



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 29, 2020 – 12:17 PM EST

PDB ID : 6VGM  
Title : Crystal structure of DPO4 with 8-oxoadenine (oxoA) and dTTP\*  
Authors : Jung, H.; Lee, S.  
Deposited on : 2020-01-08  
Resolution : 2.84 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 : 2.16  
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) : 2.16

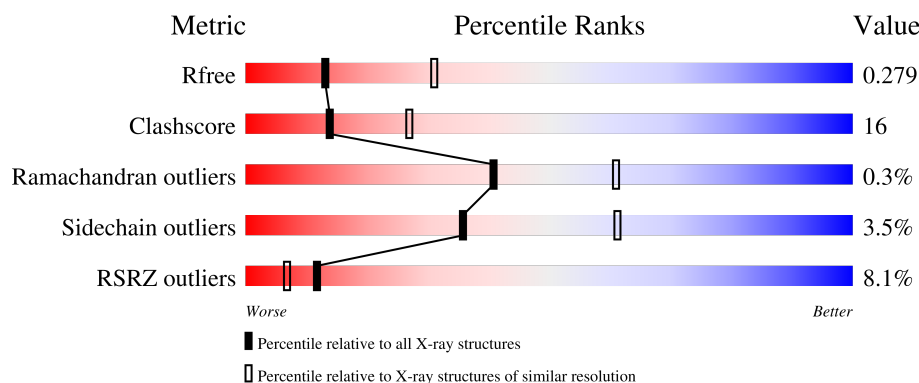
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.84 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	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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  $\geq 3$ , 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	341	<div> <div>8%</div> <div>67%</div> <div>31%</div> <div>.</div> </div>
1	D	341	<div> <div>10%</div> <div>70%</div> <div>27%</div> <div>.</div> </div>
2	B	13	<div> <div>62%</div> <div>38%</div> </div>
2	P	13	<div> <div>69%</div> <div>31%</div> </div>
3	C	18	<div> <div>6%</div> <div>44%</div> <div>33%</div> <div>11%</div> <div>11%</div> </div>

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Mol	Chain	Length	Quality of chain
3	T	18	<div><div></div><div>61%</div><div>17%</div><div>11%</div><div>11%</div></div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6744 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	341	Total	C	N	O	S	0	0	0
			2743	1760	472	504	7			
1	D	341	Total	C	N	O	S	0	0	0
			2743	1760	472	504	7			

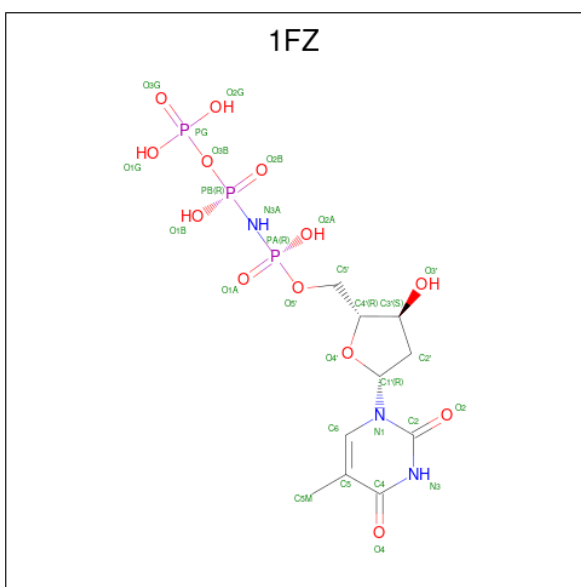
- Molecule 2 is a DNA chain called DNA (5'-D(\*GP\*GP\*GP\*GP\*GP\*AP\*AP\*GP\*GP\*AP\*TP\*TP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	13	Total	C	N	O	P	0	0	0
			273	129	57	75	12			
2	P	13	Total	C	N	O	P	0	0	0
			273	129	57	75	12			

- Molecule 3 is a DNA chain called DNA (5'-D(\*TP\*CP\*AP\*TP\*(A38)P\*GP\*AP\*AP\*TP\*CP\*CP\*TP\*TP\*CP\*CP\*CP\*CP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	16	Total	C	N	O	P	0	0	0
			320	153	54	97	16			
3	T	16	Total	C	N	O	P	0	0	0
			320	153	54	97	16			

- Molecule 4 is 5'-O-[(R)-hydroxy{[(R)-hydroxy(phosphonooxy)phosphoryl]amino}phosphoryl]thymidine (three-letter code: 1FZ) (formula: C<sub>10</sub>H<sub>18</sub>N<sub>3</sub>O<sub>13</sub>P<sub>3</sub>).



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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Mg 1 1	0	0
5	A	2	Total Mg 2 2	0	0
5	D	1	Total Mg 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	4	Total O 4 4	0	0
6	B	2	Total O 2 2	0	0
6	C	1	Total O 1 1	0	0
6	D	2	Total O 2 2	0	0

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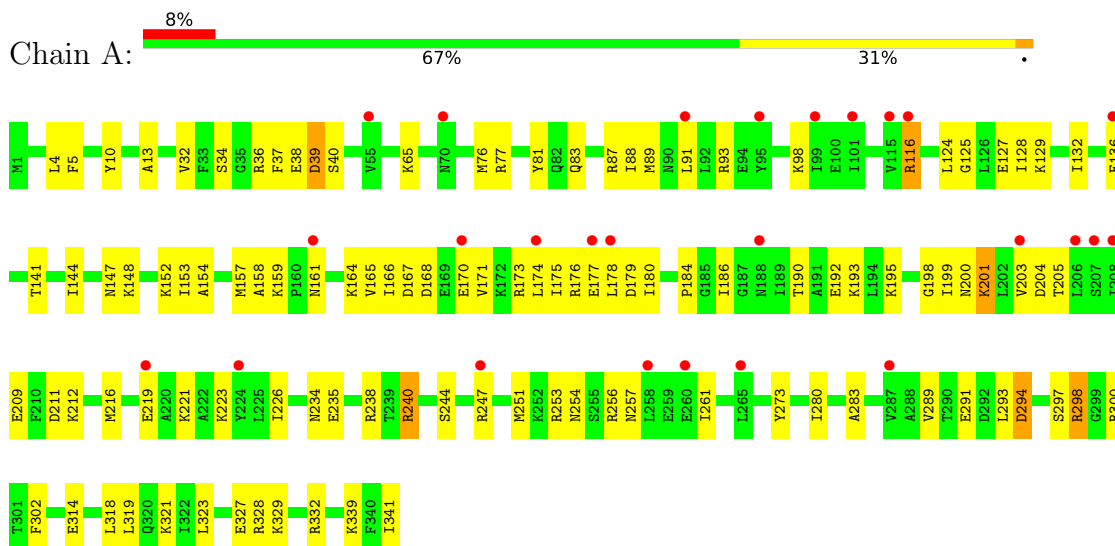
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	T	1	Total	O	0	0
			1	1		

