



Full wwPDB X-ray Structure Validation Report i

May 22, 2020 – 05:04 am BST

PDB ID : 6JUL
Title : MsDpo4-DNA complex 1
Authors : Nair, D.T.; Johnson, M.K.
Deposited on : 2019-04-15
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>
with specific help available everywhere you see the i symbol.

The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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

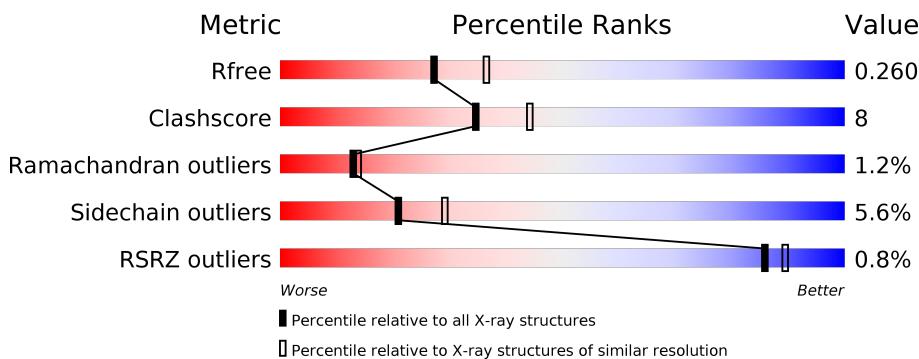
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6472 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.

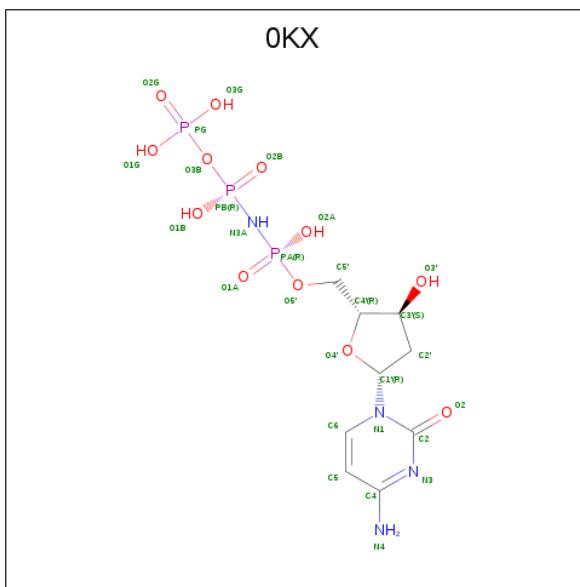
- Molecule 1 is a protein called DNA polymerase IV.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	F	347	Total	C 2645	N 1663	O 465	S 506	Se 3	0	0	0
1	A	347	Total	C 2645	N 1663	O 465	S 506	Se 3	0	0	0

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	H	8	Total	C 163	N 77	O 31	P 47		0	0	0
2	G	11	Total	C 226	N 107	O 40	P 68		0	0	0
2	C	10	Total	C 201	N 95	O 37	P 59		0	0	0
2	B	12	Total	C 248	N 117	O 45	P 74		0	0	0

- Molecule 3 is 2'-deoxy-5'-O-[(R)-hydroxy{|(R)-hydroxy(phosphonoxy)phosphoryl]amino}p phosphoryl]cytidine (three-letter code: 0KX) (formula: C₉H₁₇N₄O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	F	1	28	9	4	12	3	0	0
3	A	1	28	9	4	12	3	0	0

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

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	113	Total O 113 113		0	0
5	H	5	Total O 5 5		0	0
5	G	15	Total O 15 15		0	0
5	A	128	Total O 128 128		0	0
5	C	11	Total O 11 11		0	0

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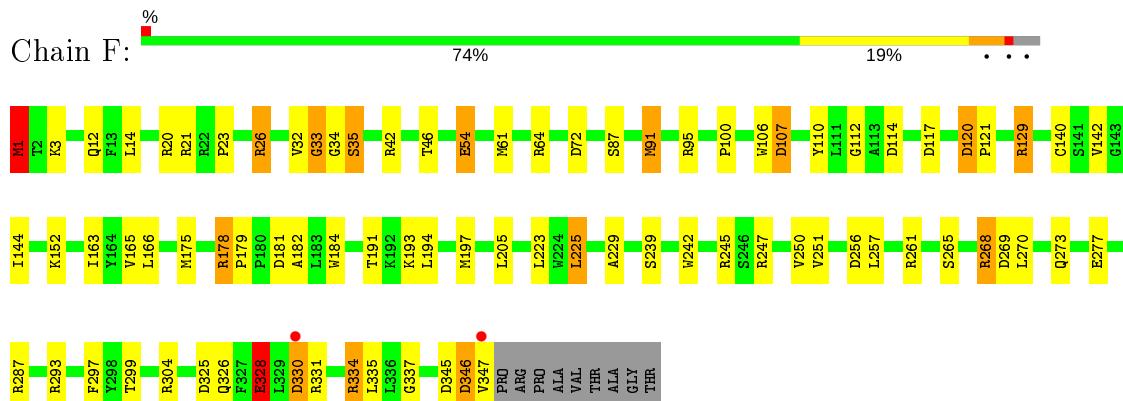
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	12	Total O 12 12	0	0

