



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 29, 2024 – 09:52 PM EDT

PDB ID : 3U60  
Title : Structure of T4 Bacteriophage Clamp Loader Bound To Open Clamp, DNA and ATP Analog  
Authors : Kelch, B.A.; Makino, D.L.; O'Donnell, M.; Kuriyan, J.  
Deposited on : 2011-10-11  
Resolution : 3.34 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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.

The types of validation reports are described at

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

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

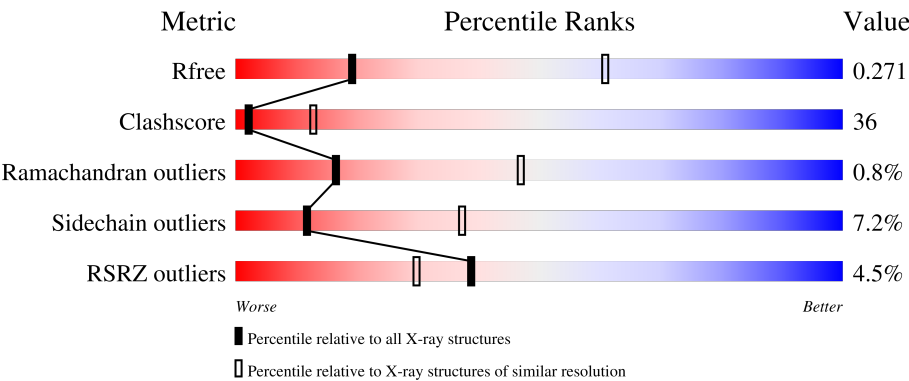
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

# 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 3.34 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 <sub>free</sub>	164625	1325 (3.38-3.30)
Clashscore	180529	1376 (3.38-3.30)
Ramachandran outliers	177936	1376 (3.38-3.30)
Sidechain outliers	177891	1375 (3.38-3.30)
RSRZ outliers	164620	1325 (3.38-3.30)

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  $\geq 3$ , 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	B	324	<div><div>5%</div><div><div></div><div></div><div></div><div></div></div><div>60%33%5%</div></div>
1	C	324	<div><div>2%</div><div><div></div><div></div><div></div><div></div></div><div>54%40%</div></div>
1	D	324	<div><div>3%</div><div><div></div><div></div><div></div><div></div></div><div>58%36%</div></div>
1	E	324	<div><div>8%</div><div><div></div><div></div><div></div><div></div></div><div>51%38%5%6%</div></div>
2	I	30	<div><div>3%</div><div><div></div><div></div><div></div><div></div></div><div>30%47%20%</div></div>

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Mol	Chain	Length	Quality of chain
3	J	20	
4	A	195	
5	F	228	
5	G	228	
5	H	228	

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 17695 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 accessory protein 44.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	319	Total	C	N	O	S	0	0	0
			2509	1587	431	474	17			
1	C	320	Total	C	N	O	S	0	0	0
			2515	1590	432	476	17			
1	D	319	Total	C	N	O	S	0	0	0
			2503	1584	428	474	17			
1	E	305	Total	C	N	O	S	0	0	0
			2409	1527	413	453	16			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLY	-	expression tag	UNP P04526
B	-3	PRO	-	expression tag	UNP P04526
B	-2	GLY	-	expression tag	UNP P04526
B	-1	GLY	-	expression tag	UNP P04526
B	0	SER	-	expression tag	UNP P04526
C	-4	GLY	-	expression tag	UNP P04526
C	-3	PRO	-	expression tag	UNP P04526
C	-2	GLY	-	expression tag	UNP P04526
C	-1	GLY	-	expression tag	UNP P04526
C	0	SER	-	expression tag	UNP P04526
D	-4	GLY	-	expression tag	UNP P04526
D	-3	PRO	-	expression tag	UNP P04526
D	-2	GLY	-	expression tag	UNP P04526
D	-1	GLY	-	expression tag	UNP P04526
D	0	SER	-	expression tag	UNP P04526
E	-4	GLY	-	expression tag	UNP P04526
E	-3	PRO	-	expression tag	UNP P04526
E	-2	GLY	-	expression tag	UNP P04526
E	-1	GLY	-	expression tag	UNP P04526
E	0	SER	-	expression tag	UNP P04526

- Molecule 2 is a DNA chain called Template DNA strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	24	Total	C	N	O	P	0	0	0
			489	236	76	153	24			

