	1.70	1.63
3	F	401	0KX	C3'-C4'	2.68	1.60	1.53
3	F	401	0KX	C2'-C3'	-2.64	1.45	1.52
3	A	401	0KX	C2'-C3'	-2.60	1.46	1.52
3	F	401	0KX	C1'-N1	-2.55	1.41	1.49
3	F	401	0KX	PA-O1A	2.41	1.50	1.46
3	A	401	0KX	PA-N3A	2.39	1.69	1.63
3	F	401	0KX	PG-O1G	-2.36	1.45	1.54
3	F	401	0KX	PA-N3A	2.20	1.69	1.63
3	A	401	0KX	C5-C4	2.10	1.46	1.41

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	0KX	O2A-PA-O1A	9.06	128.91	109.92
3	F	401	0KX	C2-N3-C4	6.62	123.05	116.34
3	F	401	0KX	C4'-O4'-C1'	-4.72	98.05	109.45
3	A	401	0KX	O1A-PA-N3A	-4.31	105.42	111.77
3	A	401	0KX	C2-N3-C4	4.30	120.70	116.34
3	F	401	0KX	O2A-PA-O1A	3.86	118.02	109.92
3	F	401	0KX	O3G-PG-O1G	3.64	121.54	107.64
3	A	401	0KX	O1B-PB-O2B	3.38	117.01	109.92
3	A	401	0KX	O2B-PB-N3A	3.29	116.62	111.77
3	F	401	0KX	O4'-C1'-C2'	3.17	112.23	106.25
3	F	401	0KX	O4'-C4'-C3'	3.14	113.00	105.67
3	F	401	0KX	O4'-C4'-C5'	-3.00	99.51	109.37
3	A	401	0KX	C3'-C2'-C1'	2.98	110.01	102.54
3	F	401	0KX	O1A-PA-N3A	-2.78	107.67	111.77
3	A	401	0KX	O3B-PB-N3A	-2.72	99.05	106.59
3	A	401	0KX	C4'-O4'-C1'	-2.68	102.99	109.45
3	F	401	0KX	O3'-C3'-C4'	2.48	119.59	110.10
3	F	401	0KX	C2'-C3'-C4'	-2.42	97.71	102.76
3	F	401	0KX	PA-O5'-C5'	-2.29	111.97	120.47
3	F	401	0KX	O3'-C3'-C2'	2.22	118.83	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	0KX	O5'-PA-O1A	-2.02	106.46	114.24

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	0KX	PB-O3B-PG-O1G
3	A	401	0KX	PB-N3A-PA-O5'
3	F	401	0KX	PB-O3B-PG-O1G
3	F	401	0KX	PB-N3A-PA-O1A
3	F	401	0KX	PB-N3A-PA-O5'
3	F	401	0KX	PB-O3B-PG-O2G
3	A	401	0KX	PB-O3B-PG-O3G
3	F	401	0KX	PB-O3B-PG-O3G
3	A	401	0KX	PB-O3B-PG-O2G