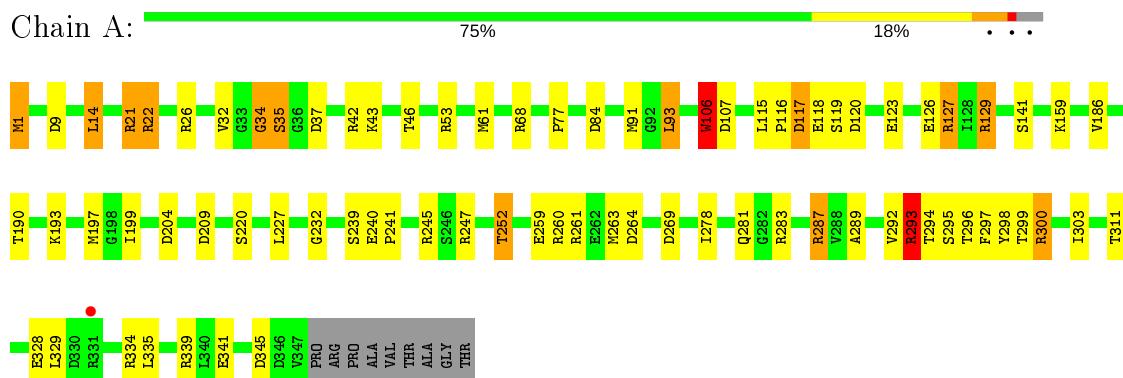
3 Residue-property plots

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.

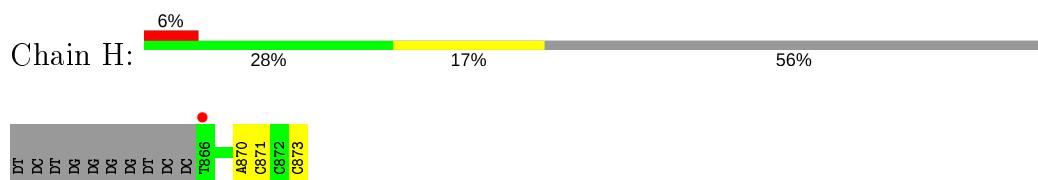
- Molecule 1: DNA polymerase IV



- Molecule 1: DNA polymerase IV



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



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





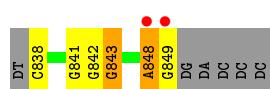
- Molecule 2: DNA ($5'$ -D(P*CP*CP*TP*AP*GP*GP*AP*CP*CP*C)- $3'$)

Chain C:
22% 22% 11% 44%



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

Chain B:
11% 33% 22% 11% 33%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	53.96 Å 80.78 Å 210.52 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.17 – 2.30 64.08 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (70.17-2.30) 100.0 (64.08-2.30)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ ¹	2.22 (at 2.29 Å)	Xtriage
Refinement program	REFMAC 5.8.0155, PHENIX	Depositor
R , R_{free}	0.200 , 0.259 0.202 , 0.260	Depositor DCC
R_{free} test set	2145 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	32.5	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 36.1	EDS
L-test for twinning ²	$< L > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6472	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $< |L| >$, $< L^2 >$ 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	1.25	6/2691 (0.2%)	1.30	32/3659 (0.9%)
1	F	1.22	4/2691 (0.1%)	1.33	34/3659 (0.9%)
2	B	1.25	1/277 (0.4%)	1.53	4/426 (0.9%)
2	C	0.87	0/224	1.34	4/342 (1.2%)
2	G	0.88	0/252	1.20	1/387 (0.3%)
2	H	0.74	0/182	1.10	0/278
All	All	1.20	11/6317 (0.2%)	1.31	75/8751 (0.9%)

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
1	F	0	2
All	All	0	3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	1	MSE	N-CA	8.18	1.62	1.46
2	B	848	DA	P-OP2	-6.37	1.38	1.49
1	A	106	TRP	CB-CG	-6.22	1.39	1.50
1	A	68	ARG	CZ-NH1	5.97	1.40	1.33
1	A	1	MSE	N-CA	5.63	1.57	1.46
1	F	328	GLU	CG-CD	5.55	1.60	1.51
1	F	223	LEU	N-CA	5.41	1.57	1.46
1	A	232	GLY	N-CA	5.36	1.54	1.46
1	A	295	SER	CB-OG	5.20	1.49	1.42
1	A	126	GLU	CG-CD	5.18	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	110	TYR	CZ-OH	-5.09	1.29	1.37

