



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:28 AM UTC

PDB ID : 6JUL / pdb_00006jul
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

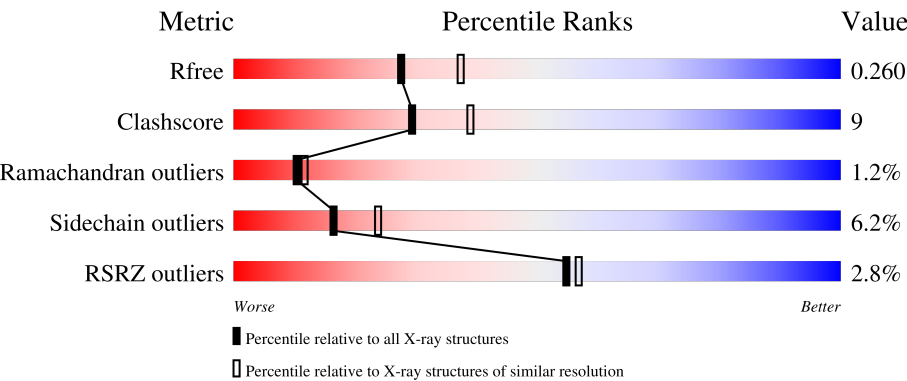
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 of 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 $\leq 5\%$. 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	3% 72% 21% . .
1	F	356	2% 73% 19% . . .
2	B	18	6% 33% 28% 6% 33%
2	C	18	6% 22% 28% 6% 44%
2	G	18	6% 33% 22% 6% 39%

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Mol	Chain	Length	Quality of chain
2	H	18	28% 11% 6% 56%

2 Entry composition

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.

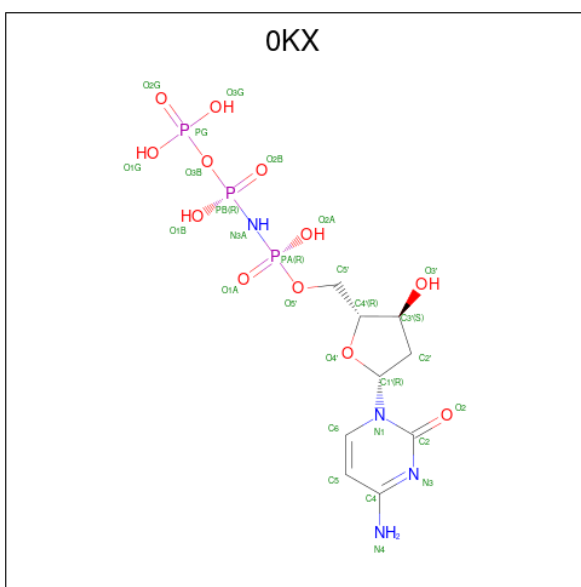
- Molecule 1 is a protein called DNA polymerase IV.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	F	347	Total	C	N	O	S	Se	0	0	0
			2645	1663	465	506	3	8			
1	A	347	Total	C	N	O	S	Se	0	0	0
			2645	1663	465	506	3	8			

- 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	N	O	P	0	0	0
			163	77	31	47	8			
2	G	11	Total	C	N	O	P	0	0	0
			226	107	40	68	11			
2	C	10	Total	C	N	O	P	0	0	0
			201	95	37	59	10			
2	B	12	Total	C	N	O	P	0	0	0
			248	117	45	74	12			

- Molecule 3 is 2'-deoxy-5'-O-[(R)-hydroxy{[(R)-hydroxy(phosphonooxy)phosphoryl]amino}phosphoryl]cytidine (CCD ID: 0KX) (formula: C₉H₁₇N₄O₁₂P₃).



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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	2	Total Mg 2 2	0	0
4	A	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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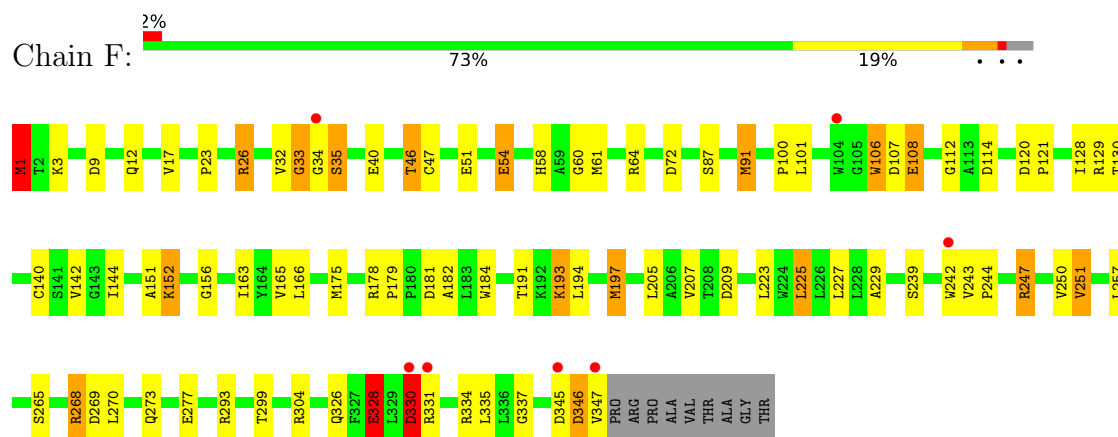
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	12	Total	O	0	0
			12	12		