- Molecule 3 is a DNA chain called Primer DNA strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	20	Total	C	N	O	P	0	0	0
			408	195	81	113	19			

- Molecule 4 is a protein called DNA polymerase accessory protein 62.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	186	Total	C	N	O	S	0	0	0
			1488	959	244	279	6			

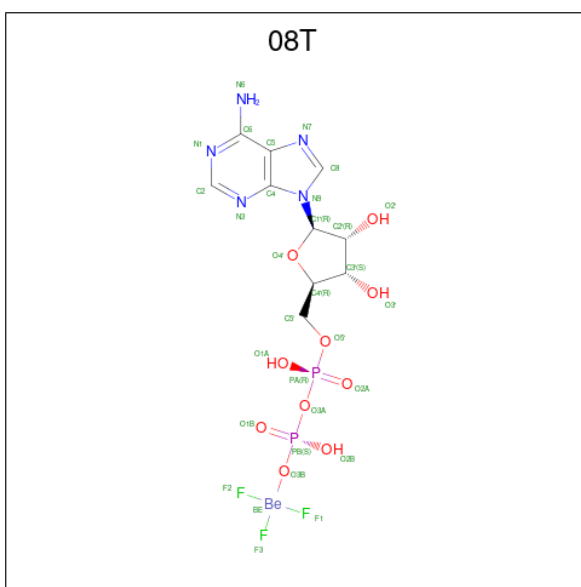
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	188	GLY	-	expression tag	UNP P04527
A	189	LEU	-	expression tag	UNP P04527
A	190	GLU	-	expression tag	UNP P04527
A	191	HIS	-	expression tag	UNP P04527
A	192	HIS	-	expression tag	UNP P04527
A	193	HIS	-	expression tag	UNP P04527
A	194	HIS	-	expression tag	UNP P04527
A	195	HIS	-	expression tag	UNP P04527
A	196	HIS	-	expression tag	UNP P04527

- Molecule 5 is a protein called DNA polymerase processivity component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	G	228	Total	C	N	O	Se	0	0	0
			1750	1113	288	343	6			
5	H	228	Total	C	N	O	Se	0	0	0
			1750	1113	288	343	6			
5	F	228	Total	C	N	O	Se	0	0	0
			1750	1113	288	343	6			

- Molecule 6 is [|(2R,3S,4R,5R)-5-(6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl]oxy-oxidanyl-phosphoryl]oxy-tris(fluoranyl)beryllium (three-letter code: 08T) (formula: C<sub>10</sub>H<sub>14</sub>BeF<sub>3</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
6	B	1	Total	Be	C	F	N	O	P	0	0
			31	1	10	3	5	10	2		
6	C	1	Total	Be	C	F	N	O	P	0	0
			31	1	10	3	5	10	2		
6	D	1	Total	Be	C	F	N	O	P	0	0
			31	1	10	3	5	10	2		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Mg	0	0
			1	1		
7	C	1	Total	Mg	0	0
			1	1		
7	D	1	Total	Mg	0	0
			1	1		
7	E	1	Total	Mg	0	0
			1	1		

- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).