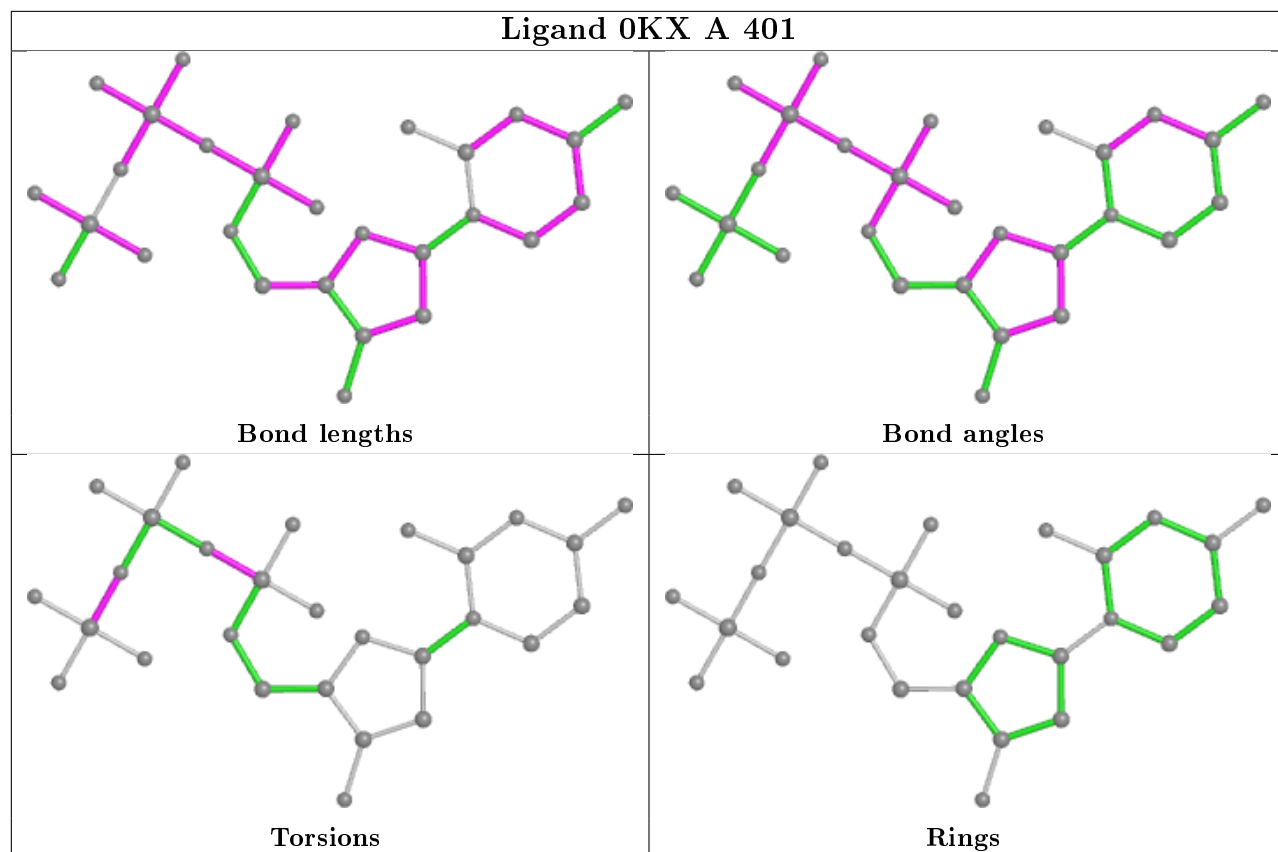
There are no ring outliers.

1 monomer is involved in 1 short contact:

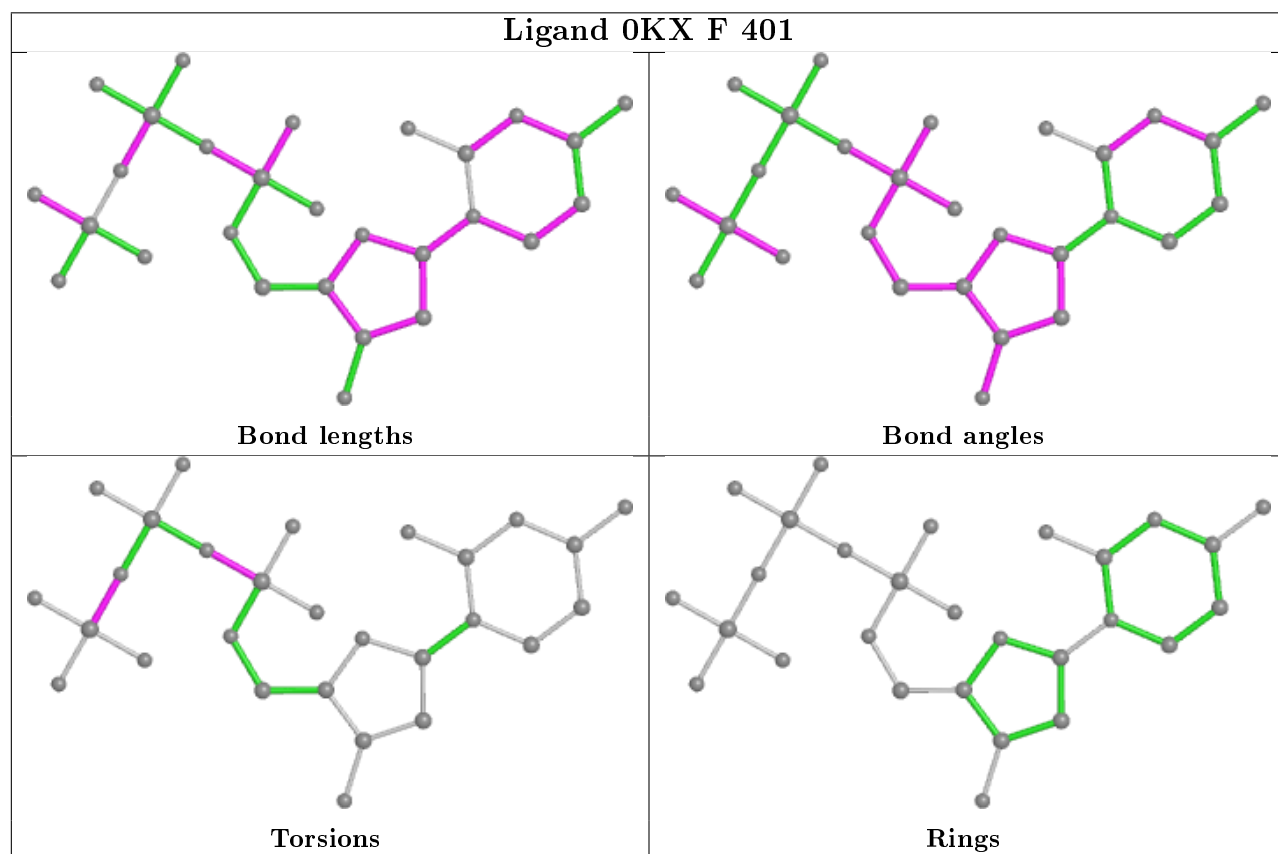
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	401	0KX	1	0

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.

## Ligand 0KX A 401



## Ligand 0KX F 401



## 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%)	0.10	15 (4%) 35 45	19, 36, 65, 106	0
1	F	347/356 (97%)	-0.04	6 (1%) 70 76	22, 37, 60, 95	0
2	B	13/18 (72%)	0.78	2 (15%) 2 2	36, 48, 103, 113	0
2	C	12/18 (66%)	1.00	3 (25%) 0 0	39, 65, 137, 156	0
2	G	11/18 (61%)	-0.01	1 (9%) 9 13	35, 49, 75, 104	0
2	H	8/18 (44%)	0.28	1 (12%) 3 5	38, 50, 87, 93	0
All	All	738/784 (94%)	0.06	28 (3%) 40 49	19, 37, 70, 156	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	862	DG	6.1
1	A	347	VAL	5.9
2	B	850	DG	4.9
1	A	346	ASP	3.9
1	A	196	ALA	3.8
1	A	172	MET	3.7
2	B	849	DG	3.6
1	F	347	VAL	3.5
1	F	175	MET	3.4
2	G	848	DA	3.3
1	A	332	PRO	3.1
1	A	331	ARG	3.0
2	C	864	DC	2.8
1	A	175	MET	2.7
1	A	298	TYR	2.6
1	A	92	GLY	2.6
1	F	177	ASP	2.6
1	F	192	LYS	2.5
1	F	330	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	345	ASP	2.3
1	A	21	ARG	2.3
2	C	863	DT	2.2
1	A	197	MET	2.2
1	F	242	TRP	2.1
1	A	91	MET	2.1
1	A	300	ARG	2.1
2	H	866	DT	2.0
1	A	299	THR	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