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	848	DA	O5'-P-OP1	13.45	126.84	110.70
1	F	334	ARG	NE-CZ-NH2	-12.78	113.91	120.30
1	F	334	ARG	NE-CZ-NH1	11.48	126.04	120.30
1	F	287	ARG	NE-CZ-NH1	10.53	125.56	120.30
1	A	293	ARG	NE-CZ-NH2	-10.32	115.14	120.30
1	F	129	ARG	NE-CZ-NH2	-9.85	115.38	120.30
1	F	129	ARG	NE-CZ-NH1	9.59	125.09	120.30
1	F	64	ARG	NE-CZ-NH1	9.39	124.99	120.30
1	A	68	ARG	NE-CZ-NH2	-9.32	115.64	120.30
1	A	245	ARG	NE-CZ-NH1	8.45	124.52	120.30
1	F	268	ARG	NE-CZ-NH1	8.21	124.41	120.30
1	A	287	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	A	120	ASP	CB-CG-OD1	7.96	125.47	118.30
1	A	37	ASP	CB-CG-OD1	7.86	125.37	118.30
1	F	178	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	A	107	ASP	CB-CG-OD2	7.66	125.19	118.30
2	B	849	DG	C1'-O4'-C4'	-7.41	102.69	110.10
1	F	33	GLY	N-CA-C	7.29	131.33	113.10
1	F	42	ARG	NE-CZ-NH2	-7.29	116.65	120.30
1	A	107	ASP	OD1-CG-OD2	-7.15	109.71	123.30
1	A	107	ASP	CB-CG-OD1	7.06	124.66	118.30
1	A	129	ARG	NE-CZ-NH2	-7.05	116.78	120.30
1	A	247	ARG	NE-CZ-NH1	-7.01	116.79	120.30
1	F	26	ARG	NE-CZ-NH2	6.98	123.79	120.30
1	A	68	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	A	245	ARG	NE-CZ-NH2	-6.73	116.93	120.30
1	F	245	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	A	37	ASP	CB-CG-OD2	-6.55	112.40	118.30
1	A	61	MSE	CG-SE-CE	6.54	113.29	98.90
1	A	9	ASP	CB-CG-OD2	6.52	124.17	118.30
1	F	95	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	A	14	LEU	CB-CG-CD1	6.36	121.81	111.00
1	F	178	ARG	NE-CZ-NH2	-6.25	117.17	120.30
1	A	247	ARG	NE-CZ-NH2	6.25	123.42	120.30
2	B	843	DG	O5'-P-OP2	-6.13	100.19	105.70
1	A	53	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	F	1	MSE	CG-SE-CE	-6.07	85.54	98.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	166	LEU	CB-CG-CD2	-6.01	100.78	111.00
1	A	93	LEU	CA-CB-CG	-5.96	101.60	115.30
1	F	21	ARG	NE-CZ-NH2	5.90	123.25	120.30
1	A	26	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	F	256	ASP	CB-CG-OD1	5.85	123.57	118.30
1	A	84	ASP	CB-CG-OD1	5.79	123.51	118.30
1	A	293	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	F	91	MSE	CG-SE-CE	5.75	111.55	98.90
2	C	873	DC	O4'-C4'-C3'	5.70	109.42	106.00
1	F	107	ASP	CB-CG-OD1	5.65	123.39	118.30
1	F	268	ARG	CG-CD-NE	5.61	123.59	111.80
1	A	209	ASP	CB-CG-OD1	5.54	123.29	118.30
1	A	328	GLU	N-CA-C	-5.52	96.08	111.00
1	F	325	ASP	CB-CG-OD1	5.50	123.25	118.30
2	G	838	DC	C2'-C3'-O3'	-5.49	94.48	112.60
1	A	204	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	F	42	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	F	61	MSE	CA-CB-CG	-5.43	104.06	113.30
1	F	107	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	106	TRP	N-CA-CB	-5.36	100.95	110.60
1	A	1	MSE	N-CA-CB	5.36	120.25	110.60
1	A	22	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	F	20	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	F	21	ARG	NE-CZ-NH1	-5.33	117.63	120.30
1	F	261	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	1	MSE	CB-CG-SE	5.30	128.61	112.70
2	C	871	DC	O5'-P-OP1	-5.27	100.96	105.70
1	F	120	ASP	CB-CG-OD1	5.24	123.02	118.30
2	C	872	DC	C1'-O4'-C4'	-5.22	104.88	110.10
1	F	14	LEU	CB-CG-CD1	5.21	119.86	111.00
1	F	107	ASP	OD1-CG-OD2	-5.17	113.48	123.30
2	C	864	DC	N1-C1'-C2'	5.13	122.35	112.60
1	F	117	ASP	CB-CG-OD1	5.11	122.90	118.30
1	A	269	ASP	CB-CG-OD1	5.08	122.87	118.30
2	B	849	DG	OP1-P-OP2	5.06	127.19	119.60
1	F	225	LEU	CB-CG-CD1	5.05	119.58	111.00
1	A	21	ARG	NE-CZ-NH2	5.03	122.81	120.30
1	F	54	GLU	CA-CB-CG	5.02	124.45	113.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	106	TRP	Peptide
1	F	106	TRP	Peptide
1	F	330	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	2659	46	0
1	F	2645	0	2659	41	0
2	B	248	0	136	10	0
2	C	201	0	111	4	0
2	G	226	0	125	5	0
2	H	163	0	89	3	0
3	A	28	0	15	0	0
3	F	28	0	14	1	0
4	A	2	0	0	0	0
4	F	2	0	0	0	0
5	A	128	0	0	9	0
5	B	12	0	0	0	0
5	C	11	0	0	1	0
5	F	113	0	0	2	0
5	G	15	0	0	0	0
5	H	5	0	0	0	0
All	All	6472	0	5808	100	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 (100) 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:194:LEU:HA	1:F:197:MSE:HE3	1.55	0.89
1:F:268:ARG:NH1	1:F:269:ASP:OD1	2.10	0.84
1:A:300:ARG:O	5:A:501:HOH:O	1.98	0.82
1:F:193:LYS:CE	2:B:838:DC:H5	1.93	0.81
