



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 06:05 am BST

PDB ID : 2Y1T  
Title : Bacillus subtilis prophage dUTPase in complex with dUDP  
Authors : Garcia-Nafria, J.; Harkiolaki, M.; Persson, R.; Fogg, M.J.; Wilson, K.S.  
Deposited on : 2010-12-10  
Resolution : 1.89 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

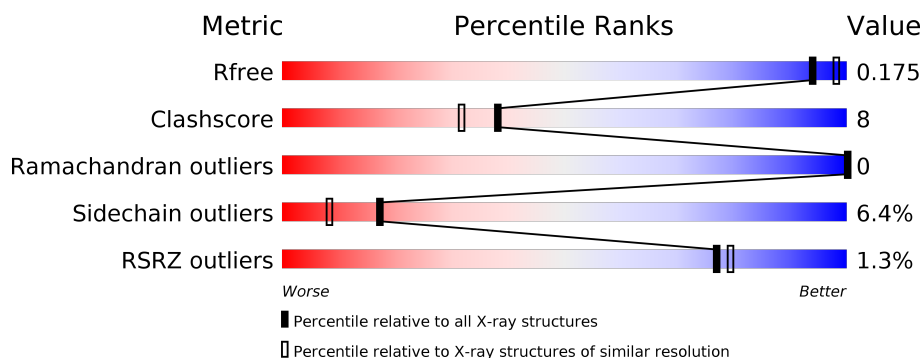
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.89 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	142	<div> <div>2%</div> <div> <div></div> <div>70%</div> <div>18%</div> <div>•</div> <div>10%</div> </div> </div>
1	B	142	<div> <div>%</div> <div> <div></div> <div>77%</div> <div>11%</div> <div>•</div> <div>10%</div> </div> </div>
1	C	142	<div> <div>%</div> <div> <div></div> <div>74%</div> <div>11%</div> <div>•</div> <div>12%</div> </div> </div>
1	D	142	<div> <div>%</div> <div> <div></div> <div>74%</div> <div>14%</div> <div>•</div> <div>10%</div> </div> </div>
1	E	142	<div> <div></div> <div> <div></div> <div>77%</div> <div>12%</div> <div>•</div> <div>11%</div> </div> </div>
1	F	142	<div> <div>%</div> <div> <div></div> <div>73%</div> <div>15%</div> <div>•</div> <div>11%</div> </div> </div>

## 2 Entry composition [i](#)

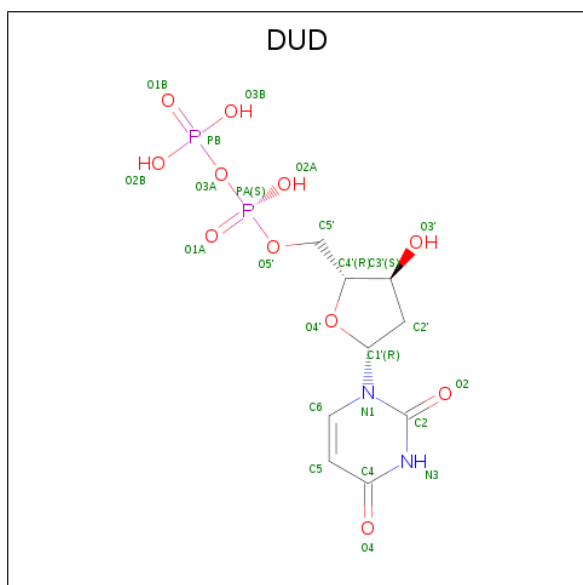
There are 3 unique types of molecules in this entry. The entry contains 6896 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SPBC2 PROPHAGE-DERIVED DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YOSS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	128	Total	C	N	O	S	12	3	0
			1058	678	179	194	7			
1	B	128	Total	C	N	O	S	26	2	0
			1051	672	178	194	7			
1	C	125	Total	C	N	O	S	6	2	0
			1028	659	174	189	6			
1	D	128	Total	C	N	O	S	12	1	0
			1049	671	178	193	7			
1	E	127	Total	C	N	O	S	25	1	0
			1037	665	174	191	7			
1	F	127	Total	C	N	O	S	22	2	0
			1046	670	177	193	6			

- Molecule 2 is DEOXYURIDINE-5'-DIPHOSPHATE (three-letter code: DUD) (formula:  $C_9H_{14}N_2O_{11}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			24	9	2	11	2		
2	C	1	Total	C	N	O	P	0	0
			24	9	2	11	2		
2	D	1	Total	C	N	O	P	0	0
			24	9	2	11	2		
2	E	1	Total	C	N	O	P	0	0
			24	9	2	11	2		
2	E	1	Total	C	N	O	P	0	0
			24	9	2	11	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	86	Total	O	0	0
			86	86		
3	B	92	Total	O	0	0
			92	92		
3	C	80	Total	O	0	0
			80	80		
3	D	75	Total	O	0	0
			75	75		
3	E	97	Total	O	0	0
			97	97		
3	F	77	Total	O	0	0
			77	77		

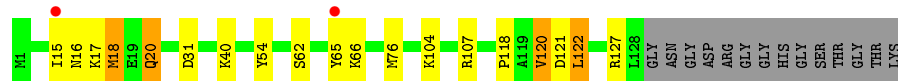
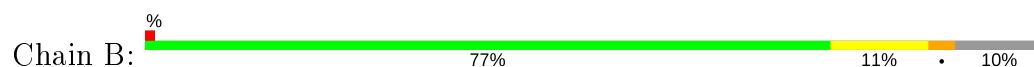
### 3 Residue-property plots [i](#)

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

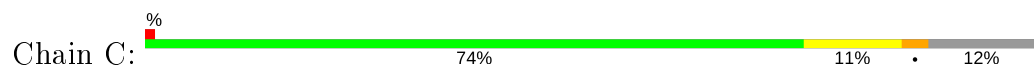
- Molecule 1: SPBC2 PROPHAGE-DERIVED DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YOSS