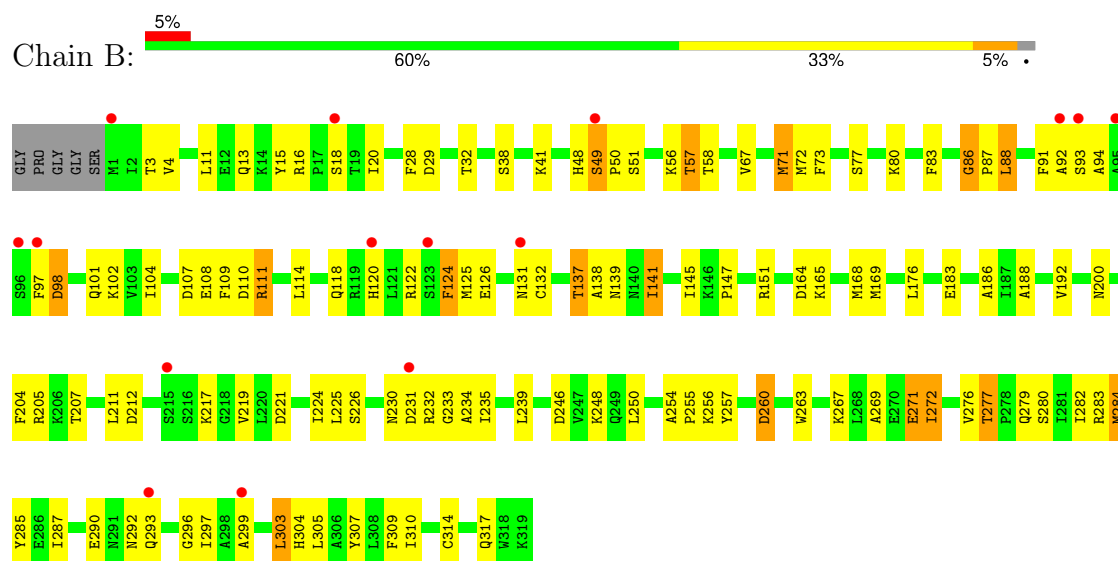


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

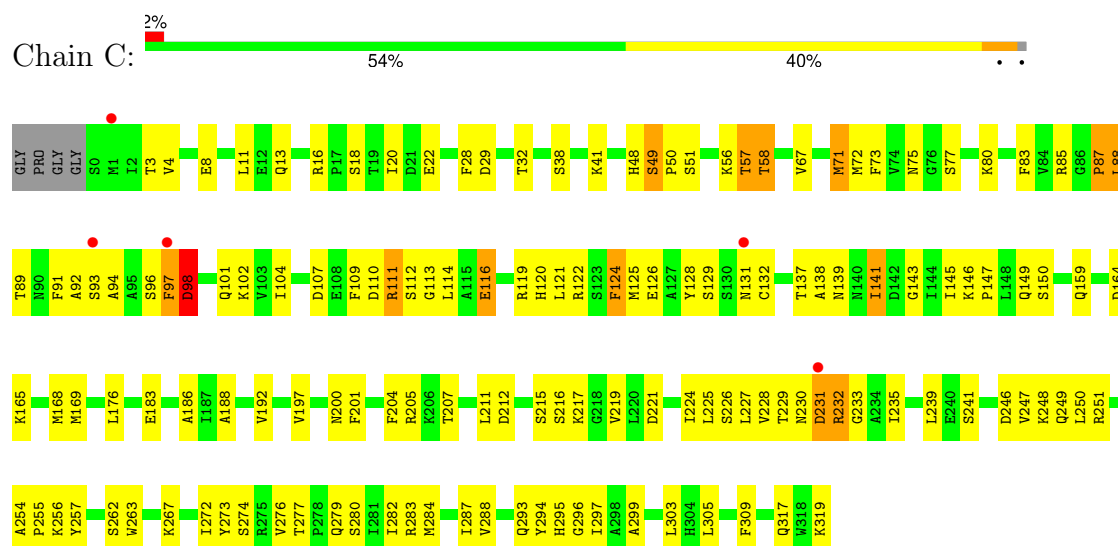
### 3 Residue-property plots [i](#)

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 accessory protein 44



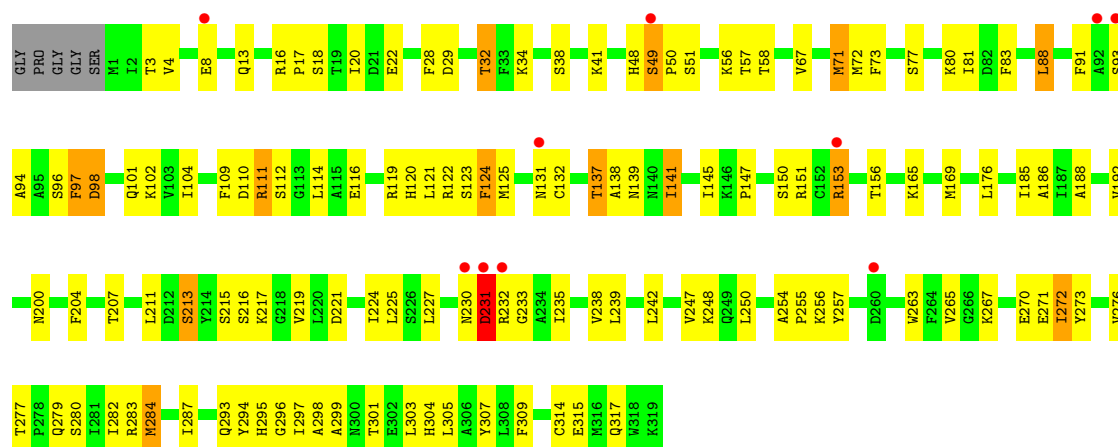
- Molecule 1: DNA polymerase accessory protein 44