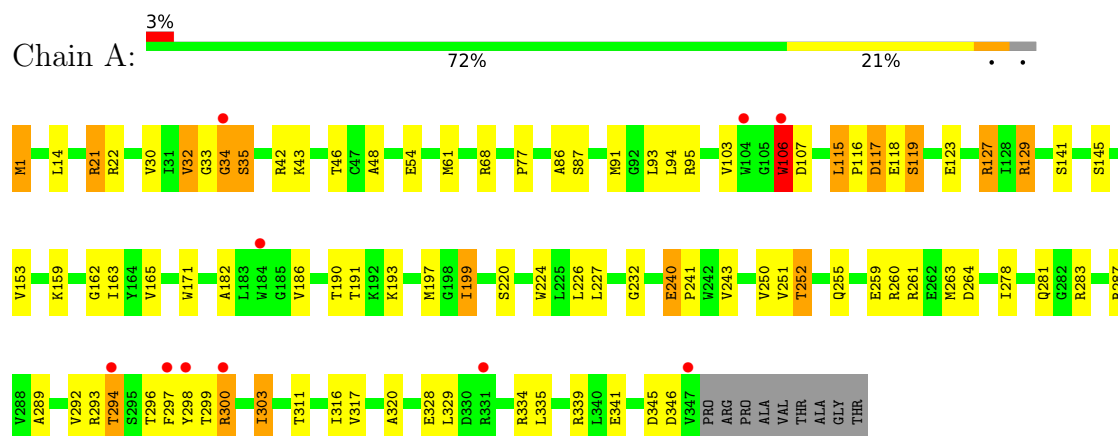
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

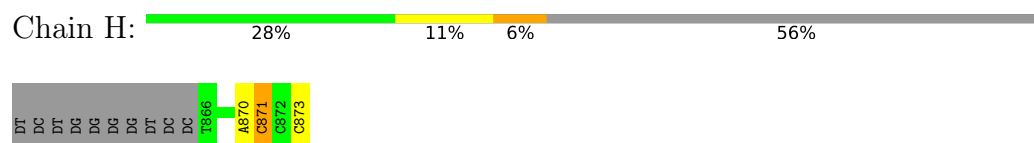
• Molecule 1: DNA polymerase IV



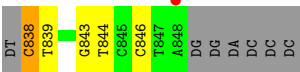
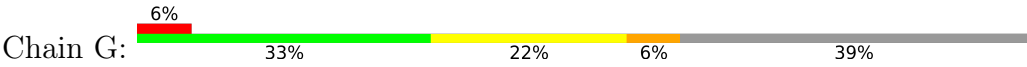
• Molecule 1: DNA polymerase IV



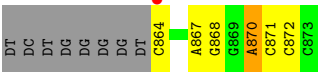
• Molecule 2: DNA (5'-D(P*CP*CP*TP*AP*GP*GP*AP*CP*CP*C)-3')



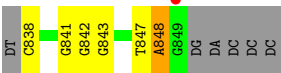
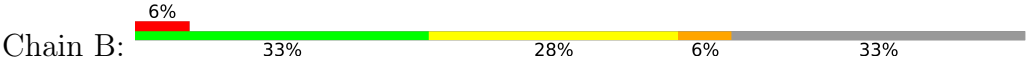
• Molecule 2: DNA (5'-D(P*CP*CP*TP*AP*GP*GP*AP*CP*CP*C)-3')



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	53.96Å 80.78Å 210.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.17 – 2.30 70.17 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (70.17-2.30) 100.0 (70.17-2.30)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 2.29Å)	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)	0.36 , 33.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	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 $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.62	26/2691 (1.0%)	1.51	22/3659 (0.6%)
1	F	1.58	17/2691 (0.6%)	1.51	24/3659 (0.7%)
2	B	0.85	1/277 (0.4%)	1.34	3/426 (0.7%)
2	C	0.65	0/224	1.33	3/342 (0.9%)
2	G	0.61	0/252	1.33	2/387 (0.5%)
2	H	0.57	0/182	1.18	1/278 (0.4%)
All	All	1.50	44/6317 (0.7%)	1.48	55/8751 (0.6%)