2:C:870:DA:H2"	2:C:871:DC:H5"	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:ARG:HD3	1:A:341:GLU:OE1	1.84	0.77
1:A:252:THR:HG22	1:A:335:LEU:HD12	1.69	0.74
1:F:23:PRO:O	1:F:26:ARG:NH1	2.21	0.72
1:A:293:ARG:HB3	1:A:335:LEU:HB3	1.73	0.71
1:F:193:LYS:HE3	2:B:838:DC:H5	1.55	0.70
1:F:304:ARG:NH2	1:F:326:GLN:OE1	2.23	0.70
1:F:328:GLU:CD	1:F:328:GLU:H	1.95	0.70
1:A:240:GLU:HG3	1:A:241:PRO:HD2	1.74	0.69
1:A:116:PRO:O	1:A:117:ASP:HB2	1.94	0.67
1:A:197:MSE:HE2	1:A:199:ILE:HD12	1.77	0.67
2:H:870:DA:H2"	2:H:871:DC:H5'	1.79	0.65
1:F:193:LYS:HE3	2:B:838:DC:C5	2.33	0.62
1:F:193:LYS:NZ	2:B:838:DC:H5	1.98	0.62
1:A:292:VAL:N	5:A:501:HOH:O	2.29	0.62
2:C:870:DA:N7	5:C:901:HOH:O	2.31	0.61
2:G:838:DC:H2'	2:G:839:DT:C6	2.35	0.61
1:A:263:MSE:HE1	1:A:329:LEU:HD22	1.83	0.60
1:A:293:ARG:HD3	1:A:299:THR:OG1	2.01	0.60
1:A:339:ARG:HD3	5:A:556:HOH:O	2.00	0.60
1:F:194:LEU:HA	1:F:197:MSE:CE	2.28	0.60
1:A:281:GLN:NE2	5:A:504:HOH:O	2.34	0.59
1:F:46:THR:HG21	5:F:520:HOH:O	2.02	0.59
2:B:842:DG:H2"	2:B:843:DG:H5"	1.84	0.59
1:A:294:THR:CG2	1:A:298:TYR:HB3	2.35	0.57
1:F:152:LYS:HG2	1:F:184:TRP:CD1	2.40	0.56
1:F:152:LYS:HE3	1:F:184:TRP:NE1	2.22	0.54
1:A:32:VAL:O	1:A:46:THR:HG22	2.07	0.54
1:A:186:VAL:O	5:A:502:HOH:O	2.18	0.54
1:A:252:THR:HG23	2:B:841:DG:OP2	2.08	0.53
1:A:34:GLY:HA3	1:A:43:LYS:HD2	1.90	0.53
1:F:345:ASP:O	1:F:346:ASP:HB2	2.10	0.52
1:A:123:GLU:HB3	1:A:127:ARG:NH2	2.24	0.52
1:A:292:VAL:O	5:A:501:HOH:O	2.19	0.52
1:F:144:ILE:HD12	1:F:165:VAL:HG22	1.92	0.52
1:A:287:ARG:HB2	1:A:341:GLU:HB2	1.91	0.51
1:A:252:THR:HG21	5:A:565:HOH:O	2.11	0.51
2:H:870:DA:C2'	2:H:871:DC:H5'	2.40	0.51
1:A:42:ARG:HH21	1:A:334:ARG:HG3	1.74	0.51
1:F:178:ARG:HB3	1:F:179:PRO:HD2	1.92	0.51
1:F:152:LYS:HE3	1:F:184:TRP:HE1	1.75	0.51
1:A:294:THR:HG22	1:A:298:TYR:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:MSE:CE	1:A:329:LEU:HD22	2.41	0.50
1:F:87:SER:O	1:F:91:MSE:HG2	2.11	0.50
2:G:838:DC:H2'	2:G:839:DT:H6	1.75	0.50
1:F:242:TRP:CZ2	2:G:844:DT:H5"	2.47	0.49
1:A:240:GLU:HG3	1:A:241:PRO:CD	2.41	0.49
1:F:293:ARG:HB3	1:F:335:LEU:HB3	1.94	0.49
1:A:260:ARG:NH1	1:A:264:ASP:OD1	2.45	0.49
1:A:289:ALA:HB2	1:A:303:ILE:HD12	1.94	0.49
1:F:3:LYS:HG2	1:F:114:ASP:OD1	2.12	0.49
1:A:42:ARG:NH2	5:A:506:HOH:O	2.45	0.48
2:G:843:DG:H2"	2:G:844:DT:H5'	1.96	0.48
1:F:194:LEU:HD23	1:F:197:MSE:HE1	1.95	0.48
1:F:129:ARG:HD2	1:F:140:CYS:O	2.13	0.48
1:F:251:VAL:HG23	1:F:270:LEU:HD21	1.96	0.48
1:F:293:ARG:HD3	1:F:299:THR:OG1	2.14	0.48
1:A:345:ASP:N	1:A:345:ASP:OD1	2.41	0.48
1:F:205:LEU:HD23	1:F:229:ALA:HB2	1.96	0.48
1:A:294:THR:HG22	1:A:298:TYR:H	1.79	0.47
1:F:181:ASP:HB3	1:F:191:THR:OG1	2.13	0.47
1:A:294:THR:HG23	1:A:296:THR:H	1.79	0.47
1:F:175:MSE:HE1	1:F:182:ALA:HB1	1.95	0.47
1:F:26:ARG:HG2	1:F:26:ARG:HH11	1.79	0.47
1:F:273:GLN:O	1:F:277:GLU:HG3	2.15	0.47
1:A:252:THR:HG23	2:B:841:DG:P	2.55	0.47
1:A:116:PRO:HD2	1:A:119:SER:HB3	1.96	0.47
1:F:194:LEU:HD23	1:F:197:MSE:CE	2.44	0.47
1:F:250:VAL:HG12	1:F:337:GLY:HA3	1.97	0.47
3:F:401:0KX:H15	3:F:401:0KX:O5'	2.15	0.46
2:G:838:DC:C4	1:A:193:LYS:HG3	2.50	0.46
1:A:260:ARG:NH2	1:A:329:LEU:HD12	2.31	0.46
1:F:142:VAL:O	1:F:163:ILE:HA	2.16	0.46
2:B:838:DC:O2	2:B:838:DC:O4'	2.32	0.45
1:A:186:VAL:HG13	1:A:190:THR:HB	1.98	0.45
1:A:141:SER:HB2	1:A:159:LYS:HD3	1.99	0.45
1:A:278:ILE:HB	1:A:283:ARG:HB2	1.99	0.45
1:A:115:LEU:HA	1:A:116:PRO:HD3	1.86	0.44
1:A:35:SER:HA	1:A:77:PRO:HB3	1.99	0.44
2:B:848:DA:H2'	2:B:848:DA:OP2	2.18	0.44
2:C:871:DC:H2"	2:C:872:DC:O4'	2.18	0.43
1:F:152:LYS:NZ	2:H:873:DC:OP1	2.42	0.43
1:F:120:ASP:OD1	1:F:121:PRO:HD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:TYR:CE2	1:A:300:ARG:HD3	2.54	0.43
1:F:100:PRO:HD2	1:F:112:GLY:O	2.18	0.43
1:F:32:VAL:O	1:F:46:THR:HG22	2.19	0.42
1:A:294:THR:HG21	1:A:298:TYR:HB3	2.02	0.42
1:A:197:MSE:HE2	1:A:199:ILE:CD1	2.46	0.42
1:A:141:SER:CB	1:A:159:LYS:HD3	2.49	0.42
1:F:1:MSE:HE1	1:F:3:LYS:HE2	2.01	0.42
1:F:12:GLN:HG3	1:F:12:GLN:O	2.20	0.42
1:A:129:ARG:HB3	1:A:129:ARG:CZ	2.50	0.41
1:A:22:ARG:HD3	5:A:531:HOH:O	2.21	0.41
2:C:867:DA:C2	2:B:848:DA:C2	3.09	0.41
1:F:107:ASP:HB3	5:F:577:HOH:O	2.21	0.40
1:F:26:ARG:HG2	1:F:26:ARG:NH1	2.35	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%)	330 (96%)	13 (4%)	2 (1%)	25 31
1	F	345/356 (97%)	334 (97%)	5 (1%)	6 (2%)	9 8
All	All	690/712 (97%)	664 (96%)	18 (3%)	8 (1%)	13 14