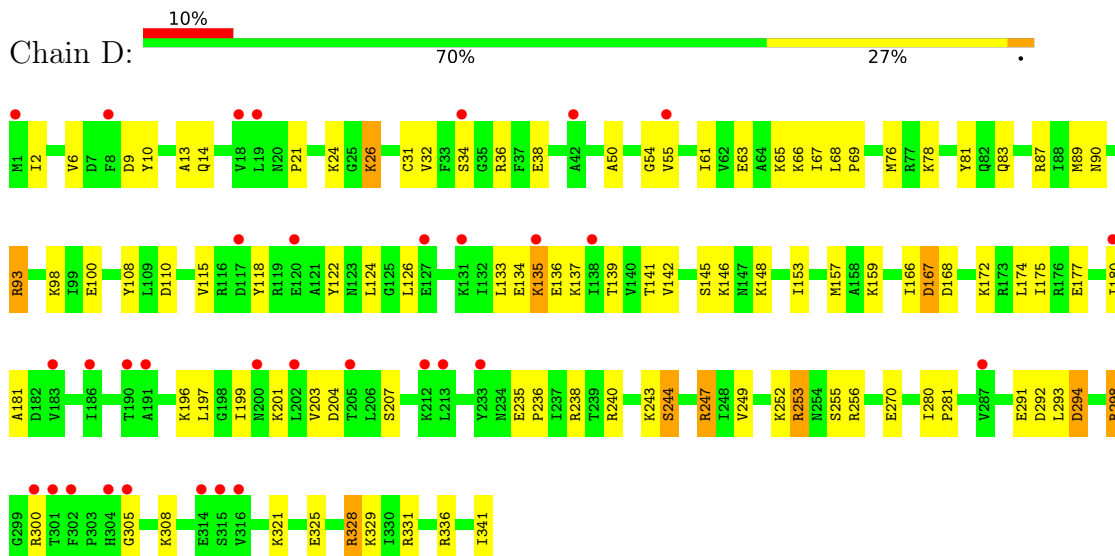
### 3 Residue-property plots

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

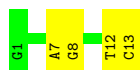


#### • Molecule 2: DNA (5'-D(\*GP\*GP\*GP\*GP\*GP\*AP\*AP\*GP\*GP\*AP\*TP\*TP\*C)-3')

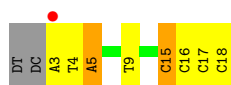
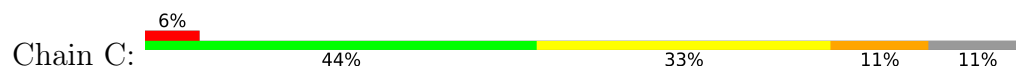




- Molecule 2: DNA (5'-D(\*GP\*GP\*GP\*GP\*GP\*AP\*AP\*GP\*GP\*AP\*TP\*TP\*C)-3')



- Molecule 3: DNA (5'-D(\*TP\*CP\*AP\*TP\*(A38)P\*GP\*AP\*AP\*TP\*CP\*CP\*TP\*TP\*CP\*CP\*CP\*CP\*C)-3')



- Molecule 3: DNA (5'-D(\*TP\*CP\*AP\*TP\*(A38)P\*GP\*AP\*AP\*TP\*CP\*CP\*TP\*TP\*CP\*CP\*CP\*CP\*C)-3')





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.84Å 97.46Å 101.24Å 90.00° 90.05° 90.00°	Depositor
Resolution (Å)	42.23 – 2.84 42.23 – 2.84	Depositor EDS
% Data completeness (in resolution range)	98.5 (42.23-2.84) 98.3 (42.23-2.84)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.60 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.17	Depositor
R, $R_{free}$	0.230 , 0.280 0.230 , 0.279	Depositor DCC
$R_{free}$ test set	1208 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	74.7	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 27.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k 0.016 for -h,-l,-k 0.458 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6744	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.02% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, A38, 1FZ

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	0.31	0/2782	0.51	0/3736
1	D	0.32	0/2782	0.54	0/3736
2	B	0.57	0/308	0.86	0/476
2	P	0.55	0/308	0.88	0/476
3	C	0.67	0/330	1.05	2/502 (0.4%)
3	T	0.64	0/330	1.03	1/502 (0.2%)
All	All	0.39	0/6840	0.64	3/9428 (0.0%)

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	D	0	3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	15	DC	C3'-C2'-C1'	-5.66	95.71	102.50
3	C	15	DC	C4'-C3'-C2'	-5.36	98.28	103.10
3	T	4	DT	O4'-C1'-N1	5.20	111.64	108.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	167	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	D	298	ARG	Sidechain
1	D	54	GLY	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	2743	0	2889	88	0
1	D	2743	0	2889	106	0
2	B	273	0	146	6	0
2	P	273	0	147	3	0
3	C	320	0	181	6	0
3	T	320	0	181	5	0
4	A	29	0	14	1	0
4	D	29	0	14	2	0
5	A	2	0	0	0	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
6	A	4	0	0	1	0
6	B	2	0	0	0	0
6	C	1	0	0	0	0
6	D	2	0	0	0	0
6	T	1	0	0	0	0
All	All	6744	0	6461	207	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 16.