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 (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	232	GLY	N-CA	9.57	1.54	1.44
1	F	1	MSE	N-CA	8.67	1.62	1.46
1	F	223	LEU	N-CA	8.48	1.57	1.46
1	A	182	ALA	C-O	-7.20	1.14	1.24
1	A	119	SER	N-CA	-7.00	1.36	1.45
1	A	86	ALA	CA-C	6.92	1.62	1.52
1	F	151	ALA	CA-C	6.32	1.60	1.52
1	A	303	ILE	CA-C	6.29	1.60	1.52
1	A	30	VAL	C-O	6.25	1.30	1.24
1	A	171	TRP	N-CA	-6.20	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	145	SER	C-O	-6.12	1.19	1.24
1	F	128	ILE	CA-C	6.08	1.60	1.52
1	F	101	LEU	CA-C	-6.04	1.45	1.52
1	F	130	THR	N-CA	6.00	1.53	1.46
1	A	1	MSE	N-CA	5.98	1.57	1.46
1	F	247	ARG	CA-C	-5.96	1.45	1.52
1	F	251	VAL	CA-C	5.96	1.59	1.52
1	A	94	LEU	CA-C	5.96	1.60	1.52
1	A	224	TRP	C-O	5.88	1.31	1.24
1	A	199	ILE	C-O	-5.85	1.17	1.24
1	A	68	ARG	CZ-NH1	5.76	1.40	1.32
1	F	244	PRO	CA-C	5.60	1.60	1.52
1	F	330	ASP	CA-C	5.59	1.60	1.52
1	A	103	VAL	C-O	-5.58	1.17	1.24
1	F	166	LEU	CA-C	5.54	1.58	1.52
1	A	153	VAL	N-CA	5.49	1.53	1.46
1	A	129	ARG	N-CA	5.48	1.52	1.46
1	A	48	ALA	CA-C	-5.47	1.46	1.52
1	A	33	GLY	N-CA	5.40	1.51	1.45
1	A	320	ALA	CA-C	5.33	1.59	1.52
1	F	47	CYS	N-CA	-5.33	1.40	1.46
1	A	54	GLU	C-O	-5.22	1.17	1.24
1	F	156	GLY	N-CA	5.20	1.52	1.45
1	F	58	HIS	CA-C	5.20	1.58	1.52
1	A	255	GLN	N-CA	5.18	1.52	1.46
1	A	191	THR	N-CA	-5.16	1.40	1.46
2	B	848	DA	P-OP2	-5.16	1.38	1.48
1	F	9	ASP	CA-C	5.08	1.58	1.52
1	A	32	VAL	C-O	-5.08	1.17	1.24
1	A	224	TRP	CA-C	5.07	1.59	1.52
1	F	227	LEU	N-CA	5.05	1.52	1.46
1	A	317	VAL	CA-CB	5.04	1.60	1.54
1	A	226	LEU	C-O	5.04	1.29	1.24
1	F	207	VAL	CA-C	-5.00	1.46	1.53