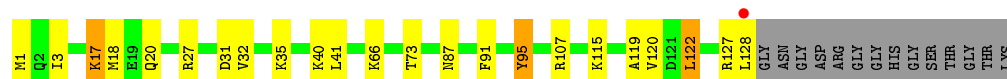
- Molecule 1: SPBC2 PROPHAGE-DERIVED DEOXYURIDINE 5'-TRIPHOSPHATE NUCLEOTIDOHYDROLASE YOSS



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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.52Å 99.34Å 99.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.31 – 1.89 19.89 – 1.89	Depositor EDS
% Data completeness (in resolution range)	98.9 (70.31-1.89) 99.1 (19.89-1.89)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.21 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.6.0086	Depositor
R, $R_{free}$	0.140 , 0.166 0.150 , 0.175	Depositor DCC
$R_{free}$ test set	3943 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.2	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 26.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.078 for k,h,-l 0.077 for -l,-k,-h 0.077 for -h,l,k 0.279 for l,h,k 0.279 for k,l,h	Xtriage
Reported twinning fraction	0.555 for H, K, L 0.408 for -L, -H, K 0.037 for K, -L, -H	Depositor
Outliers	0 of 78442 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	6896	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	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: DUD

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	1.32	3/1089 (0.3%)	1.05	4/1462 (0.3%)
1	B	1.23	1/1080 (0.1%)	1.00	1/1451 (0.1%)
1	C	1.31	2/1053 (0.2%)	1.09	3/1415 (0.2%)
1	D	1.29	1/1074 (0.1%)	1.10	3/1443 (0.2%)
1	E	1.38	3/1059 (0.3%)	1.11	4/1422 (0.3%)
1	F	1.23	0/1071	1.05	1/1438 (0.1%)
All	All	1.29	10/6426 (0.2%)	1.07	16/8631 (0.2%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	30	GLU	CD-OE1	-5.98	1.19	1.25
1	E	39	PHE	CD2-CE2	5.62	1.50	1.39
1	A	33	ALA	CA-CB	5.29	1.63	1.52
1	E	90	TRP	CB-CG	5.26	1.59	1.50
1	E	33	ALA	CA-CB	5.24	1.63	1.52
1	A	42	VAL	CB-CG1	5.20	1.63	1.52
1	C	33	ALA	CA-CB	5.18	1.63	1.52
1	C	35	LYS	CB-CG	-5.15	1.38	1.52
1	D	95	TYR	CD1-CE1	5.06	1.47	1.39
1	B	54	TYR	CG-CD1	5.03	1.45	1.39

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	25	ASP	CB-CG-OD2	-5.86	113.03	118.30
1	C	112	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	D	107	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	F	99	ASP	CB-CG-OD1	5.74	123.47	118.30
1	A	61	ARG	NE-CZ-NH1	5.66	123.13	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	31	ASP	CB-CG-OD1	5.64	123.37	118.30
1	E	114	MET	CG-SD-CE	-5.60	91.24	100.20
1	A	25	ASP	CB-CG-OD1	5.35	123.11	118.30
1	C	117	MET	CG-SD-CE	-5.32	91.68	100.20
1	C	31	ASP	CB-CG-OD1	5.27	123.05	118.30
1	E	80	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	D	27	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	B	107	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	E	117	MET	CG-SD-CE	-5.05	92.12	100.20
1	E	9	ASP	CB-CG-OD1	-5.04	113.76	118.30
1	A	65	TYR	CA-CB-CG	-5.04	103.83	113.40