All (207) 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:D:135:LYS:HA	1:D:135:LYS:CE	1.00	1.29
1:D:135:LYS:CA	1:D:135:LYS:CE	1.90	1.27
1:D:135:LYS:CA	1:D:135:LYS:HE2	1.41	1.25
1:D:252:LYS:NZ	1:D:253:ARG:HE	1.48	1.10
1:D:135:LYS:HA	1:D:135:LYS:HE3	1.12	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:GLU:OE2	1:A:318:LEU:HD11	1.60	1.00
1:D:32:VAL:HG22	1:D:76:MET:CE	1.91	1.00
4:A:401:1FZ:H13	4:A:401:1FZ:H1	1.48	0.95
1:D:32:VAL:HG22	1:D:76:MET:HE3	1.46	0.94
1:D:135:LYS:CA	1:D:135:LYS:HE3	1.77	0.92
1:D:252:LYS:HZ3	1:D:253:ARG:HE	1.14	0.91
1:A:257:ASN:O	1:A:261:ILE:CD1	2.22	0.88
1:A:314:GLU:OE2	1:A:318:LEU:CD1	2.23	0.88
1:D:134:GLU:C	1:D:135:LYS:HE3	1.98	0.84
1:D:135:LYS:N	1:D:135:LYS:HE3	1.96	0.81
1:A:124:LEU:HA	1:A:127:GLU:HG3	1.61	0.80
1:A:257:ASN:O	1:A:261:ILE:HD12	1.81	0.79
1:D:252:LYS:NZ	1:D:253:ARG:NE	2.29	0.79
1:A:235:GLU:HG3	1:A:238:ARG:HH12	1.47	0.78
1:A:170:GLU:HG3	1:A:173:ARG:HD3	1.67	0.76
1:D:252:LYS:HZ2	1:D:253:ARG:HE	1.34	0.73
1:D:100:GLU:OE1	1:D:240:ARG:NH1	2.22	0.72
1:D:89:MET:HB3	1:D:93:ARG:NH1	2.05	0.72
1:D:38:GLU:HA	1:D:38:GLU:OE2	1.89	0.70
1:D:236:PRO:HD2	1:D:238:ARG:NH1	2.06	0.70
1:D:244:SER:OG	1:D:336:ARG:HD3	1.92	0.69
1:A:289:VAL:HG11	1:A:332:ARG:HH21	1.58	0.69
1:A:240:ARG:NH2	3:T:10:DC:OP1	2.26	0.69
1:D:135:LYS:HE2	1:D:135:LYS:C	2.14	0.68
1:A:153:ILE:HD13	1:A:178:LEU:HD11	1.77	0.67
1:D:32:VAL:CG2	1:D:76:MET:CE	2.72	0.66
1:A:235:GLU:CG	1:A:238:ARG:HH12	2.08	0.66
1:D:6:VAL:HG12	1:D:142:VAL:HG22	1.77	0.66
1:D:252:LYS:HD3	1:D:253:ARG:HD2	1.77	0.65
3:C:17:DC:H2"	3:C:18:DC:OP2	1.97	0.64
1:D:135:LYS:HA	1:D:135:LYS:HE2	0.65	0.64
1:A:298:ARG:HD2	1:A:321:LYS:HD2	1.78	0.64
1:D:199:ILE:HG23	1:D:204:ASP:HB3	1.79	0.64
1:D:134:GLU:O	1:D:135:LYS:HE3	1.96	0.63
1:D:244:SER:HG	1:D:336:ARG:HH11	1.44	0.63
1:D:159:LYS:HE2	4:D:401:1FZ:O3G	1.98	0.63
1:D:252:LYS:HZ2	1:D:253:ARG:NE	1.94	0.63
1:A:261:ILE:HD12	1:A:261:ILE:H	1.64	0.62
1:A:76:MET:HG2	1:A:81:TYR:HE2	1.63	0.62
1:A:36:ARG:NH1	1:A:251:MET:O	2.32	0.62
1:D:89:MET:CB	1:D:93:ARG:NH1	2.62	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:32:VAL:HG22	1:D:76:MET:HE2	1.82	0.62
1:A:32:VAL:HG22	1:A:76:MET:HE2	1.82	0.60
1:D:252:LYS:HZ3	1:D:253:ARG:NE	1.92	0.60
1:A:219:GLU:HG2	1:A:223:LYS:HD2	1.85	0.59
1:A:171:VAL:O	1:A:175:ILE:HG13	2.03	0.59
1:A:173:ARG:NE	1:A:177:GLU:OE2	2.33	0.59
1:D:235:GLU:HA	1:D:235:GLU:OE2	2.03	0.59
1:A:257:ASN:O	1:A:261:ILE:HD13	2.00	0.58
2:B:12:DT:H2''	2:B:13:DC:H5'	1.84	0.58
1:D:36:ARG:HH11	1:D:331:ARG:HH22	1.52	0.58
1:D:247:ARG:NH1	1:D:249:VAL:HG12	2.19	0.58
3:T:3:DA:H4'	3:T:4:DT:H5''	1.85	0.57
1:D:65:LYS:HG3	1:D:69:PRO:HA	1.86	0.57
1:A:283:ALA:HB2	1:A:339:LYS:HD2	1.86	0.57
1:A:186:ILE:O	1:A:186:ILE:HG13	2.04	0.57
1:A:291:GLU:OE2	1:A:329:LYS:HB2	2.04	0.57
1:D:115:VAL:CG1	1:D:124:LEU:HD12	2.34	0.57
1:D:166:ILE:HD12	1:D:174:LEU:CD1	2.35	0.56
1:D:36:ARG:HH11	1:D:331:ARG:NH2	2.03	0.56
1:A:166:ILE:HG22	1:A:171:VAL:HG23	1.87	0.55
1:D:294:ASP:HB2	1:D:328:ARG:NH1	2.22	0.55
1:A:176:ARG:O	1:A:201:LYS:HD2	2.05	0.55