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	838	DC	C2'-C3'-O3'	-11.35	94.48	111.50
1	F	40	GLU	CA-C-N	-10.04	110.24	120.98
1	F	40	GLU	C-N-CA	-10.04	110.24	120.98
1	F	33	GLY	N-CA-C	7.66	131.33	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	107	ASP	N-CA-C	-7.49	105.05	114.56
1	A	87	SER	N-CA-C	-7.10	103.47	111.14
1	A	328	GLU	N-CA-C	-7.06	96.08	108.23
1	A	243	VAL	CA-C-N	-7.03	112.52	119.76
1	A	243	VAL	C-N-CA	-7.03	112.52	119.76
1	F	108	GLU	N-CA-C	6.72	119.15	109.14
2	C	870	DA	C4'-C3'-O3'	-6.63	100.05	110.00
1	A	61	MSE	CG-SE-CE	6.53	113.29	98.92
1	F	328	GLU	N-CA-C	-6.46	100.09	109.59
1	A	316	ILE	N-CA-C	6.36	117.11	110.62
1	F	51	GLU	N-CA-C	-6.33	104.46	111.36
2	B	847	DT	C4'-C3'-O3'	-6.33	100.50	110.00
1	A	107	ASP	N-CA-CB	-6.26	102.67	111.00
1	F	193	LYS	N-CA-C	-6.24	104.39	111.07
2	B	847	DT	O3'-P-O5'	-6.20	94.69	104.00
1	F	1	MSE	CG-SE-CE	-6.08	85.54	98.92
1	A	106	TRP	N-CA-CB	-6.02	100.95	110.28
2	B	848	DA	O5'-P-OP1	5.95	126.84	109.00
1	A	232	GLY	N-CA-C	-5.90	103.26	112.58
2	C	864	DC	N1-C1'-C2'	5.90	122.35	113.50
1	F	334	ARG	NE-CZ-NH2	-5.88	113.91	119.20
1	F	91	MSE	CG-SE-CE	5.74	111.55	98.92
1	F	152	LYS	N-CA-C	-5.74	104.94	111.14
1	A	1	MSE	N-CA-CB	5.73	120.25	110.50
1	A	251	VAL	CA-C-N	-5.70	114.85	122.72
1	A	251	VAL	C-N-CA	-5.70	114.85	122.72
1	A	345	ASP	N-CA-C	5.58	117.04	111.07
2	C	868	DG	C2'-C3'-O3'	-5.54	103.20	111.50
1	F	243	VAL	N-CA-C	5.53	113.02	107.55
1	A	107	ASP	OD1-CG-OD2	-5.50	109.71	122.90
1	A	115	LEU	N-CA-C	5.48	117.57	109.62
2	G	846	DC	C2'-C3'-O3'	5.47	119.70	111.50
1	F	197	MSE	N-CA-C	-5.42	105.89	112.88
1	A	32	VAL	N-CA-C	5.42	117.10	108.87
1	F	225	LEU	CA-C-N	5.40	127.46	120.44
1	F	225	LEU	C-N-CA	5.40	127.46	120.44
1	F	60	GLY	N-CA-C	-5.37	107.60	114.37
1	A	1	MSE	CB-CG-SE	5.30	128.61	112.70
1	F	33	GLY	O-C-N	-5.28	115.83	122.70
1	F	268	ARG	CG-CD-NE	5.27	123.59	112.00
1	A	346	ASP	N-CA-C	5.23	118.71	111.55
1	F	209	ASP	N-CA-C	5.23	116.00	109.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	871	DC	C5'-C4'-O4'	-5.19	101.61	109.40
1	F	54	GLU	CA-CB-CG	5.17	124.45	114.10
1	A	21	ARG	N-CA-C	-5.16	107.03	113.38
1	F	17	VAL	N-CA-C	-5.13	105.54	110.72
1	A	165	VAL	CA-C-N	-5.11	115.56	122.77
1	A	165	VAL	C-N-CA	-5.11	115.56	122.77
1	F	26	ARG	NE-CZ-NH2	5.10	123.79	119.20
1	F	54	GLU	N-CA-C	-5.03	106.25	112.38
1	F	61	MSE	CA-CB-CG	-5.02	104.06	114.10

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	44	0
2	B	248	0	136	12	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	5	0	0	0	0
All	All	6472	0	5808	103	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 9.