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1058	0	1081	40	0
1	B	1051	0	1064	28	0
1	C	1028	0	1043	19	0
1	D	1049	0	1063	13	0
1	E	1037	0	1052	6	0
1	F	1046	0	1062	21	0
2	B	24	0	11	0	0
2	C	24	0	11	1	0
2	D	24	0	11	0	0
2	E	48	0	22	3	0
3	A	86	0	0	0	0
3	B	92	0	0	1	0
3	C	80	0	0	1	0
3	D	75	0	0	2	0
3	E	97	0	0	2	0
3	F	77	0	0	0	0
All	All	6896	0	6420	96	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 (96) 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:B:65:TYR:CE2	1:C:39:PHE:CD1	2.40	1.09
1:B:65:TYR:HE2	1:C:39:PHE:CG	1.75	1.04
1:B:65:TYR:CE2	1:C:39:PHE:CG	2.57	0.93
1:A:126:ASP:C	1:A:127:ARG:HG3	1.89	0.91
1:B:65:TYR:OH	1:C:95:TYR:HD2	1.58	0.84
1:A:76:MET:CE	1:B:76:MET:CE	2.56	0.83
1:A:76:MET:HE3	1:B:76:MET:HE3	1.69	0.74
1:A:76:MET:HE3	1:B:76:MET:CE	2.17	0.74
1:B:65:TYR:OH	1:C:95:TYR:CD2	2.37	0.74
1:D:41:LEU:HD22	1:D:91:PHE:HB3	1.69	0.73
1:A:33:ALA:O	1:A:40[B]:LYS:HE3	1.89	0.73
1:B:65:TYR:HH	1:C:95:TYR:HD2	0.76	0.70
1:F:15:ILE:CG2	1:F:16:ASN:N	2.56	0.69
1:A:76:MET:HE1	1:B:76:MET:CE	2.24	0.67
1:D:119:ALA:HB1	1:F:19:GLU:HA	1.77	0.67
1:E:62[A]:SER:HB2	2:E:143:DUD:O1B	1.96	0.65
1:E:1:MET:HG2	1:F:120:VAL:HG23	1.80	0.64
1:D:41:LEU:HD22	1:D:91:PHE:CB	2.28	0.64
1:A:18:MET:SD	1:A:24:ILE:CD1	2.86	0.64
1:B:31:ASP:OD1	1:B:104:LYS:N	2.22	0.63
1:A:76:MET:CE	1:B:76:MET:HE1	2.29	0.63
1:B:65:TYR:CD2	1:C:39:PHE:CE1	2.87	0.62
1:A:76:MET:CE	1:B:76:MET:HE3	2.27	0.62
1:A:18:MET:CE	1:A:24:ILE:HD11	2.31	0.61
1:B:15:ILE:HG23	3:B:2025:HOH:O	2.01	0.59
1:A:83:TYR:CE2	1:A:88:ASP:HB3	2.38	0.59
1:B:65:TYR:CD2	1:C:39:PHE:CD1	2.89	0.59
1:D:66:LYS:NZ	3:D:2042:HOH:O	2.22	0.58
1:A:18:MET:CG	1:A:24:ILE:HD11	2.33	0.58
1:A:41:LEU:HD22	1:A:91:PHE:HB3	1.85	0.58
1:E:62[B]:SER:OG	2:E:143:DUD:O1B	2.22	0.58
1:A:18:MET:HG2	1:A:24:ILE:CD1	2.35	0.56
1:A:76:MET:HE1	1:B:76:MET:HE1	1.85	0.56
1:A:126:ASP:O	1:A:127:ARG:HG3	2.06	0.56
1:B:18:MET:HB3	1:B:20:GLN:CG	2.36	0.56
1:A:18:MET:HG2	1:A:24:ILE:HD11	1.87	0.56
1:B:18:MET:HB3	1:B:20:GLN:HG3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:ILE:HG21	1:B:122:LEU:HD22	1.89	0.54
1:F:59:VAL:CG1	1:F:76:MET:HG3	2.38	0.54
1:A:18:MET:SD	1:A:24:ILE:HD11	2.48	0.53
1:A:76:MET:HE1	1:B:76:MET:SD	2.48	0.53
1:F:42:VAL:HG11	1:F:108:ILE:HD13	1.90	0.53
1:C:126:ASP:O	1:C:127:ARG:HD2	2.09	0.52
1:F:15:ILE:HG23	1:F:16:ASN:N	2.22	0.52
1:F:10:GLU:O	1:F:10:GLU:HG3	2.08	0.52
1:B:65:TYR:HE2	1:C:39:PHE:CB	2.23	0.52
1:A:120:VAL:HG21	1:C:3:ILE:HG13	1.92	0.51
1:D:17:LYS:NZ	1:E:120:VAL:O	2.32	0.51
1:A:44:LEU:CD2	1:A:108:ILE:HD11	2.41	0.50
1:A:18:MET:CE	1:A:24:ILE:CD1	2.89	0.50
1:A:123:ILE:HD12	1:C:2:GLN:OE1	2.11	0.49
1:D:119:ALA:CB	1:F:19:GLU:HA	2.42	0.49
1:F:44:LEU:HD21	1:F:108:ILE:HD11	1.95	0.49
1:F:61:ARG:HG3	1:F:109:CYS:HA	1.93	0.49
1:A:83:TYR:CZ	1:A:88:ASP:HB3	2.48	0.48
1:D:32:VAL:HG11	1:D:40:LYS:HG2	1.95	0.48
1:F:42:VAL:HG11	1:F:108:ILE:CD1	2.44	0.47
1:A:42:VAL:HG11	1:A:108:ILE:HD13	1.96	0.47
1:A:18:MET:HE3	1:A:24:ILE:CD1	2.44	0.47
1:A:83:TYR:CD2	1:A:88:ASP:HB3	2.50	0.46
1:F:59:VAL:HG12	1:F:76:MET:HG3	1.98	0.46
1:F:61:ARG:O	1:F:63:SER:N	2.48	0.46
1:C:56:ALA:HB3	1:C:79:ILE:HB	1.97	0.46
1:D:1:MET:HE3	3:E:2085:HOH:O	2.15	0.46
1:A:123:ILE:CD1	1:C:2:GLN:OE1	2.64	0.46
1:B:118:PRO:O	1:B:120:VAL:HG12	2.16	0.45
1:D:35:LYS:HE2	3:D:2026:HOH:O	2.16	0.45
1:D:122:LEU:HD12	1:F:5:ILE:HG21	1.98	0.45
1:A:44:LEU:HD21	1:A:108:ILE:HD11	1.98	0.45
1:F:60:PRO:HD3	1:F:72:GLN:OE1	2.16	0.45
1:A:126:ASP:O	1:A:127:ARG:CG	2.65	0.45
1:F:15:ILE:HG22	1:F:16:ASN:N	2.26	0.44
2:E:144:DUD:O2A	3:E:2097:HOH:O	2.21	0.44
1:A:18:MET:CG	1:A:24:ILE:CD1	2.96	0.44
1:B:65:TYR:OH	1:C:39:PHE:HB2	2.17	0.44
1:B:20:GLN:HG2	1:B:20:GLN:H	0.99	0.43
1:C:115:LYS:HD3	1:C:116:LYS:N	2.33	0.43
1:D:3:ILE:HB	1:E:122:LEU:HD23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:114:MET:HE3	1:F:114:MET:HB2	1.81	0.43
1:F:15:ILE:HD13	1:F:15:ILE:HG21	1.72	0.43
1:A:18:MET:HE3	1:A:24:ILE:HD12	2.01	0.43
1:A:76:MET:CE	1:B:76:MET:SD	3.07	0.42
1:A:126:ASP:C	1:A:127:ARG:CG	2.71	0.42
1:A:123:ILE:HD12	1:C:2:GLN:CD	2.40	0.42
1:A:18:MET:HE1	1:B:120:VAL:HG11	2.01	0.42
1:D:73:THR:CG2	1:D:95:TYR:HB2	2.50	0.42
1:C:33:ALA:O	1:C:40:LYS:HE2	2.20	0.41
1:A:32:VAL:HG11	1:A:40[A]:LYS:HG2	2.03	0.41
1:F:5:ILE:HD11	1:F:46:VAL:CG1	2.50	0.41
1:C:32:VAL:HG13	1:C:40:LYS:HD3	2.03	0.40
1:A:117:MET:HE3	3:C:2017:HOH:O	2.21	0.40
1:A:32:VAL:HG13	1:A:40[B]:LYS:HD2	2.04	0.40
1:D:128:LEU:CD1	1:F:6:LYS:HB2	2.51	0.40
1:B:62[A]:SER:OG	2:C:143:DUD:O2B	2.39	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	129/142 (91%)	124 (96%)	5 (4%)	0	100	100
1	B	128/142 (90%)	127 (99%)	1 (1%)	0	100	100
1	C	123/142 (87%)	120 (98%)	3 (2%)	0	100	100
1	D	127/142 (89%)	125 (98%)	2 (2%)	0	100	100
1	E	124/142 (87%)	121 (98%)	3 (2%)	0	100	100
1	F	125/142 (88%)	123 (98%)	2 (2%)	0	100	100
All	All	756/852 (89%)	740 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	116/121 (96%)	110 (95%)	6 (5%)	23	14
1	B	115/121 (95%)	105 (91%)	10 (9%)	10	4
1	C	112/121 (93%)	106 (95%)	6 (5%)	22	13
1	D	114/121 (94%)	106 (93%)	8 (7%)	15	7
1	E	113/121 (93%)	106 (94%)	7 (6%)	18	9
1	F	114/121 (94%)	108 (95%)	6 (5%)	22	13
All	All	684/726 (94%)	641 (94%)	43 (6%)	17	8