1:A:36:ARG:NH2	1:A:254:ASN:OD1	2.39	0.55
1:D:89:MET:HB3	1:D:93:ARG:HH11	1.71	0.55
3:C:5:A38:H4'	1:D:34:SER:HB3	1.88	0.55
1:A:176:ARG:HA	1:A:203:VAL:CG2	2.37	0.54
1:D:292:ASP:O	1:D:293:LEU:HB2	2.07	0.54
1:A:4:LEU:HG	1:A:144:ILE:HD11	1.89	0.54
1:D:108:TYR:CD1	1:D:148:LYS:HG2	2.43	0.54
1:A:167:ASP:OD1	1:A:168:ASP:N	2.41	0.54
1:A:261:ILE:HD12	1:A:261:ILE:N	2.23	0.54
1:D:167:ASP:CG	1:D:168:ASP:H	2.12	0.53
1:A:177:GLU:HA	1:A:201:LYS:HD2	1.89	0.53
1:A:256:ARG:NH1	1:A:327:GLU:OE2	2.33	0.53
1:D:204:ASP:O	1:D:207:SER:N	2.27	0.53
1:A:88:ILE:HG23	1:A:132:ILE:HD12	1.90	0.53
3:T:3:DA:N3	3:T:3:DA:H2'	2.22	0.53
1:D:175:ILE:HG22	1:D:203:VAL:HB	1.90	0.52
1:D:83:GLN:OE1	1:D:87:ARG:NH1	2.40	0.52
1:A:144:ILE:HB	1:A:165:VAL:HA	1.92	0.52
1:D:141:THR:HG21	1:D:159:LYS:HG2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:252:LYS:HZ2	1:D:253:ARG:HH21	1.56	0.51
1:D:294:ASP:HB2	1:D:328:ARG:HH12	1.75	0.50
1:D:236:PRO:HD2	1:D:238:ARG:HH12	1.72	0.50
1:D:252:LYS:HZ2	1:D:253:ARG:NH2	2.09	0.50
1:D:177:GLU:O	1:D:201:LYS:HE3	2.12	0.50
1:A:314:GLU:OE2	1:A:318:LEU:CG	2.60	0.50
1:D:256:ARG:HG2	1:D:329:LYS:HA	1.94	0.50
1:D:50:ALA:HB1	1:D:55:VAL:HG21	1.94	0.50
1:A:38:GLU:O	1:A:39:ASP:HB2	2.12	0.50
1:D:21:PRO:O	1:D:24:LYS:HB2	2.12	0.49
1:D:252:LYS:NZ	1:D:253:ARG:HH21	2.10	0.49
1:D:298:ARG:HG3	1:D:321:LYS:HG2	1.92	0.49
1:A:125:GLY:O	1:A:129:LYS:HG3	2.12	0.49
3:C:9:DT:H3'	1:D:243:LYS:HE3	1.93	0.48
1:D:115:VAL:HG11	1:D:124:LEU:HD12	1.95	0.48
1:A:83:GLN:O	1:A:87:ARG:HG3	2.13	0.48
1:D:87:ARG:NE	1:D:136:GLU:OE2	2.43	0.48
2:B:6:DA:H5''	1:D:300:ARG:NH1	2.29	0.48
1:D:298:ARG:NH1	1:D:325:GLU:OE2	2.46	0.48
3:C:15:DC:H2''	3:C:16:DC:OP2	2.13	0.48
1:D:122:TYR:CE1	1:D:126:LEU:HD11	2.49	0.48
1:D:89:MET:CB	1:D:93:ARG:HH11	2.24	0.48
3:C:9:DT:OP2	1:D:244:SER:HB3	2.14	0.47
1:A:177:GLU:HA	1:A:201:LYS:CD	2.43	0.47
1:A:280:ILE:HD13	1:A:341:ILE:HD11	1.96	0.47
1:A:87:ARG:NE	1:A:136:GLU:OE1	2.47	0.47
1:D:168:ASP:O	1:D:172:LYS:HG2	2.14	0.47
1:D:63:GLU:OE1	1:D:66:LYS:NZ	2.46	0.47
1:A:170:GLU:HA	1:A:173:ARG:HB3	1.95	0.47
2:P:12:DT:H2''	2:P:13:DC:H5'	1.96	0.47
1:D:280:ILE:HB	1:D:341:ILE:HG12	1.97	0.47
1:A:128:ILE:O	1:A:132:ILE:HG12	2.14	0.47
1:A:148:LYS:HE2	1:A:148:LYS:HB2	1.80	0.46
1:A:199:ILE:HG23	1:A:204:ASP:HB2	1.97	0.46
1:D:10:TYR:HD2	1:D:13:ALA:HB3	1.78	0.46
1:D:2:ILE:HD12	1:D:118:TYR:CZ	2.51	0.46
1:A:289:VAL:HG11	1:A:332:ARG:NH2	2.26	0.46
1:A:298:ARG:HH11	1:A:321:LYS:NZ	2.14	0.46
1:A:154:ALA:HB2	1:A:166:ILE:HG13	1.98	0.46
1:A:198:GLY:O	1:A:200:ASN:ND2	2.49	0.46
2:P:7:DA:H2''	2:P:8:DG:H8	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:ILE:N	1:A:200:ASN:O	2.42	0.46
2:B:12:DT:H2'	2:B:13:DC:C6	2.50	0.46
1:A:116:ARG:HA	1:A:116:ARG:HD2	1.61	0.46
1:A:4:LEU:HG	1:A:144:ILE:CD1	2.45	0.46
1:D:90:ASN:HA	1:D:93:ARG:HD3	1.98	0.46
1:A:36:ARG:HG3	1:A:36:ARG:NH1	2.31	0.46
1:D:270:GLU:OE1	1:D:308:LYS:HD3	2.15	0.46
1:D:252:LYS:HZ2	1:D:253:ARG:CZ	2.29	0.46
1:A:176:ARG:HA	1:A:203:VAL:HG21	1.98	0.46
3:C:3:DA:H5''	3:C:4:DT:H5''	1.96	0.45
1:D:298:ARG:HA	1:D:298:ARG:HD3	1.74	0.45
2:B:7:DA:H2''	2:B:8:DG:H8	1.79	0.45