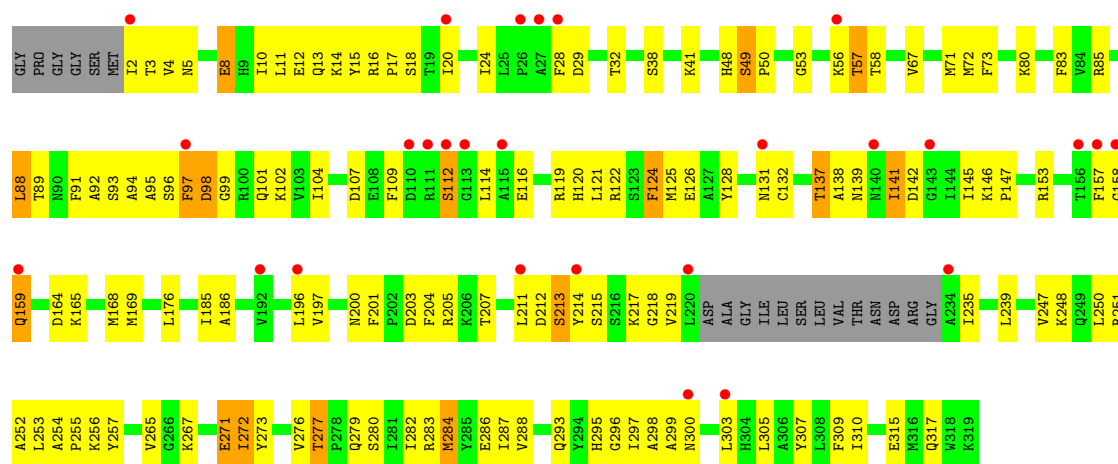
- Molecule 1: DNA polymerase accessory protein 44







• Molecule 1: DNA polymerase accessory protein 44



• Molecule 2: Template DNA strand

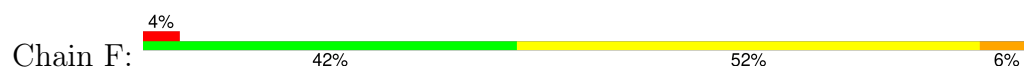


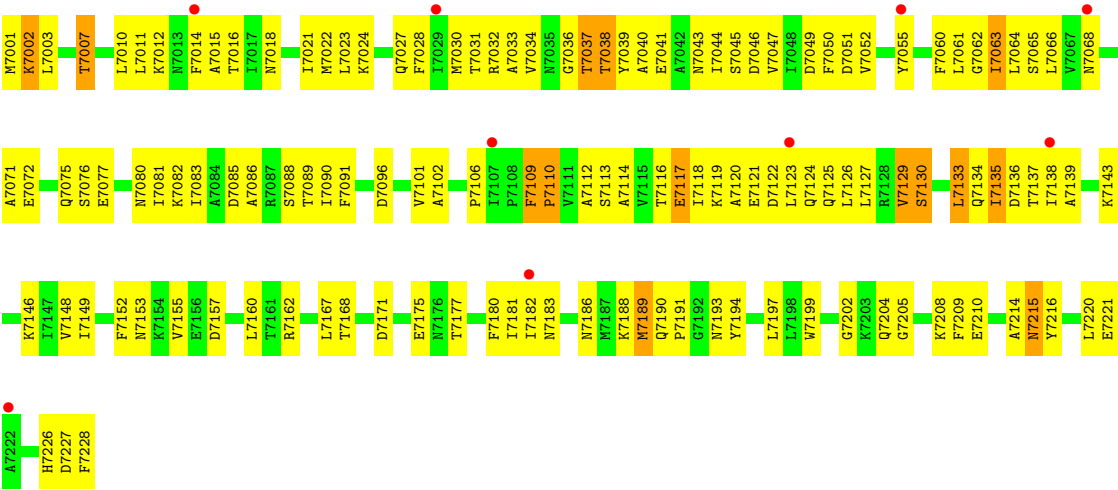
• Molecule 3: Primer DNA strand



• Molecule 4: DNA polymerase accessory protein 62







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.52Å 118.44Å 133.08Å 90.00° 102.06° 90.00°	Depositor
Resolution (Å)	49.71 – 3.34 49.71 – 3.34	Depositor EDS
% Data completeness (in resolution range)	93.8 (49.71-3.34) 93.2 (49.71-3.34)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.20	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.66 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, $R_{free}$	0.244 , 0.282 0.237 , 0.271	Depositor DCC
$R_{free}$ test set	1648 reflections (4.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.5	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 47.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	17695	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 2.94% 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: 08T, MG, ADP