All (103) 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
1:A:287:ARG:HD3	1:A:341:GLU:OE1	1.84	0.77
1:F:328:GLU:H	1:F:328:GLU:CD	1.95	0.74
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:A:240:GLU:HG3	1:A:241:PRO:HD2	1.74	0.69
1:A:197:MSE:HE2	1:A:199:ILE:HD12	1.77	0.67
1:A:116:PRO:O	1:A:117:ASP:HB2	1.94	0.66
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:F:193:LYS:HZ1	2:B:838:DC:H5	1.48	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:F:194:LEU:HA	1:F:197:MSE:CE	2.28	0.60
1:A:339:ARG:HD3	5:A:556:HOH:O	2.00	0.60
1:F:46:THR:HG21	5:F:520:HOH:O	2.02	0.59
1:A:281:GLN:NE2	5:A:504:HOH:O	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:34:GLY:HA3	1:A:43:LYS:HD2	1.90	0.53
1:A:252:THR:HG23	2:B:841:DG:OP2	2.08	0.53
1:F:345:ASP:O	1:F:346:ASP:HB2	2.10	0.52
1:F:144:ILE:HD12	1:F:165:VAL:HG22	1.92	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:A:287:ARG:HB2	1:A:341:GLU:HB2	1.91	0.51
1:F:87:SER:OG	1:F:106:TRP:O	2.25	0.51
2:H:870:DA:C2'	2:H:871:DC:H5'	2.40	0.51
1:A:252:THR:HG21	5:A:565:HOH:O	2.11	0.51
1:F:152:LYS:HE3	1:F:184:TRP:HE1	1.75	0.51
1:F:178:ARG:HB3	1:F:179:PRO:HD2	1.92	0.51
1:A:42:ARG:HH21	1:A:334:ARG:HG3	1.74	0.51
1:A:294:THR:HG22	1:A:298:TYR:HB3	1.92	0.50
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:F:293:ARG:HB3	1:F:335:LEU:HB3	1.94	0.49
1:A:240:GLU:HG3	1:A:241:PRO:CD	2.41	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:F:205:LEU:HD23	1:F:229:ALA:HB2	1.96	0.48
1:F:181:ASP:HB3	1:F:191:THR:OG1	2.13	0.47
1:A:294:THR:HG22	1:A:298:TYR:H	1.79	0.47
1:F:175:MSE:HE1	1:F:182:ALA:HB1	1.95	0.47
1:A:294:THR:HG23	1:A:296:THR:H	1.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:250:VAL:HG12	1:F:337:GLY:HA3	1.97	0.47
3:F:401:OKX:O5'	3:F:401:OKX:H15	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:O4'	2:B:838:DC:O2	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:F:193:LYS:NZ	2:B:838:DC:C5	2.78	0.44
1:A:35:SER:HA	1:A:77:PRO:HB3	1.99	0.44
1:A:115:LEU:HA	1:A:116:PRO:HD3	1.86	0.44
2:B:848:DA:H2'	2:B:848:DA:OP2	2.18	0.44
1:F:152:LYS:NZ	2:H:873:DC:OP1	2.42	0.43
2:C:871:DC:H2''	2:C:872:DC:O4'	2.18	0.43
1:F:120:ASP:OD1	1:F:121:PRO:HD2	2.18	0.43
1:A:298:TYR:CE2	1:A:300:ARG:HD3	2.54	0.43
1:A:162:GLY:C	1:A:163:ILE:HG13	2.43	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:F:1:MSE:HE1	1:F:3:LYS:HE2	2.01	0.42
1:A:141:SER:CB	1:A:159:LYS:HD3	2.49	0.42
1:F:12:GLN:HG3	1:F:12:GLN:O	2.20	0.42
1:A:129:ARG:CZ	1:A:129:ARG:HB3	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:26:ARG:NH1	1:F:26:ARG:HG2	2.35	0.40
1:F:107:ASP:HB3	5:F:577:HOH:O	2.21	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	345/356 (97%)	330 (96%)	13 (4%)	2 (1%)	21	27
1	F	345/356 (97%)	334 (97%)	5 (1%)	6 (2%)	7	7
All	All	690/712 (97%)	664 (96%)	18 (3%)	8 (1%)	10	12

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
1	F	33	GLY
1	F	331	ARG
1	F	34	GLY

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	284/282 (101%)	263 (93%)	21 (7%)	13	17
1	F	284/282 (101%)	270 (95%)	14 (5%)	22	34
All	All	568/564 (101%)	533 (94%)	35 (6%)	16	24

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	1	MSE
1	F	35	SER
1	F	46	THR
1	F	54	GLU
1	F	64	ARG

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Mol	Chain	Res	Type
1	F	72	ASP
1	F	108	GLU
1	F	225	LEU
1	F	239	SER
1	F	247	ARG
1	F	257	LEU
1	F	265	SER
1	F	328	GLU
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	95	ARG
1	A	106	TRP
1	A	118	GLU
1	A	127	ARG
1	A	220	SER
1	A	227	LEU
1	A	240	GLU
1	A	250	VAL
1	A	252	THR
1	A	259	GLU
1	A	261	ARG
1	A	294	THR
1	A	297	PHE
1	A	300	ARG
1	A	311	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	255	GLN

5.3.3 RNA ⓘ

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 oligosaccharides 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	OKX	F	401	4	28,29,29	1.23	2 (7%)	39,45,45	1.97	6 (15%)
3	OKX	A	401	4	28,29,29	1.73	4 (14%)	39,45,45	2.28	12 (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	OKX	F	401	4	-	5/19/34/34	0/2/2/2
3	OKX	A	401	4	-	5/19/34/34	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	OKX	PB-O2B	5.86	1.55	1.46
3	F	401	OKX	PB-O2B	4.02	1.52	1.46
3	A	401	OKX	PG-O2G	3.56	1.61	1.50
3	F	401	OKX	C6-C5	2.90	1.41	1.35
3	A	401	OKX	C2-N1	2.81	1.46	1.40
3	A	401	OKX	C6-C5	2.60	1.41	1.35