1:D:252:LYS:HD3	1:D:253:ARG:CD	2.45	0.45
1:D:36:ARG:HG2	1:D:252:LYS:O	2.16	0.45
1:D:166:ILE:HD12	1:D:174:LEU:HD13	1.97	0.45
1:A:147:ASN:ND2	1:A:234:ASN:HA	2.32	0.45
1:A:36:ARG:HG3	1:A:36:ARG:HH11	1.82	0.45
1:D:98:LYS:HD2	1:D:110:ASP:OD2	2.17	0.45
1:D:197:LEU:O	1:D:199:ILE:HG13	2.17	0.45
1:D:78:LYS:HA	1:D:81:TYR:CD2	2.52	0.45
1:A:37:PHE:O	1:A:40:SER:HB2	2.17	0.45
1:D:199:ILE:H	1:D:199:ILE:HG13	1.59	0.45
1:D:67:ILE:O	1:D:68:LEU:HD13	2.17	0.45
2:P:12:DT:H2'	2:P:13:DC:C6	2.52	0.44
1:A:192:GLU:HA	1:A:195:LYS:HB2	1.99	0.44
2:B:6:DA:H2''	2:B:7:DA:H8	1.83	0.44
1:A:193:LYS:HD3	1:A:216:MET:HG3	1.99	0.44
1:A:244:SER:HB3	3:T:9:DT:OP2	2.17	0.44
1:A:235:GLU:HG3	1:A:238:ARG:NH1	2.24	0.43
1:A:152:LYS:HE2	1:A:184:PRO:HB3	2.00	0.43
1:D:36:ARG:NH1	1:D:331:ARG:HH22	2.14	0.43
1:D:281:PRO:O	1:D:305:GLY:HA2	2.17	0.43
1:A:10:TYR:HD2	1:A:13:ALA:HB3	1.82	0.43
1:A:298:ARG:NH1	1:A:321:LYS:NZ	2.65	0.43
1:A:294:ASP:HB2	1:A:328:ARG:NH1	2.34	0.43
1:A:5:PHE:CD2	1:A:152:LYS:HA	2.54	0.43
1:D:9:ASP:HB2	1:D:139:THR:HG23	2.00	0.43
1:D:26:LYS:H	1:D:26:LYS:HD2	1.82	0.43
1:D:145:SER:OG	1:D:146:LYS:N	2.52	0.43
1:A:170:GLU:O	1:A:174:LEU:HG	2.19	0.42
1:A:93:ARG:NH2	6:A:502:HOH:O	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:LYS:HA	1:A:212:LYS:HD3	1.72	0.42
1:D:10:TYR:CE2	1:D:14:GLN:HB2	2.54	0.42
1:A:300:ARG:HD3	1:A:302:PHE:CE1	2.55	0.42
1:A:190:THR:HG21	1:A:221:LYS:NZ	2.35	0.42
1:A:98:LYS:HE3	1:A:98:LYS:HB2	1.75	0.42
1:A:158:ALA:HB2	1:A:164:LYS:HB2	2.02	0.42
1:D:197:LEU:HA	1:D:197:LEU:HD23	1.66	0.42
1:A:153:ILE:O	1:A:157:MET:HG3	2.19	0.42
1:D:133:LEU:O	1:D:137:LYS:HD2	2.20	0.42
2:B:6:DA:H5''	1:D:300:ARG:HH12	1.84	0.42
1:A:256:ARG:HG2	1:A:323:LEU:HD22	2.02	0.42
1:D:180:ILE:HD12	1:D:181:ALA:N	2.34	0.42
1:D:38:GLU:CA	1:D:38:GLU:OE2	2.63	0.42
1:D:10:TYR:HA	4:D:401:1FZ:O1B	2.20	0.42
1:D:50:ALA:HB1	1:D:55:VAL:CG2	2.50	0.42
1:D:87:ARG:NH2	1:D:136:GLU:OE2	2.52	0.41
1:A:175:ILE:O	1:A:203:VAL:HG23	2.20	0.41
1:A:89:MET:O	1:A:93:ARG:HG2	2.20	0.41
1:D:196:LYS:O	1:D:197:LEU:HD23	2.21	0.41
1:A:314:GLU:OE2	1:A:318:LEU:HG	2.20	0.41
1:A:205:THR:HG22	1:A:226:ILE:HG13	2.03	0.41
1:D:83:GLN:O	1:D:87:ARG:HG3	2.21	0.41
1:D:89:MET:HB2	1:D:93:ARG:NH1	2.35	0.41
1:A:141:THR:HG21	1:A:159:LYS:HG2	2.03	0.41
1:A:319:LEU:O	1:A:323:LEU:HD12	2.20	0.41
1:D:255:SER:HA	1:D:329:LYS:HD3	2.02	0.41
1:A:34:SER:HB3	3:T:5:A38:H4'	2.03	0.41
1:A:39:ASP:CG	1:A:65:LYS:HZ3	2.24	0.41
1:D:292:ASP:OD1	1:D:292:ASP:C	2.58	0.41
1:D:291:GLU:O	1:D:293:LEU:HD12	2.21	0.41
1:A:209:GLU:OE1	1:A:212:LYS:NZ	2.49	0.40
1:D:153:ILE:O	1:D:157:MET:HG3	2.21	0.40
1:A:298:ARG:HH11	1:A:321:LYS:HZ2	1.69	0.40
1:A:88:ILE:O	1:A:91:LEU:HB2	2.22	0.40
1:D:98:LYS:HB2	1:D:110:ASP:HB3	2.03	0.40
1:A:291:GLU:CD	1:A:329:LYS:HB2	2.42	0.40
1:A:280:ILE:HB	1:A:341:ILE:HG12	2.04	0.40
1:D:31:CYS:HB3	1:D:61:ILE:HD13	2.03	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	339/341 (99%)	324 (96%)	13 (4%)	2 (1%)	25	46
1	D	339/341 (99%)	318 (94%)	21 (6%)	0	100	100
All	All	678/682 (99%)	642 (95%)	34 (5%)	2 (0%)	41	61