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	117	ASP
1	F	35	SER
1	A	34	GLY
1	F	330	ASP
1	F	346	ASP

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Mol	Chain	Res	Type
1	F	33	GLY
1	F	331	ARG
1	F	34	GLY

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	284/282 (101%)	265 (93%)	19 (7%)	16 21
1	F	284/282 (101%)	271 (95%)	13 (5%)	27 38
All	All	568/564 (101%)	536 (94%)	32 (6%)	21 29

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	1	MSE
1	F	35	SER
1	F	54	GLU
1	F	72	ASP
1	F	225	LEU
1	F	239	SER
1	F	247	ARG
1	F	257	LEU
1	F	265	SER
1	F	297	PHE
1	F	328	GLU
1	F	334	ARG
1	F	347	VAL
1	A	1	MSE
1	A	14	LEU
1	A	21	ARG
1	A	35	SER
1	A	91	MSE
1	A	93	LEU
1	A	106	TRP

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Mol	Chain	Res	Type
1	A	118	GLU
1	A	127	ARG
1	A	220	SER
1	A	227	LEU
1	A	239	SER
1	A	252	THR
1	A	259	GLU
1	A	261	ARG
1	A	293	ARG
1	A	297	PHE
1	A	300	ARG
1	A	311	THR

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	0KX	F	401	4	26,29,29	1.33	2 (7%)	33,45,45	2.57	6 (18%)
3	0KX	A	401	4	26,29,29	1.61	2 (7%)	33,45,45	2.29	11 (33%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	0KX	PB-O2B	5.61	1.55	1.46
3	F	401	0KX	PB-O2B	3.85	1.52	1.46
3	A	401	0KX	PG-O2G	3.41	1.61	1.50
3	F	401	0KX	C6-N1	3.37	1.40	1.35

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	401	0KX	C2-N3-C4	8.71	125.17	116.34
3	F	401	0KX	O1A-PA-N3A	-6.99	101.47	111.77
3	A	401	0KX	O2A-PA-O1A	5.70	121.86	109.92
3	A	401	0KX	O2B-PB-N3A	-5.62	103.50	111.77
3	F	401	0KX	O2A-PA-O1A	5.49	121.43	109.92
3	A	401	0KX	O1A-PA-N3A	-4.11	105.71	111.77
3	A	401	0KX	C2-N3-C4	3.57	119.96	116.34
3	F	401	0KX	O1G-PG-O2G	3.34	123.74	110.68
3	A	401	0KX	O1B-PB-O2B	3.24	116.71	109.92
3	A	401	0KX	O5'-PA-O1A	-2.99	102.73	114.24
3	F	401	0KX	C6-N1-C2	-2.97	116.48	121.20
3	A	401	0KX	C6-N1-C2	-2.91	116.57	121.20
3	A	401	0KX	C2'-C1'-N1	-2.89	107.59	114.27
3	A	401	0KX	O3'-C3'-C4'	2.80	120.81	110.10
3	F	401	0KX	C2'-C1'-N1	-2.33	108.91	114.27
3	A	401	0KX	O1B-PB-O3B	2.30	112.32	104.64
3	A	401	0KX	O3B-PG-O2G	-2.17	99.16	111.19

There are no chirality outliers.