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	401	0KX	O1A-PA-N3A	-6.99	101.47	111.77
3	A	401	0KX	O2B-PB-N3A	-5.62	103.50	111.77
3	A	401	0KX	O2A-PA-O1A	5.59	121.86	109.87
3	F	401	0KX	O2A-PA-O1A	5.39	121.43	109.87
3	A	401	0KX	O2-C2-N3	-4.47	115.28	122.33
3	A	401	0KX	O1A-PA-N3A	-4.11	105.71	111.77
3	A	401	0KX	O5'-PA-O1A	-3.89	102.73	114.27
3	F	401	0KX	O1G-PG-O2G	3.31	123.74	110.83
3	A	401	0KX	O1B-PB-O2B	3.19	116.71	109.87
3	F	401	0KX	C4-N3-C2	3.12	125.17	120.26
3	A	401	0KX	O4'-C1'-N1	3.06	113.30	107.86
3	A	401	0KX	O3'-C3'-C4'	2.83	120.81	110.07
3	A	401	0KX	C2'-C1'-N1	-2.49	107.59	113.81
3	F	401	0KX	C6-N1-C2	-2.36	116.48	120.46
3	A	401	0KX	C6-N1-C2	-2.30	116.57	120.46
3	A	401	0KX	O1B-PB-O3B	2.30	112.32	104.64
3	A	401	0KX	O3B-PG-O2G	-2.26	99.16	111.04
3	F	401	0KX	O5'-C5'-C4'	2.00	115.82	108.99

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	F	401	0KX	PB-O3B-PG-O2G
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

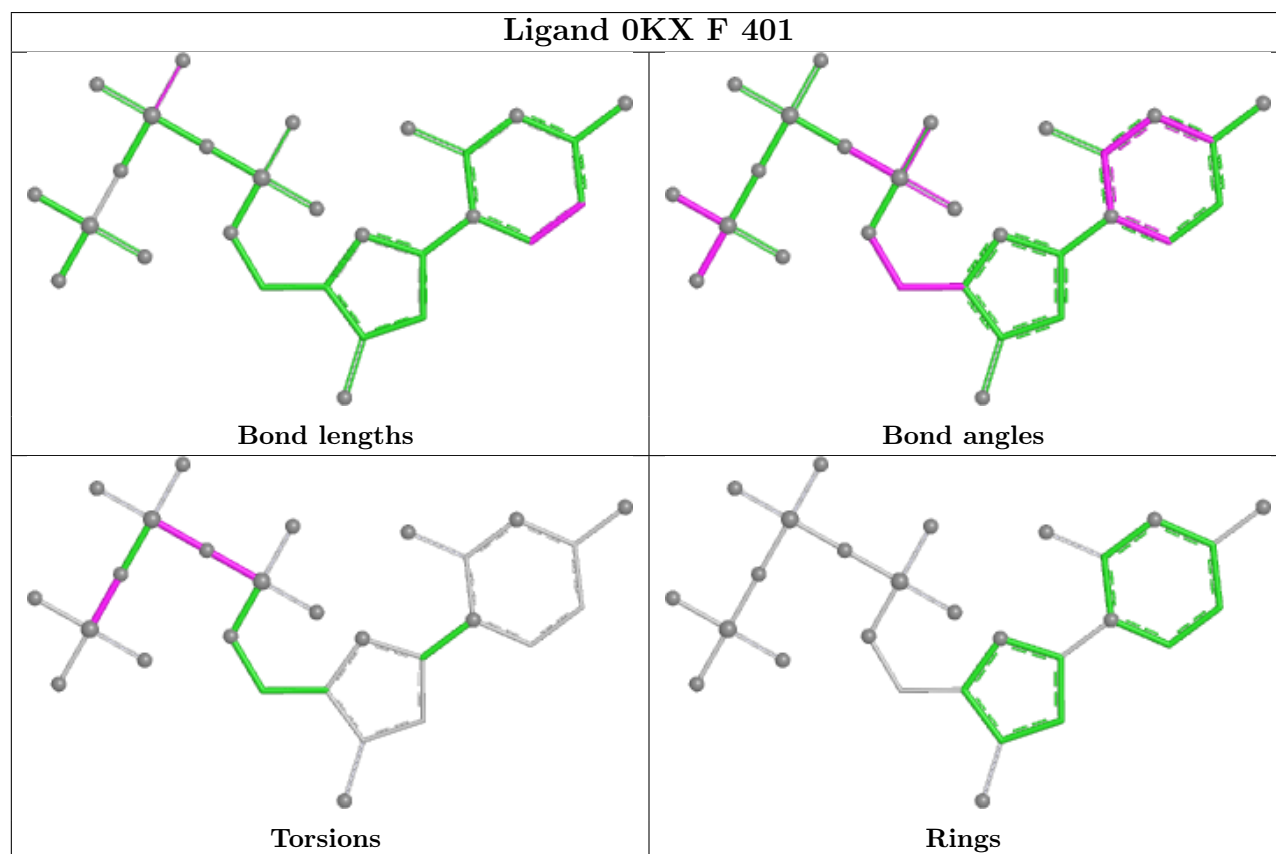
There are no ring outliers.