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	ASP
1	A	161	ASN

### 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	300/300 (100%)	287 (96%)	13 (4%)	29	54
1	D	300/300 (100%)	292 (97%)	8 (3%)	44	69
All	All	600/600 (100%)	579 (96%)	21 (4%)	36	61

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	ARG
1	A	116	ARG
1	A	179	ASP
1	A	201	LYS

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Mol	Chain	Res	Type
1	A	211	ASP
1	A	240	ARG
1	A	247	ARG
1	A	253	ARG
1	A	273	TYR
1	A	293	LEU
1	A	294	ASP
1	A	297	SER
1	A	298	ARG
1	D	26	LYS
1	D	93	ARG
1	D	135	LYS
1	D	244	SER
1	D	247	ARG
1	D	253	ARG
1	D	294	ASP
1	D	328	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	20	ASN
1	D	304	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	A38	T	5	3	18,24,25	4.01	8 (44%)	19,35,38	2.05	4 (21%)
3	A38	C	5	3	18,24,25	4.03	8 (44%)	19,35,38	2.04	4 (21%)

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	A38	T	5	3	-	0/3/21/22	0/3/3/3
3	A38	C	5	3	-	0/3/21/22	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	5	A38	C8-N7	9.19	1.44	1.34
3	T	5	A38	C8-N7	9.18	1.44	1.34
3	C	5	A38	C3'-C4'	-7.82	1.31	1.53
3	T	5	A38	C3'-C4'	-7.77	1.31	1.53
3	T	5	A38	C2'-C1'	-7.15	1.32	1.52
3	C	5	A38	C2'-C1'	-7.04	1.32	1.52
3	C	5	A38	O4'-C1'	5.65	1.55	1.42
3	T	5	A38	O4'-C1'	5.54	1.54	1.42
3	C	5	A38	O4'-C4'	5.22	1.56	1.45
3	T	5	A38	O4'-C4'	5.22	1.56	1.45
3	C	5	A38	C2'-C3'	3.77	1.62	1.52
3	T	5	A38	C2'-C3'	3.69	1.62	1.52
3	T	5	A38	C6-N6	2.92	1.44	1.34
3	C	5	A38	C6-N6	2.88	1.44	1.34
3	C	5	A38	C5-N7	2.51	1.48	1.39
3	T	5	A38	C5-N7	2.50	1.48	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	5	A38	N3-C2-N1	-5.59	119.94	128.68
3	C	5	A38	C2'-C1'-N9	-5.54	109.96	116.01
3	C	5	A38	N3-C2-N1	-5.33	120.34	128.68
3	T	5	A38	C2'-C1'-N9	-5.23	110.30	116.01
3	T	5	A38	C2-N1-C6	2.59	123.19	118.75
3	C	5	A38	C2-N1-C6	2.31	122.70	118.75
3	T	5	A38	C4'-O4'-C1'	-2.10	104.38	109.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	5	A38	C4'-O4'-C1'	-2.07	104.46	109.45

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	T	5	A38	1	0
3	C	5	A38	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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
4	1FZ	D	401	5	26,30,30	1.87	4 (15%)	32,47,47	1.85	5 (15%)
4	1FZ	A	401	5	26,30,30	1.81	4 (15%)	32,47,47	2.08	7 (21%)

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
4	1FZ	D	401	5	-	4/16/34/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	1FZ	A	401	5	-	7/16/34/34	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	401	1FZ	C5M-C5	-6.17	1.39	1.51
4	D	401	1FZ	C5M-C5	-6.10	1.39	1.51
4	D	401	1FZ	C4-N3	3.97	1.40	1.33
4	A	401	1FZ	C4-N3	3.46	1.39	1.33
4	D	401	1FZ	PA-O2A	2.19	1.62	1.56
4	A	401	1FZ	O4'-C1'	2.18	1.47	1.42
4	D	401	1FZ	PG-O1G	2.13	1.63	1.54
4	A	401	1FZ	PG-O2G	2.01	1.62	1.54

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	401	1FZ	C4-N3-C2	8.05	121.94	115.14
4	D	401	1FZ	C4-N3-C2	7.43	121.41	115.14
4	A	401	1FZ	O2B-PB-N3A	4.35	118.18	111.77
4	D	401	1FZ	O2B-PB-N3A	3.70	117.21	111.77
4	A	401	1FZ	PG-O3B-PB	-3.64	119.80	132.62
4	D	401	1FZ	PG-O3B-PB	-3.42	120.57	132.62
4	A	401	1FZ	O4'-C1'-C2'	-3.21	100.19	106.25
4	A	401	1FZ	C6-N1-C1'	2.52	124.90	119.24
4	D	401	1FZ	O4'-C4'-C3'	-2.44	99.97	105.67
4	D	401	1FZ	C2'-C3'-C4'	-2.37	97.82	102.76
4	A	401	1FZ	O1A-PA-N3A	2.32	115.18	111.77
4	A	401	1FZ	O3B-PB-N3A	-2.20	100.50	106.59

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	401	1FZ	PB-N3A-PA-O1A
4	D	401	1FZ	PB-O3B-PG-O1G
4	A	401	1FZ	C5'-O5'-PA-O2A
4	A	401	1FZ	PB-N3A-PA-O1A
4	A	401	1FZ	PB-O3B-PG-O1G
4	A	401	1FZ	C3'-C4'-C5'-O5'
4	A	401	1FZ	C5'-O5'-PA-O1A

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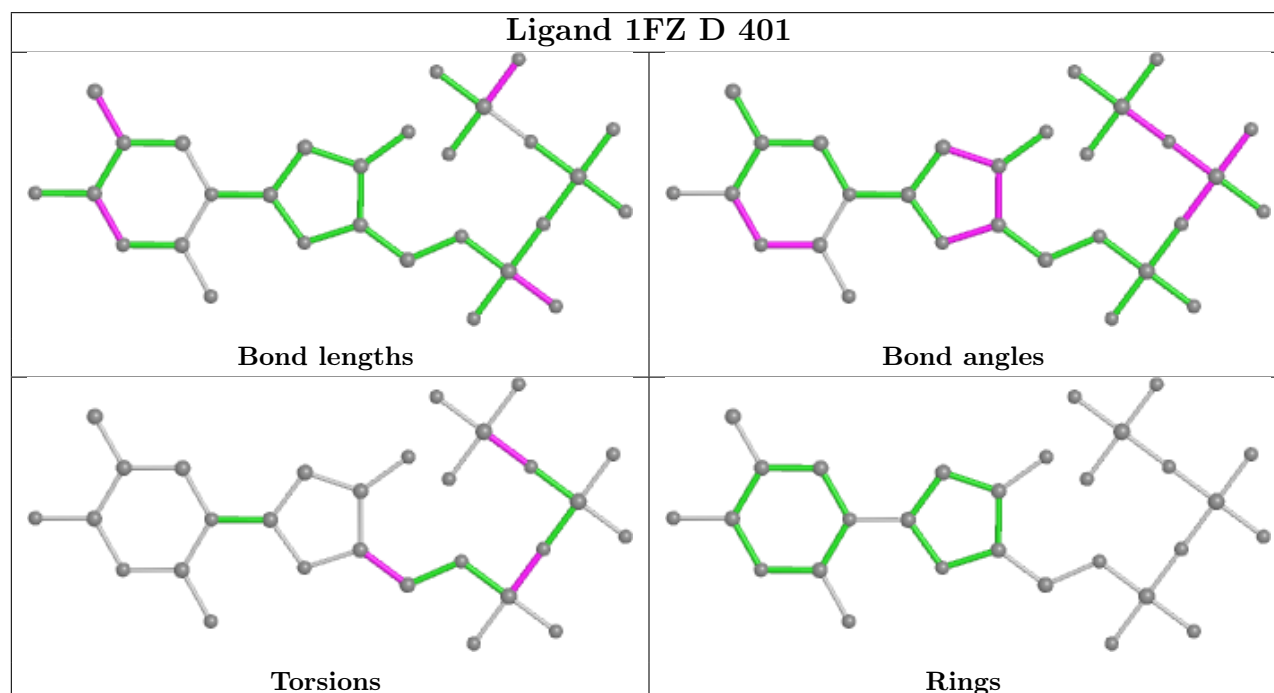
Mol	Chain	Res	Type	Atoms
4	D	401	1FZ	PB-O3B-PG-O3G
4	A	401	1FZ	O4'-C4'-C5'-O5'
4	A	401	1FZ	PB-O3B-PG-O3G
4	D	401	1FZ	O4'-C4'-C5'-O5'