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	B	0.56	0/2553	0.76	3/3441 (0.1%)
1	C	0.55	1/2559 (0.0%)	0.75	5/3449 (0.1%)
1	D	0.57	0/2547	0.74	4/3434 (0.1%)
1	E	0.58	0/2452	0.76	3/3303 (0.1%)
2	I	1.01	0/544	2.02	26/838 (3.1%)
3	J	1.03	0/459	1.82	17/706 (2.4%)
4	A	0.58	0/1516	0.86	1/2042 (0.0%)
5	F	0.43	0/1774	0.78	7/2395 (0.3%)
5	G	0.43	0/1774	0.76	4/2395 (0.2%)
5	H	0.45	0/1774	0.73	2/2395 (0.1%)
All	All	0.57	1/17952 (0.0%)	0.88	72/24398 (0.3%)

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	B	0	3
1	C	0	2
1	D	0	3
1	E	0	2
4	A	0	1
All	All	0	11

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	87	PRO	N-CD	5.39	1.55	1.47

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	21	DT	O4'-C1'-N1	12.68	116.88	108.00
3	J	20	DA	O4'-C1'-N9	10.43	115.30	108.00
2	I	19	DC	O4'-C1'-N1	-10.11	100.93	108.00
2	I	16	DA	O4'-C1'-N9	9.96	114.97	108.00
1	E	112	SER	CB-CA-C	-9.49	92.08	110.10

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	296	GLY	Peptide
1	B	49	SER	Peptide
1	B	86	GLY	Mainchain
1	C	229	THR	Peptide
1	C	296	GLY	Peptide

## 5.2 Too-close contacts [i](#)

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	B	2509	0	2538	168	0
1	C	2515	0	2543	194	2
1	D	2503	0	2527	201	0
1	E	2409	0	2433	192	1
2	I	489	0	277	46	0
3	J	408	0	225	27	0
4	A	1488	0	1509	165	0
5	F	1750	0	1752	173	0
5	G	1750	0	1752	142	0
5	H	1750	0	1752	188	1
6	B	31	0	13	3	0
6	C	31	0	13	2	0
6	D	31	0	13	4	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	E	1	0	0	0	0
8	E	27	0	12	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	17695	0	17359	1260	3

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 36.

The worst 5 of 1260 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)
5:F:7028:PHE:CZ	5:F:7030:MSE:HE2	1.22	1.68
5:F:7028:PHE:CZ	5:F:7030:MSE:CE	1.93	1.50
4:A:167:LEU:CD1	4:A:180:LEU:HD21	1.51	1.40
4:A:167:LEU:HD11	4:A:180:LEU:CD2	1.55	1.36
5:F:7028:PHE:CE2	5:F:7030:MSE:CE	2.10	1.33

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:GLU:OE1	1:C:248:LYS:NZ[2_655]	1.58	0.62
1:C:183:GLU:CD	1:C:248:LYS:NZ[2_655]	2.14	0.06
1:E:185:ILE:C	5:H:6212:GLU:OE1[2_646]	2.19	0.01

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	317/324 (98%)	304 (96%)	13 (4%)	0	100	100
1	C	318/324 (98%)	305 (96%)	12 (4%)	1 (0%)	37	66
1	D	317/324 (98%)	303 (96%)	14 (4%)	0	100	100
1	E	301/324 (93%)	294 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	184/195 (94%)	161 (88%)	20 (11%)	3 (2%)	8	33
5	F	226/228 (99%)	179 (79%)	44 (20%)	3 (1%)	10	37
5	G	226/228 (99%)	183 (81%)	40 (18%)	3 (1%)	10	37
5	H	226/228 (99%)	184 (81%)	35 (16%)	7 (3%)	3	21
All	All	2115/2175 (97%)	1913 (90%)	185 (9%)	17 (1%)	16	47

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	232	ARG
4	A	38	ASN
4	A	150	LYS
5	G	5106	PRO
5	F	7037	THR