All (10) torsion outliers are listed below:

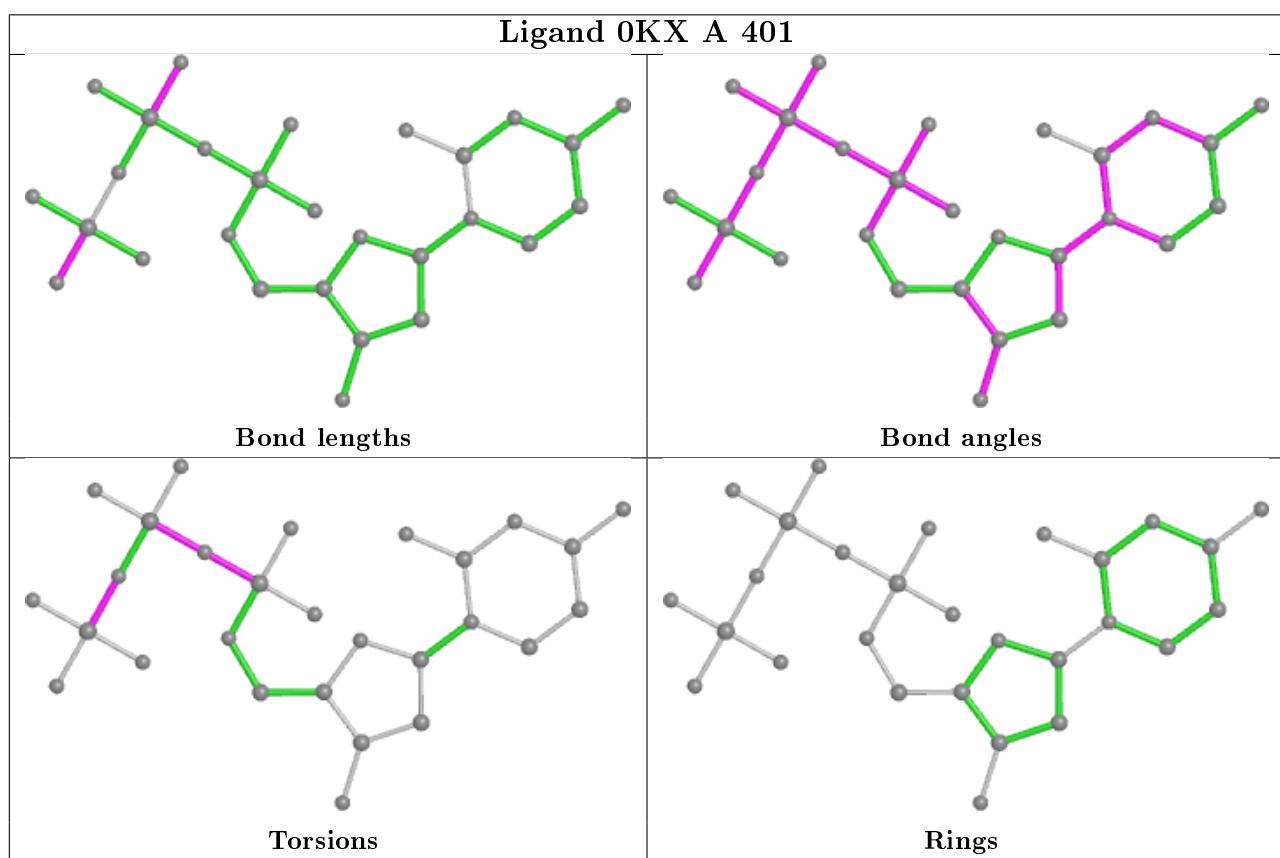
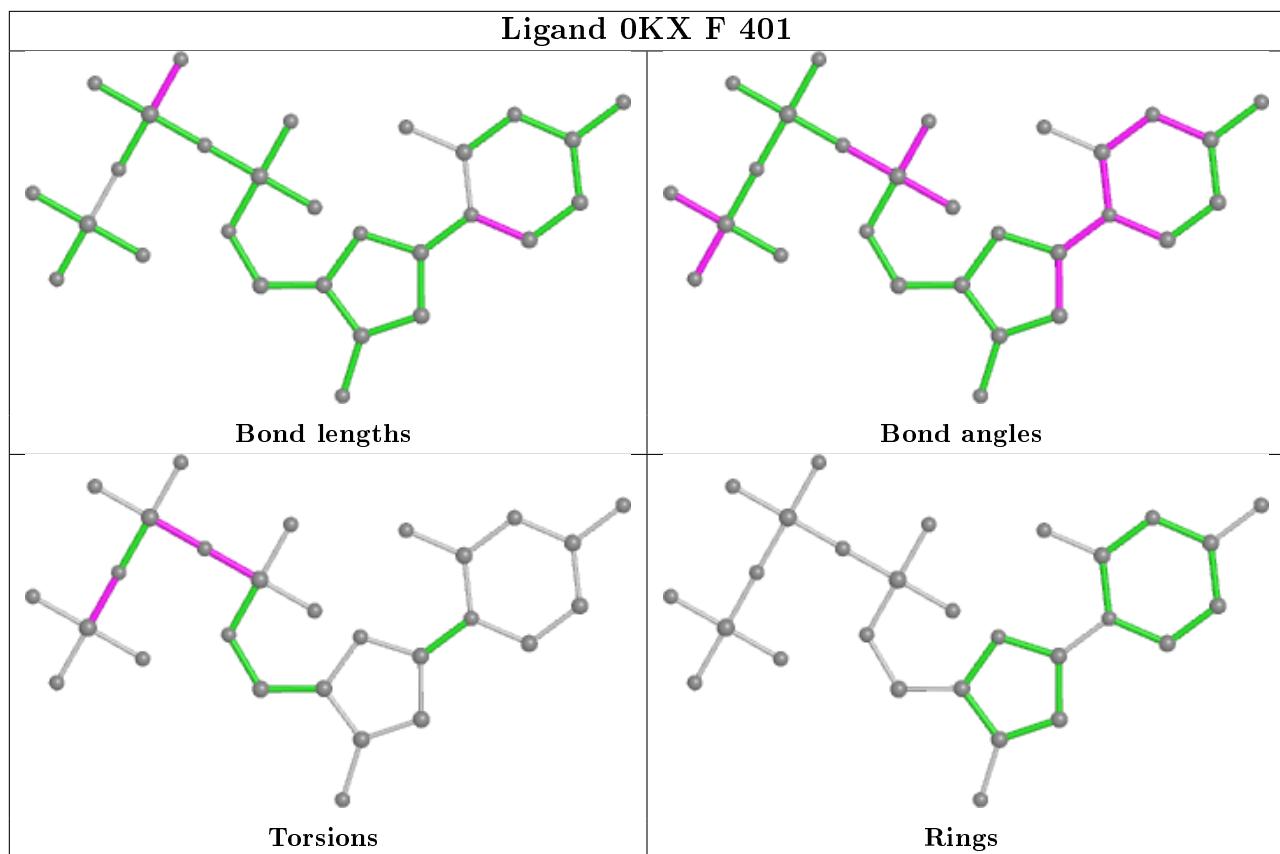
Mol	Chain	Res	Type	Atoms
3	F	401	0KX	PB-O3B-PG-O1G
3	F	401	0KX	PA-N3A-PB-O2B
3	A	401	0KX	PA-N3A-PB-O2B
3	A	401	0KX	PB-N3A-PA-O5'
3	A	401	0KX	PB-O3B-PG-O2G
3	F	401	0KX	PB-N3A-PA-O5'
3	F	401	0KX	PB-O3B-PG-O3G
3	A	401	0KX	PB-O3B-PG-O1G
3	A	401	0KX	PB-O3B-PG-O3G
3	F	401	0KX	PB-O3B-PG-O2G