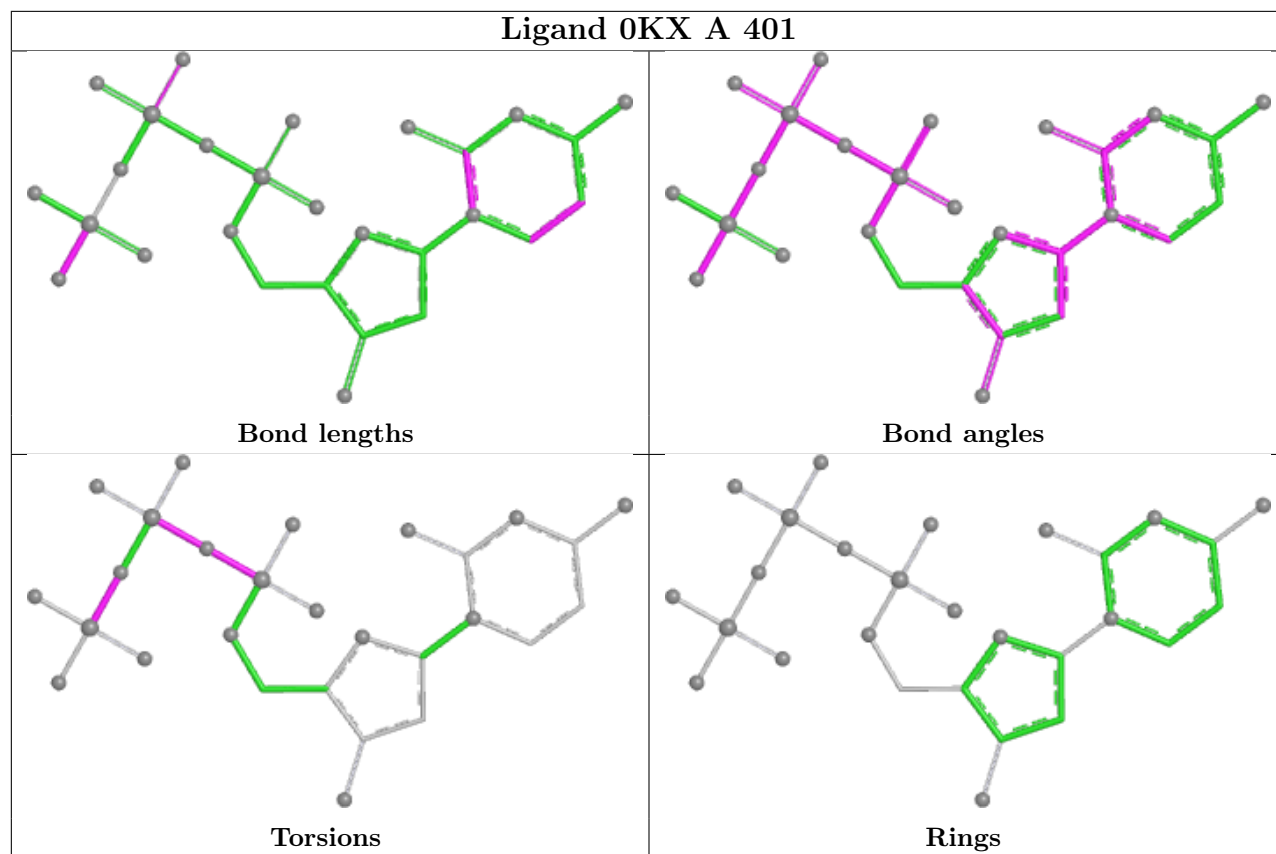
1 monomer is involved in 1 short contact:

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 ⓘ

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, 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%)	-0.13	10 (2%) 53 56	18, 32, 63, 96	0
1	F	339/356 (95%)	-0.19	7 (2%) 63 65	18, 31, 54, 91	0
2	B	12/18 (66%)	0.23	1 (8%) 17 19	31, 45, 102, 121	0
2	C	10/18 (55%)	0.17	1 (10%) 12 14	34, 60, 77, 107	0
2	G	11/18 (61%)	-0.12	1 (9%) 15 16	27, 40, 75, 111	0
2	H	8/18 (44%)	-0.11	0 100 100	30, 42, 84, 96	0
All	All	719/784 (91%)	-0.15	20 (2%) 55 57	18, 32, 63, 121	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	347	VAL	8.1
1	A	347	VAL	5.5
1	A	104	TRP	4.2
1	F	34	GLY	4.0
2	B	849	DG	3.6
1	A	331	ARG	3.6
1	A	184	TRP	3.2
1	A	298	TYR	3.1
1	F	104	TRP	3.0
1	F	242	TRP	3.0
1	F	330	ASP	2.9
1	F	331	ARG	2.9
1	A	300	ARG	2.5
2	G	848	DA	2.4
2	C	864	DC	2.3
1	A	294	THR	2.2
1	A	106	TRP	2.2
1	A	297	PHE	2.1
1	A	34	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	345	ASP	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