### 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	B	277/279 (99%)	254 (92%)	23 (8%)	9	32
1	C	278/279 (100%)	256 (92%)	22 (8%)	10	34
1	D	276/279 (99%)	255 (92%)	21 (8%)	11	35
1	E	266/279 (95%)	245 (92%)	21 (8%)	10	34
4	A	161/170 (95%)	139 (86%)	22 (14%)	3	13
5	F	189/183 (103%)	183 (97%)	6 (3%)	34	61
5	G	189/183 (103%)	182 (96%)	7 (4%)	29	57
5	H	189/183 (103%)	179 (95%)	10 (5%)	19	47
All	All	1825/1835 (100%)	1693 (93%)	132 (7%)	12	37

5 of 132 residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
5	G	5189	MSE
5	H	6116	THR
5	F	7189	MSE
1	D	38	SER
1	D	32	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
5	G	5215	ASN
5	H	6043	ASN
5	H	6027	GLN
5	H	6153	ASN
1	D	13	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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
8	ADP	E	700	7	24,29,29	0.92	1 (4%)	29,45,45	1.37	6 (20%)
6	08T	D	700	7	27,33,33	2.06	7 (25%)	27,52,52	1.54	3 (11%)
6	08T	C	700	7	27,33,33	1.90	7 (25%)	27,52,52	1.46	3 (11%)
6	08T	B	700	7	27,33,33	1.79	7 (25%)	27,52,52	1.60	3 (11%)

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
8	ADP	E	700	7	-	3/12/32/32	0/3/3/3
6	08T	D	700	7	-	0/12/38/38	0/3/3/3
6	08T	C	700	7	-	6/12/38/38	0/3/3/3
6	08T	B	700	7	-	5/12/38/38	0/3/3/3

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	700	08T	PB-O3A	-4.91	1.54	1.59
6	D	700	08T	C2'-C3'	-4.32	1.41	1.53
6	C	700	08T	C2'-C3'	-4.20	1.42	1.53
6	B	700	08T	C2'-C3'	-4.05	1.42	1.53
6	D	700	08T	F2-BE	-3.75	1.45	1.54

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	700	08T	N3-C2-N1	-6.31	120.10	128.67
6	D	700	08T	N3-C2-N1	-5.52	121.18	128.67
6	C	700	08T	N3-C2-N1	-4.82	122.13	128.67
8	E	700	ADP	C4'-O4'-C1'	2.87	112.55	109.92
8	E	700	ADP	O3'-C3'-C4'	-2.51	103.87	111.08

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	700	08T	C5'-O5'-PA-O2A
6	B	700	08T	C5'-O5'-PA-O3A