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.



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

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

6 Fit of model and data [\(i\)](#)

6.1 Protein, DNA and RNA chains [\(i\)](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	339/356 (95%)	-0.21	1 (0%)	94 96	18, 32, 63, 96	0
1	F	339/356 (95%)	-0.30	2 (0%)	89 92	18, 31, 54, 91	0
2	B	12/18 (66%)	0.37	2 (16%)	1 2	31, 45, 102, 121	0
2	C	10/18 (55%)	0.36	0	100 100	34, 60, 77, 107	0
2	G	11/18 (61%)	-0.29	0	100 100	27, 40, 75, 111	0
2	H	8/18 (44%)	0.34	1 (12%)	3 5	30, 42, 84, 96	0
All	All	719/784 (91%)	-0.23	6 (0%)	86 89	18, 32, 63, 121	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	331	ARG	5.4
1	F	330	ASP	3.8
2	B	848	DA	3.3
2	B	849	DG	3.2
2	H	866	DT	2.7
1	F	347	VAL	2.4

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 [\(i\)](#)

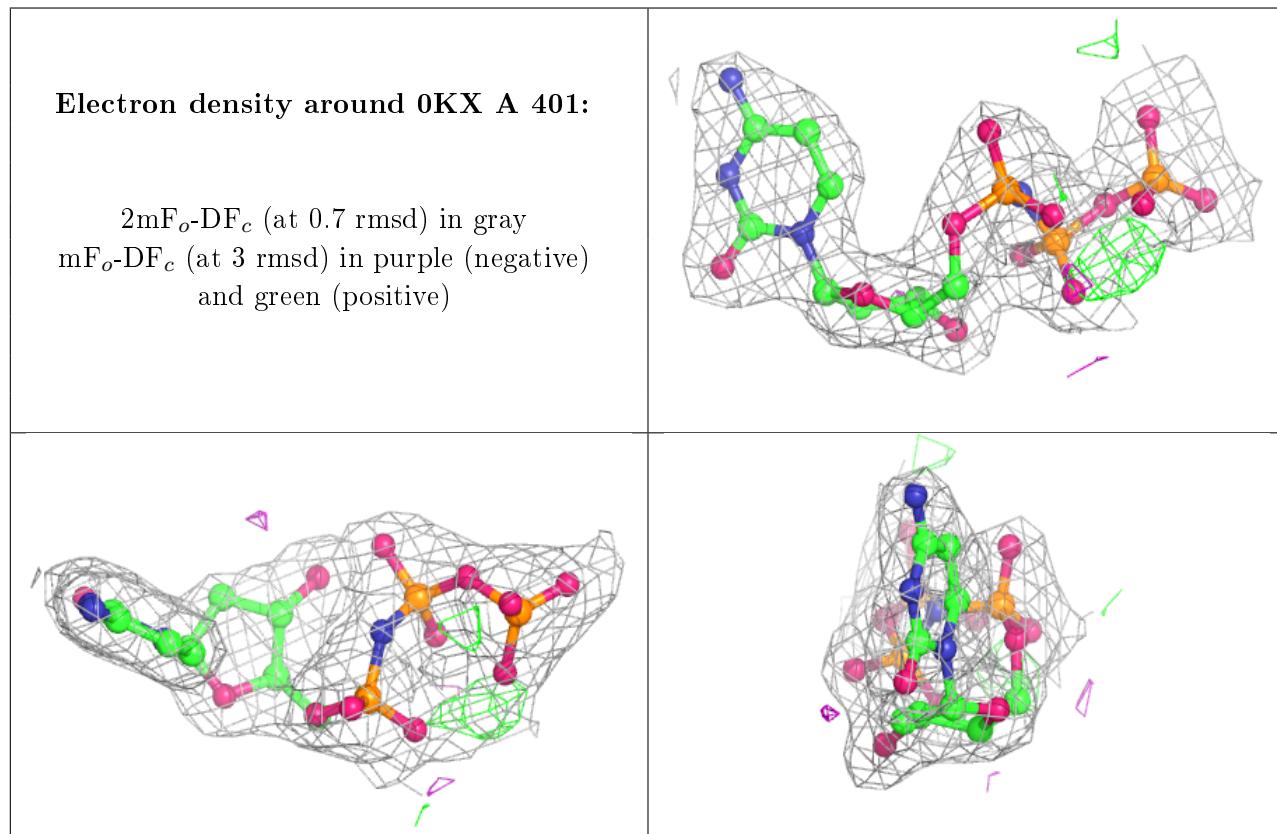
There are no carbohydrates in this entry.