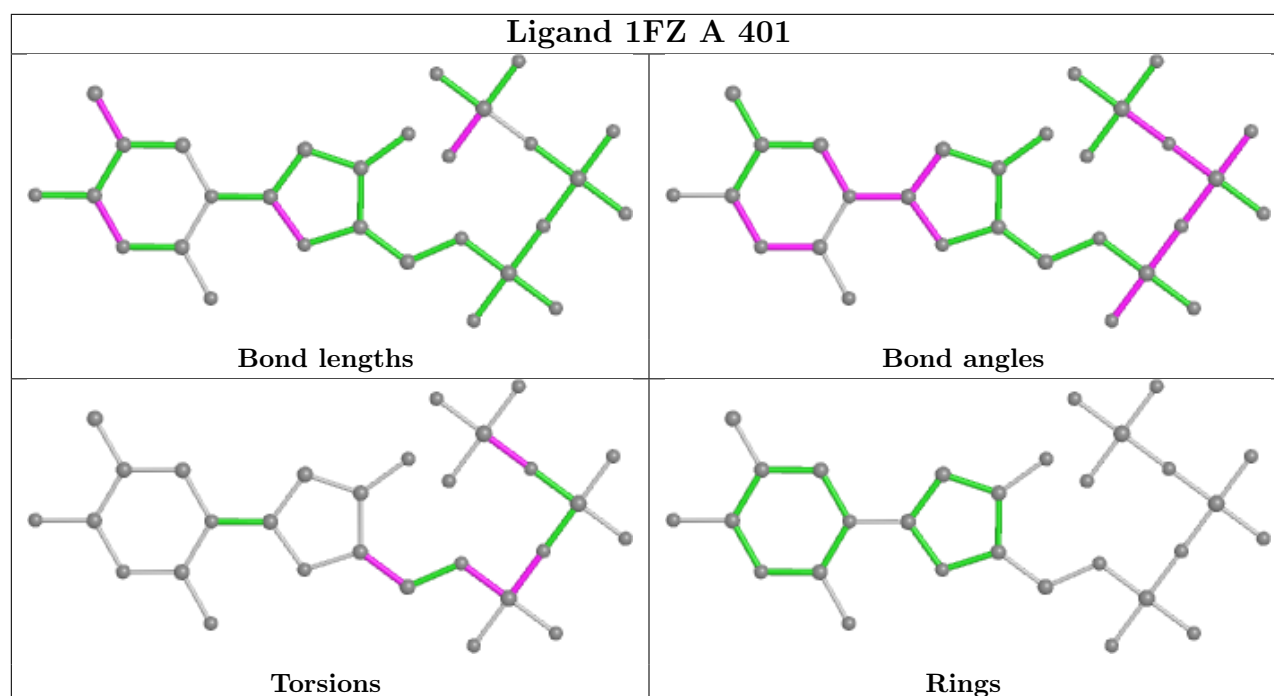
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	401	1FZ	2	0
4	A	401	1FZ	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	341/341 (100%)	0.55	26 (7%) 13 8	48, 74, 95, 106	0
1	D	341/341 (100%)	0.69	33 (9%) 7 4	50, 73, 93, 108	0
2	B	13/13 (100%)	-0.27	0 100 100	58, 81, 97, 98	0
2	P	13/13 (100%)	-0.08	0 100 100	57, 80, 96, 98	0
3	C	15/18 (83%)	-0.03	1 (6%) 17 12	52, 75, 97, 114	0
3	T	15/18 (83%)	-0.00	0 100 100	49, 74, 97, 120	0
All	All	738/744 (99%)	0.57	60 (8%) 12 7	48, 74, 95, 120	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	135	LYS	7.7
1	D	180	ILE	5.4
1	A	177	GLU	4.6
1	A	170	GLU	4.3
1	A	174	LEU	4.1
1	D	138	ILE	4.0
1	D	213	LEU	4.0
1	D	183	VAL	4.0
1	D	304	HIS	3.8
1	D	202	LEU	3.7
1	D	19	LEU	3.6
1	D	314	GLU	3.5
1	A	265	LEU	3.5
1	A	99	ILE	3.5
1	A	101	ILE	3.4
1	D	301	THR	3.3
1	D	55	VAL	3.3
1	D	200	ASN	3.2
1	D	205	THR	3.2