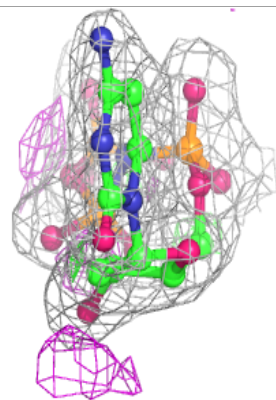
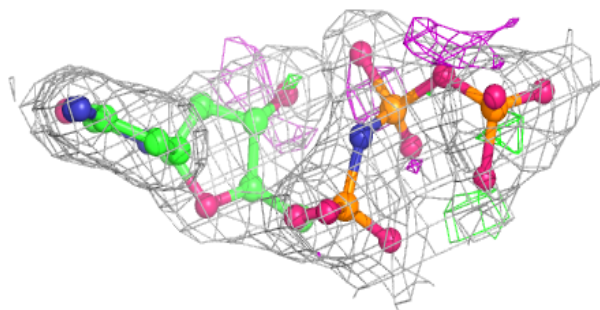
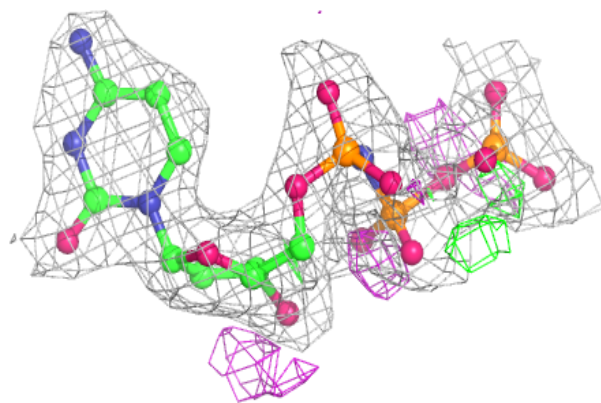
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	MG	A	403	1/1	0.93	0.19	23,23,23,23	0
4	MG	A	402	1/1	0.94	0.10	41,41,41,41	0
4	MG	F	402	1/1	0.95	0.09	45,45,45,45	0
3	0KX	A	401	28/28	0.96	0.13	26,30,31,32	0
4	MG	F	403	1/1	0.96	0.17	25,25,25,25	0
3	0KX	F	401	28/28	0.98	0.12	28,34,41,45	0

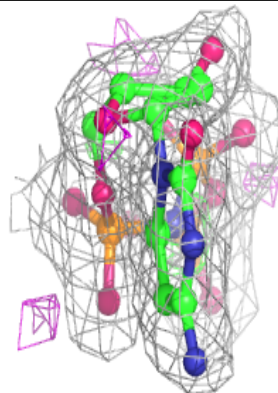
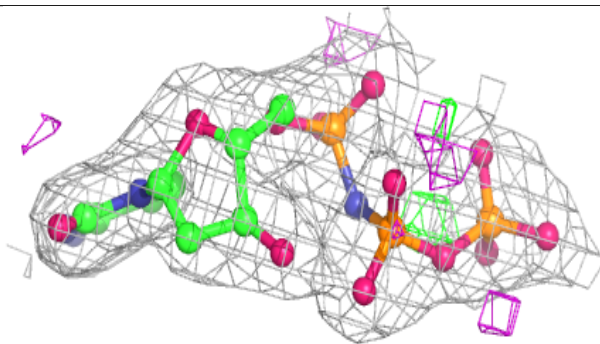
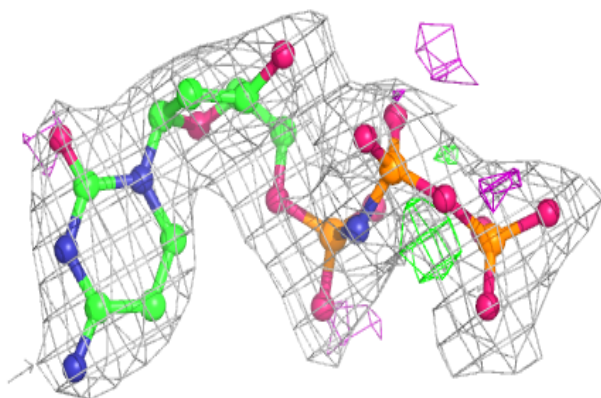
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 0KX 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 0KX 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.