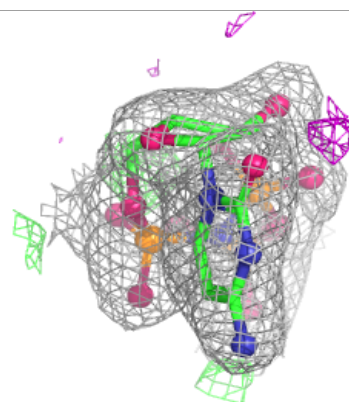
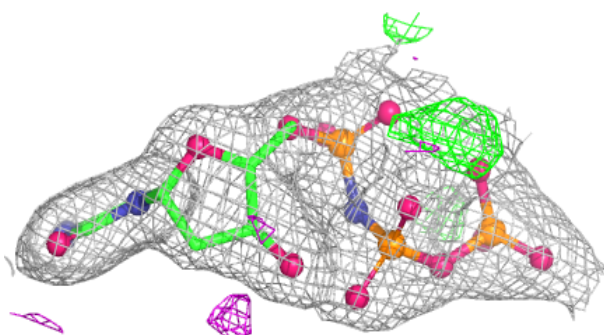
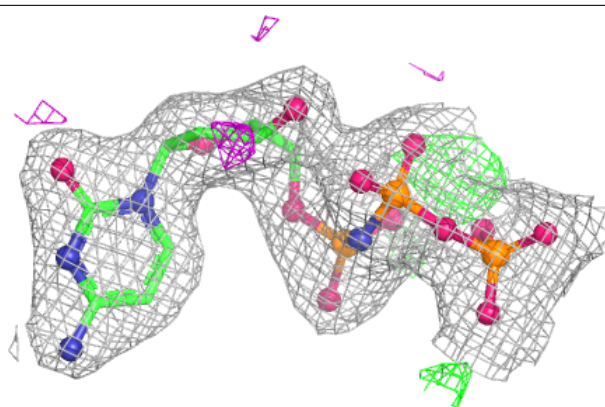
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	A	402	1/1	0.75	0.15	38,38,38,38	0
4	MG	F	402	1/1	0.93	0.12	32,32,32,32	0
4	MG	A	403	1/1	0.97	0.14	27,27,27,27	0
4	MG	F	403	1/1	0.98	0.10	25,25,25,25	0
3	OKX	A	401	28/28	0.98	0.05	25,26,28,28	0
3	OKX	F	401	28/28	0.98	0.05	25,27,31,33	0

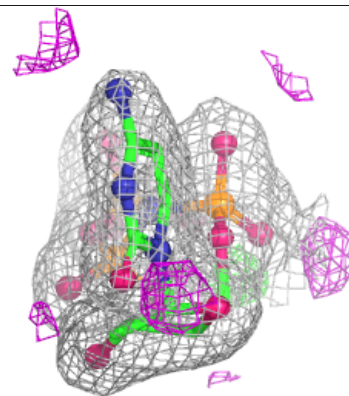
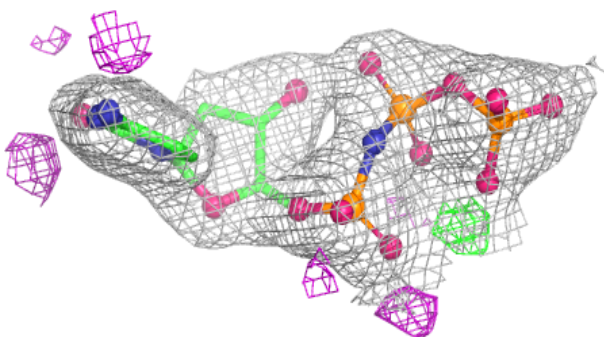
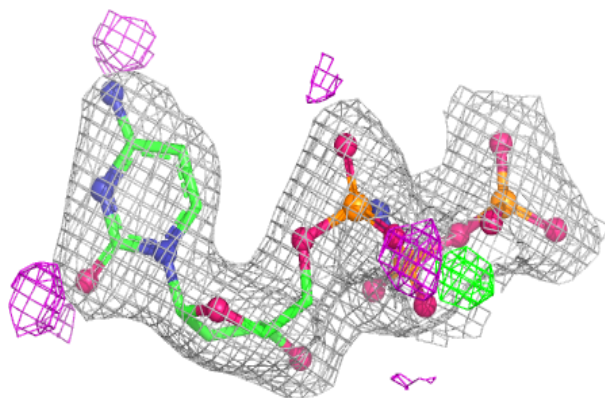
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

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.