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	20	GLN
1	A	87	ASN
1	A	115	LYS
1	A	122	LEU
1	A	127	ARG
1	B	16	ASN
1	B	17	LYS
1	B	18	MET
1	B	20	GLN
1	B	40	LYS
1	B	66	LYS
1	B	120	VAL
1	B	121	ASP
1	B	122	LEU
1	B	127	ARG
1	C	20	GLN
1	C	87	ASN
1	C	115	LYS

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Mol	Chain	Res	Type
1	C	122	LEU
1	C	126	ASP
1	C	127	ARG
1	D	17	LYS
1	D	18	MET
1	D	20	GLN
1	D	87	ASN
1	D	115	LYS
1	D	120	VAL
1	D	122	LEU
1	D	127	ARG
1	E	17	LYS
1	E	20	GLN
1	E	40	LYS
1	E	115	LYS
1	E	122	LEU
1	E	127	ARG
1	E	128	LEU
1	F	10	GLU
1	F	16	ASN
1	F	17	LYS
1	F	35	LYS
1	F	40	LYS
1	F	115	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	2	GLN
1	C	16	ASN
1	D	87	ASN
1	F	16	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

5 ligands 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
2	DUD	D	143	-	20,25,25	1.42	2 (10%)	25,38,38	1.28	4 (16%)
2	DUD	B	143	-	20,25,25	1.27	4 (20%)	25,38,38	1.64	5 (20%)
2	DUD	C	143	-	20,25,25	1.75	4 (20%)	25,38,38	1.35	2 (8%)
2	DUD	E	144	-	20,25,25	1.19	2 (10%)	25,38,38	1.43	5 (20%)
2	DUD	E	143	-	20,25,25	1.72	3 (15%)	25,38,38	1.18	4 (16%)

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
2	DUD	D	143	-	-	4/13/28/28	0/2/2/2
2	DUD	B	143	-	-	2/13/28/28	0/2/2/2
2	DUD	C	143	-	-	6/13/28/28	0/2/2/2
2	DUD	E	144	-	-	5/13/28/28	0/2/2/2
2	DUD	E	143	-	-	6/13/28/28	0/2/2/2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	143	DUD	PB-O1B	5.14	1.67	1.50
2	E	143	DUD	C6-N1	-4.49	1.30	1.35
2	D	143	DUD	C2-N3	-4.20	1.29	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	143	DUD	C2-N3	-3.91	1.30	1.38
2	D	143	DUD	C4-N3	3.73	1.39	1.33
2	C	143	DUD	C6-C5	2.78	1.44	1.38
2	C	143	DUD	O4'-C4'	-2.70	1.39	1.45
2	B	143	DUD	C2-N3	-2.61	1.33	1.38
2	E	143	DUD	PB-O2B	-2.45	1.45	1.54
2	B	143	DUD	O4-C4	2.34	1.30	1.24
2	C	143	DUD	PB-O2B	2.28	1.63	1.54
2	E	144	DUD	C6-N1	2.27	1.38	1.35
2	B	143	DUD	C1'-N1	-2.18	1.42	1.49
2	B	143	DUD	C6-N1	2.08	1.38	1.35
2	E	144	DUD	PB-O1B	2.05	1.57	1.50

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	143	DUD	O5'-PA-O1A	-4.02	93.34	109.07
2	B	143	DUD	O2A-PA-O1A	3.46	129.34	112.24
2	C	143	DUD	O3B-PB-O3A	-3.16	94.04	104.64
2	E	144	DUD	O4'-C4'-C3'	-2.94	98.81	105.67
2	E	144	DUD	O2A-PA-O1A	2.85	126.34	112.24
2	D	143	DUD	O2A-PA-O1A	2.76	125.89	112.24
2	B	143	DUD	O3A-PB-O1B	-2.66	96.41	111.19
2	B	143	DUD	O2B-PB-O3A	2.59	113.32	104.64
2	E	143	DUD	O5'-C5'-C4'	2.44	117.38	108.99
2	B	143	DUD	O3B-PB-O2B	2.43	116.94	107.64
2	E	143	DUD	C6-N1-C2	-2.43	117.34	121.20
2	E	144	DUD	O3B-PB-O3A	2.39	112.66	104.64
2	D	143	DUD	C5-C4-N3	-2.36	118.11	123.31
2	D	143	DUD	O2A-PA-O5'	2.34	118.61	107.75
2	C	143	DUD	O2A-PA-O1A	2.32	123.69	112.24
2	D	143	DUD	O3B-PB-O2B	2.29	116.38	107.64
2	E	144	DUD	O3B-PB-O2B	2.23	116.17	107.64
2	E	143	DUD	C5-C4-N3	-2.13	118.62	123.31
2	E	144	DUD	O2A-PA-O5'	-2.13	97.86	107.75
2	E	143	DUD	O3B-PB-O3A	2.06	111.55	104.64