*Continued on next page...*



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Mol	Chain	Res	Type	RSRZ
1	A	258	LEU	3.2
1	A	136	GLU	3.1
1	D	1	MET	3.1
1	A	207	SER	3.1
1	A	91	LEU	3.0
1	A	116	ARG	3.0
1	D	190	THR	3.0
1	A	203	VAL	2.9
1	D	18	VAL	2.9
1	A	115	VAL	2.9
1	D	302	PHE	2.8
1	A	208	ILE	2.8
1	D	186	ILE	2.8
1	D	131	LYS	2.8
1	A	70	ASN	2.7
1	A	95	TYR	2.6
1	D	287	VAL	2.6
1	A	188	ASN	2.6
1	D	120	GLU	2.6
1	D	233	TYR	2.6
1	D	212	LYS	2.5
1	D	300	ARG	2.5
1	A	287	VAL	2.4
1	D	117	ASP	2.4
1	A	55	VAL	2.4
1	A	260	GLU	2.4
1	A	178	LEU	2.4
1	D	316	VAL	2.3
1	A	224	TYR	2.3
1	A	247	ARG	2.3
1	D	191	ALA	2.3
1	D	305	GLY	2.3
1	A	161	ASN	2.3
1	D	8	PHE	2.2
1	D	34	SER	2.1
3	C	3	DA	2.1
1	D	42	ALA	2.1
1	D	127	GLU	2.1
1	D	315	SER	2.1
1	A	219	GLU	2.0
1	A	206	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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( $\text{\AA}^2$ )	Q<0.9
3	A38	T	5	22/23	0.93	0.20	41,55,77,83	0
3	A38	C	5	22/23	0.94	0.20	44,54,74,75	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

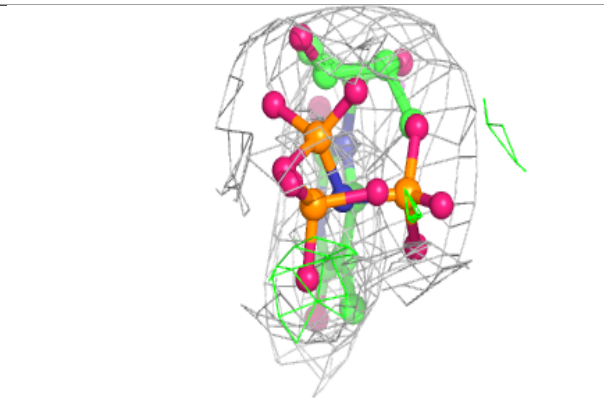
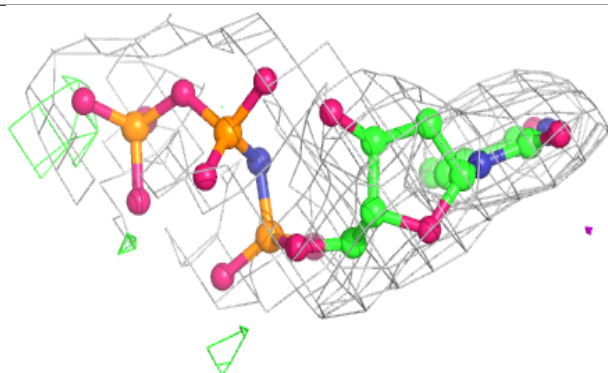
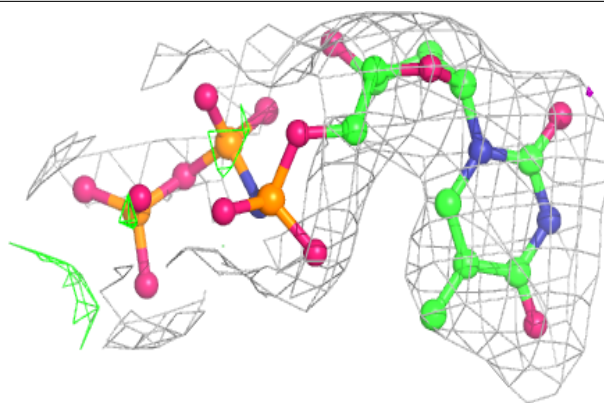
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	MG	A	403	1/1	0.83	0.15	49,49,49,49	0
5	MG	A	402	1/1	0.85	0.12	47,47,47,47	0
5	MG	B	101	1/1	0.90	0.32	48,48,48,48	0
5	MG	D	402	1/1	0.91	0.30	44,44,44,44	0
4	1FZ	A	401	29/29	0.94	0.18	42,48,57,62	0
4	1FZ	D	401	29/29	0.96	0.20	39,50,57,60	0

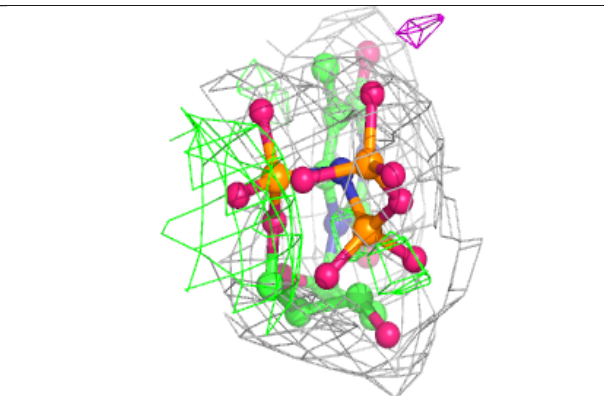
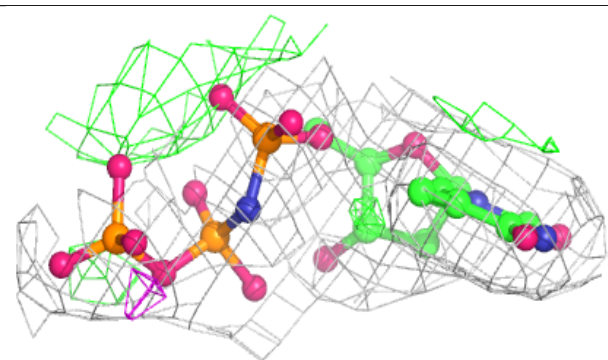
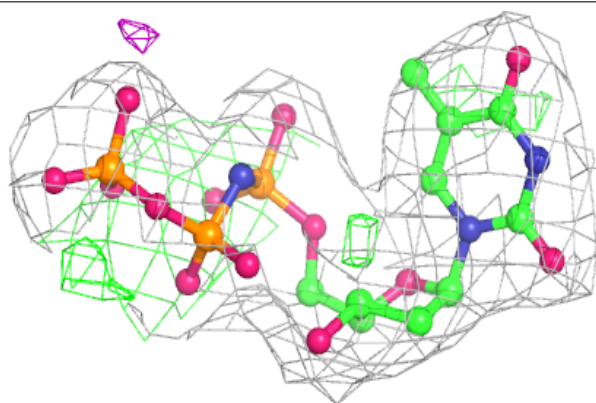
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 1FZ 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 1FZ D 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.