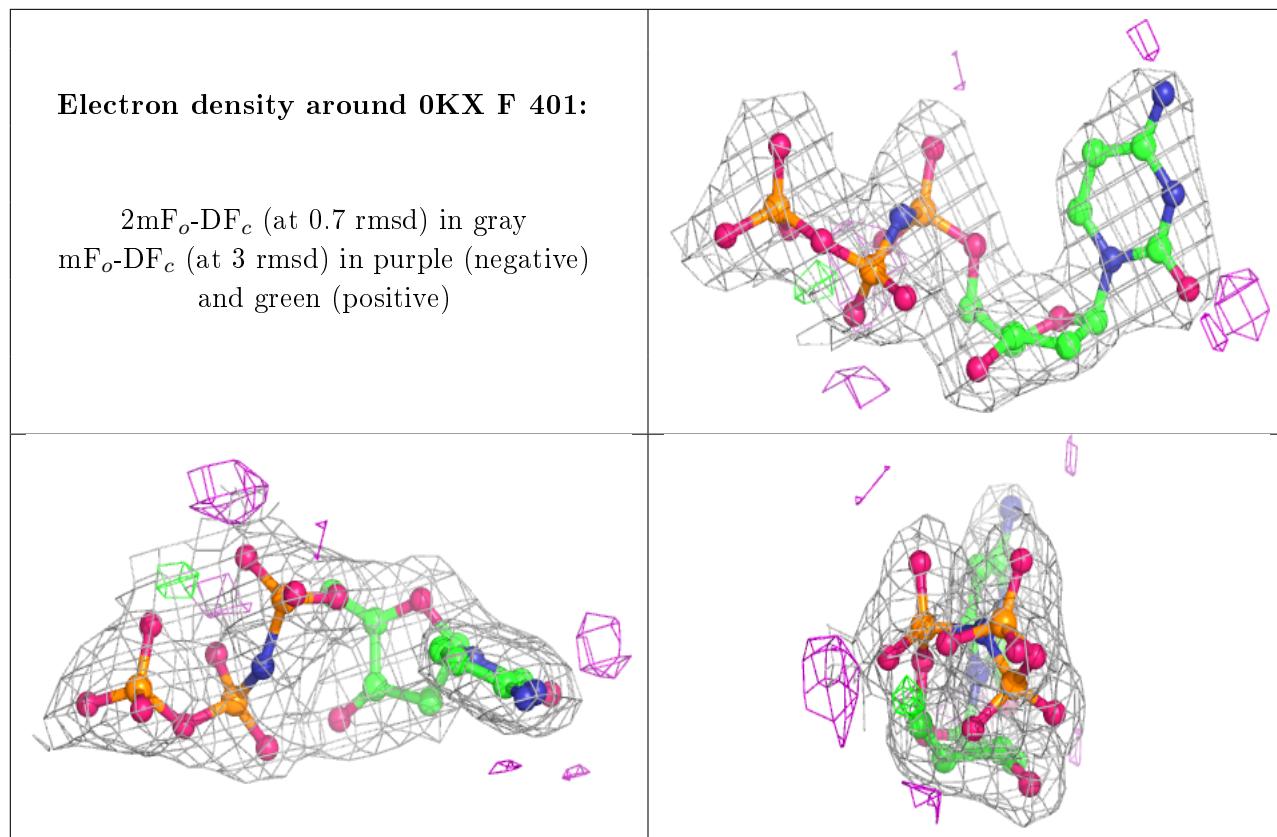
6.4 Ligands [\(i\)](#)

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MG	F	402	1/1	0.87	0.16	32,32,32,32	0
4	MG	A	402	1/1	0.88	0.22	38,38,38,38	0
4	MG	A	403	1/1	0.96	0.24	27,27,27,27	0
4	MG	F	403	1/1	0.97	0.17	25,25,25,25	0
3	0KX	A	401	28/28	0.98	0.13	25,26,28,28	0
3	0KX	F	401	28/28	0.98	0.12	25,27,31,33	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.