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	143	DUD	O4'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
2	E	144	DUD	O4'-C1'-N1-C6
2	E	144	DUD	PA-O3A-PB-O2B
2	C	143	DUD	O4'-C1'-N1-C6
2	C	143	DUD	C5'-O5'-PA-O3A
2	B	143	DUD	O4'-C1'-N1-C6
2	E	143	DUD	O4'-C1'-N1-C6
2	E	143	DUD	O4'-C4'-C5'-O5'
2	E	143	DUD	C5'-O5'-PA-O3A
2	C	143	DUD	O4'-C4'-C5'-O5'
2	E	143	DUD	C3'-C4'-C5'-O5'
2	D	143	DUD	PA-O3A-PB-O1B
2	E	144	DUD	PB-O3A-PA-O5'
2	C	143	DUD	PB-O3A-PA-O5'
2	E	143	DUD	PB-O3A-PA-O5'
2	C	143	DUD	C5'-O5'-PA-O1A
2	E	143	DUD	C5'-O5'-PA-O1A
2	D	143	DUD	O4'-C4'-C5'-O5'
2	C	143	DUD	PB-O3A-PA-O2A
2	D	143	DUD	C3'-C4'-C5'-O5'
2	B	143	DUD	O4'-C4'-C5'-O5'
2	E	144	DUD	PA-O3A-PB-O3B
2	E	144	DUD	O4'-C4'-C5'-O5'

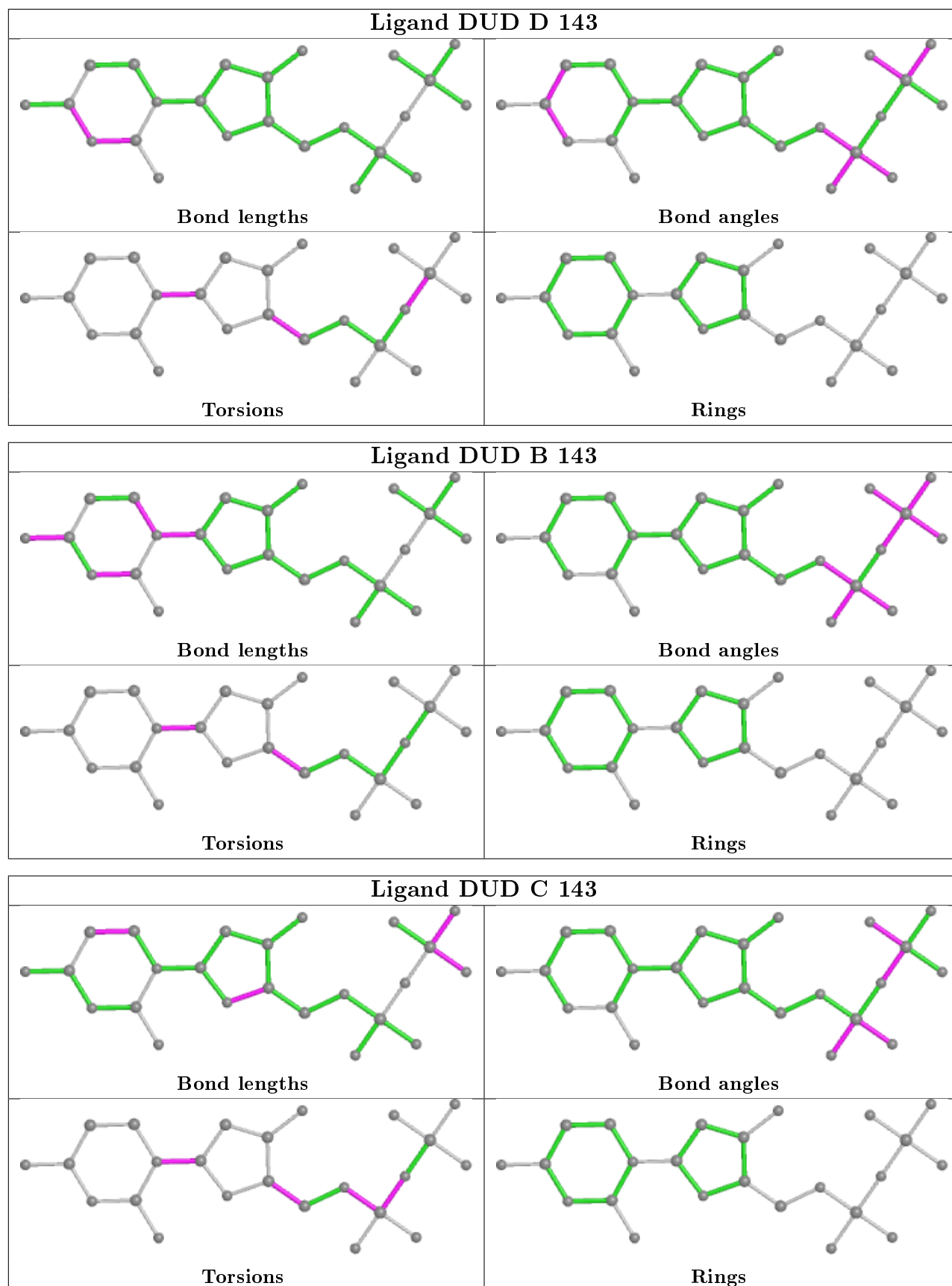
There are no ring outliers.

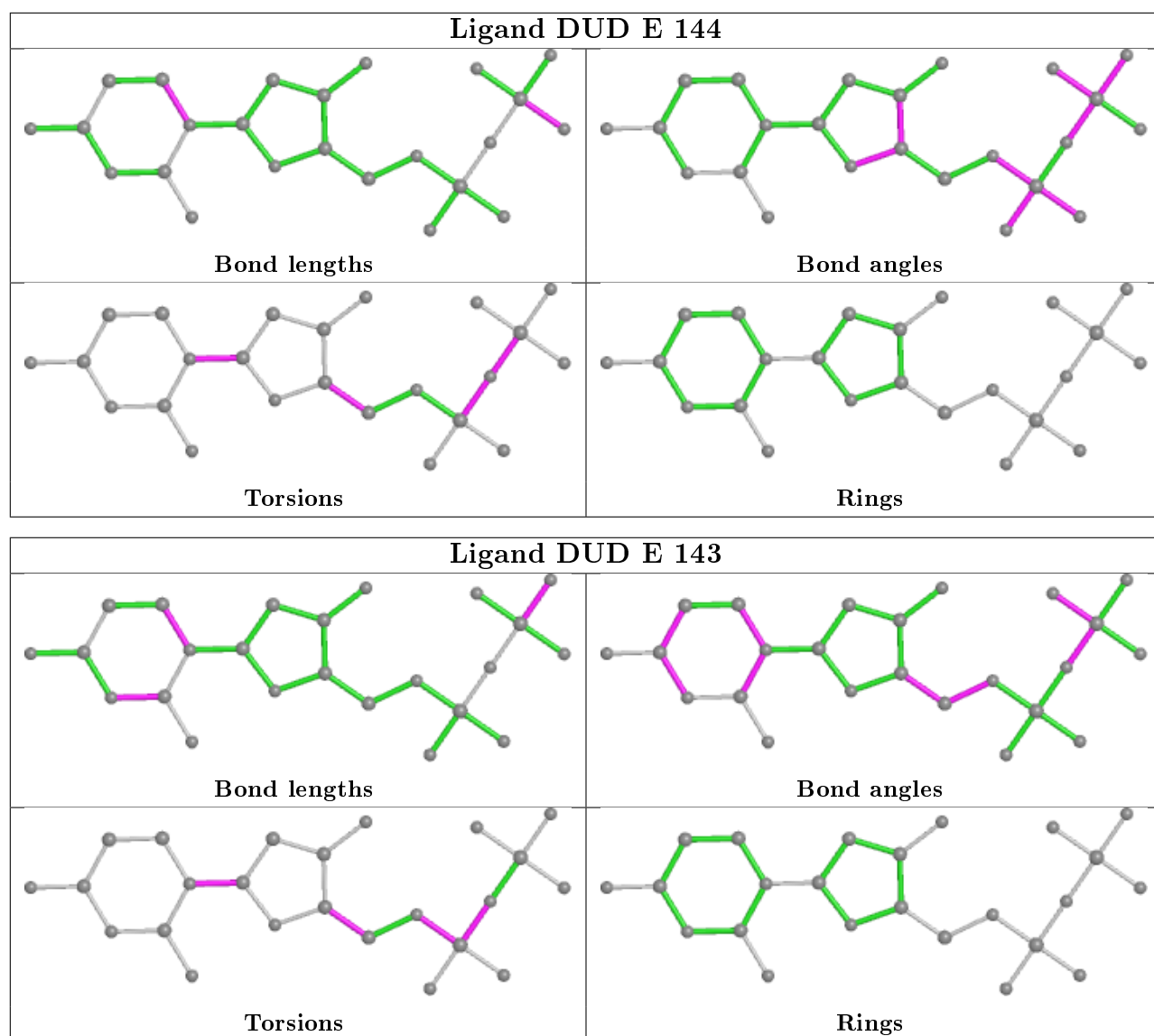
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	143	DUD	1	0
2	E	144	DUD	1	0
2	E	143	DUD	2	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	128/142 (90%)	-0.16	3 (2%) 60 63	15, 23, 40, 51	3 (2%)
1	B	128/142 (90%)	-0.21	2 (1%) 72 74	16, 23, 40, 58	7 (5%)
1	C	125/142 (88%)	-0.28	2 (1%) 72 74	16, 23, 38, 54	2 (1%)
1	D	128/142 (90%)	-0.22	1 (0%) 86 87	15, 23, 40, 58	3 (2%)
1	E	127/142 (89%)	-0.27	0 100 100	14, 21, 36, 49	7 (5%)
1	F	127/142 (89%)	-0.13	2 (1%) 72 74	15, 24, 39, 58	6 (4%)
All	All	763/852 (89%)	-0.21	10 (1%) 77 79	14, 23, 40, 58	28 (3%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	18	MET	4.6
1	B	65	TYR	4.4
1	A	17	LYS	2.4
1	F	19	GLU	2.4
1	C	16	ASN	2.3
1	B	15	ILE	2.2
1	C	127	ARG	2.1
1	F	10	GLU	2.1
1	D	128	LEU	2.1
1	A	83	TYR	2.0

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

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

## 6.3 Carbohydrates [i](#)

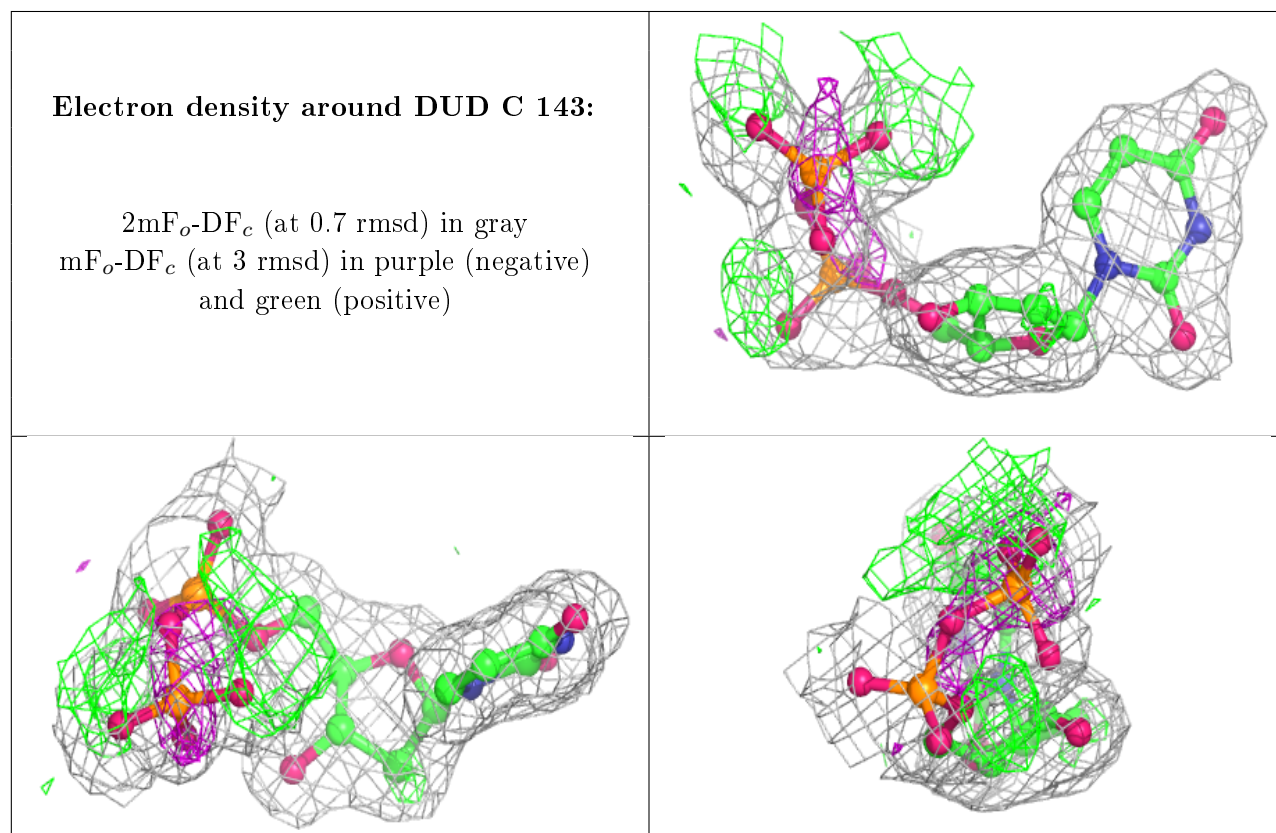
There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

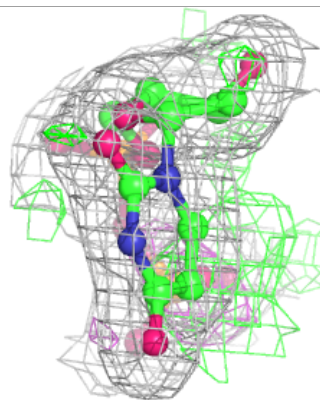
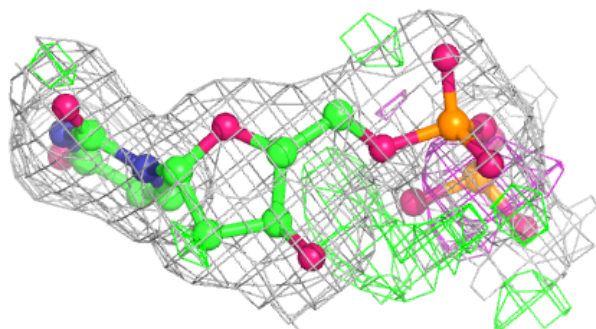
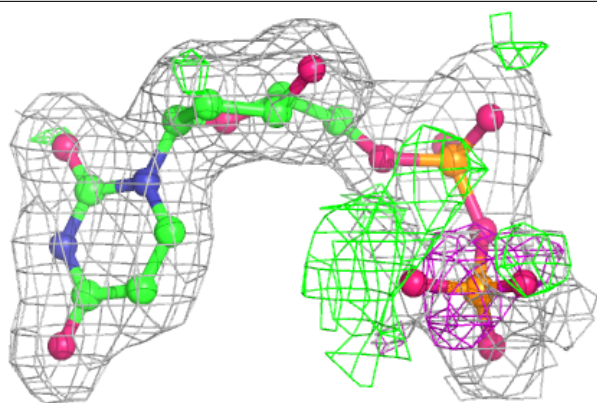
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	DUD	C	143	24/24	0.82	0.13	19,31,63,68	0
2	DUD	E	143	24/24	0.86	0.12	22,34,54,56	0
2	DUD	E	144	24/24	0.92	0.10	22,28,49,49	0
2	DUD	B	143	24/24	0.98	0.09	20,23,30,32	0
2	DUD	D	143	24/24	0.98	0.10	20,25,32,38	0

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.

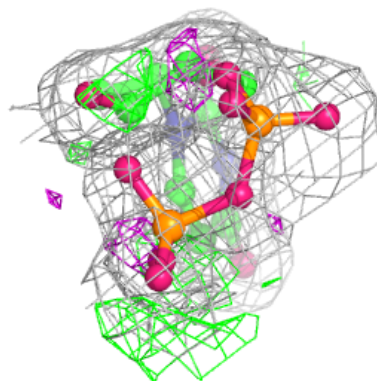
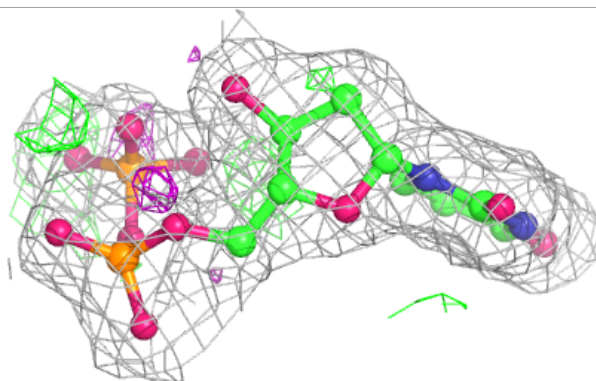
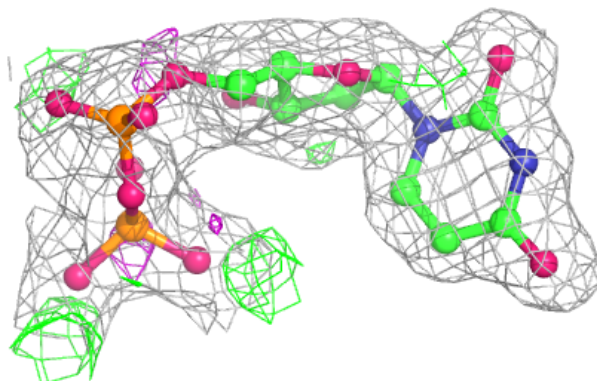


**Electron density around DUD E 143:**

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

**Electron density around DUD E 144:**

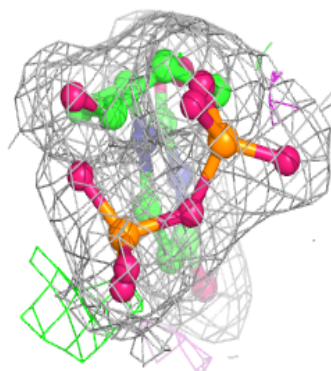
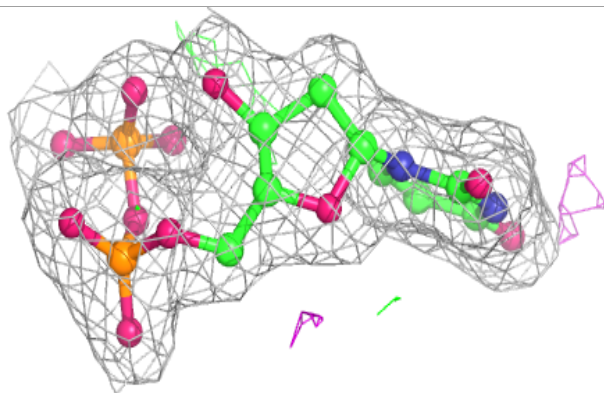
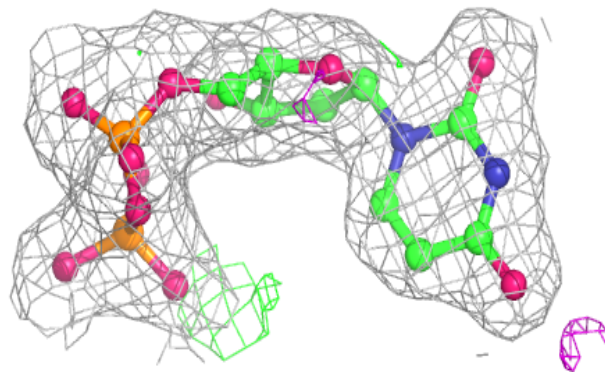
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



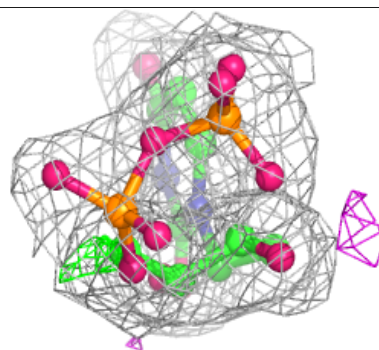
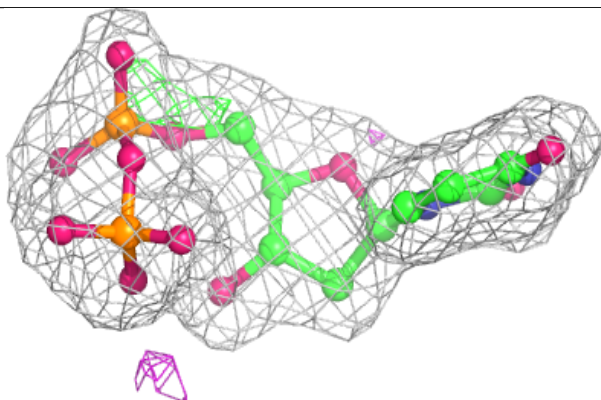
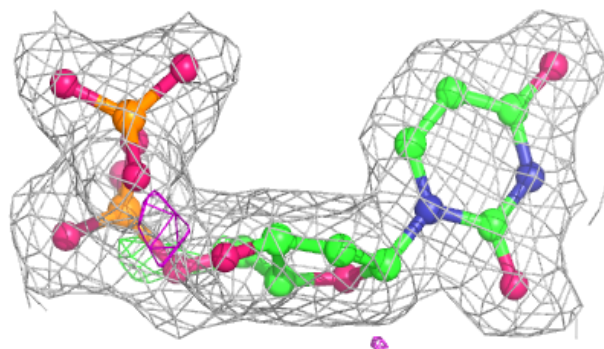


**Electron density around DUD B 143:**

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

**Electron density around DUD D 143:**

$2mF_o-DF_c$  (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.