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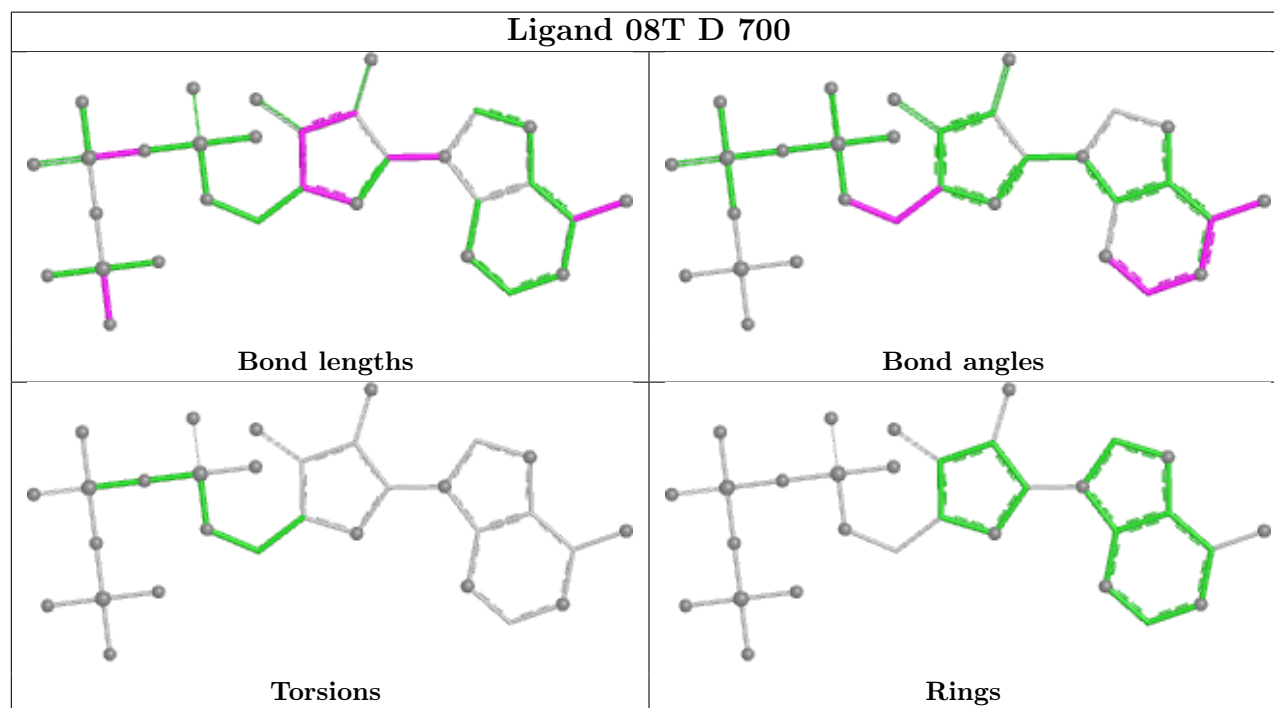
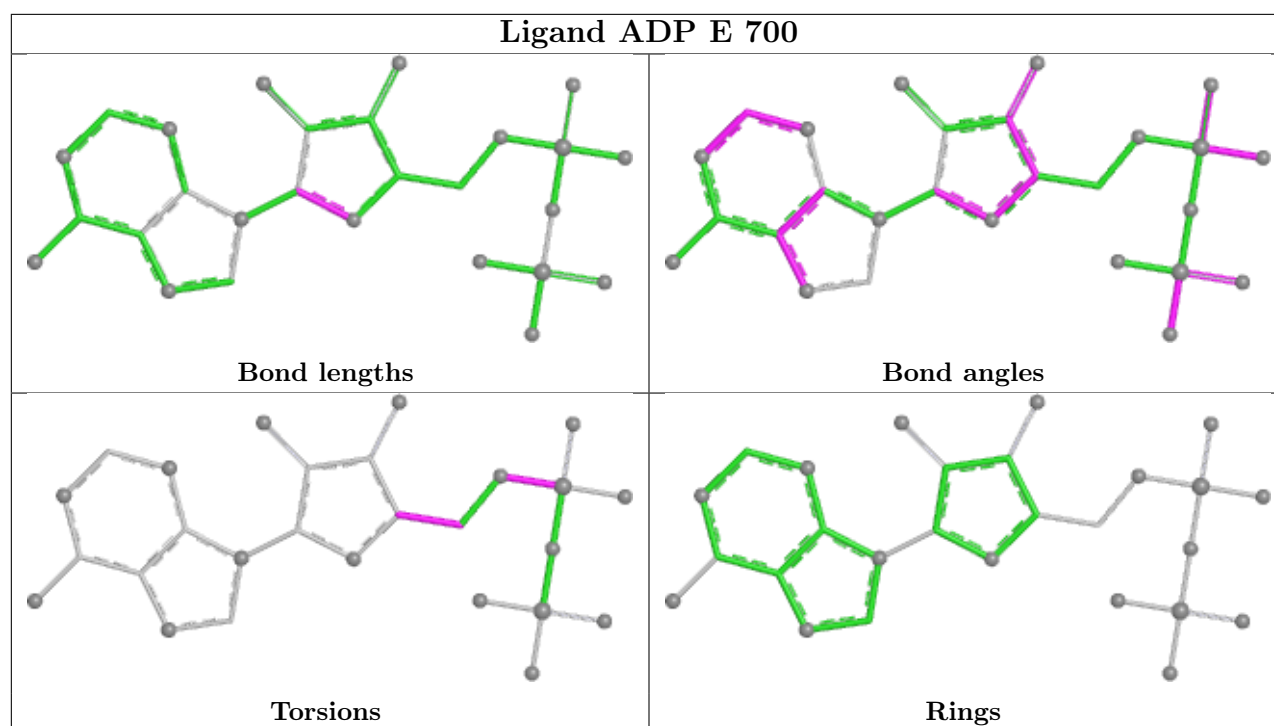
Mol	Chain	Res	Type	Atoms
6	C	700	08T	C5'-O5'-PA-O1A
6	C	700	08T	C5'-O5'-PA-O2A
6	C	700	08T	C5'-O5'-PA-O3A

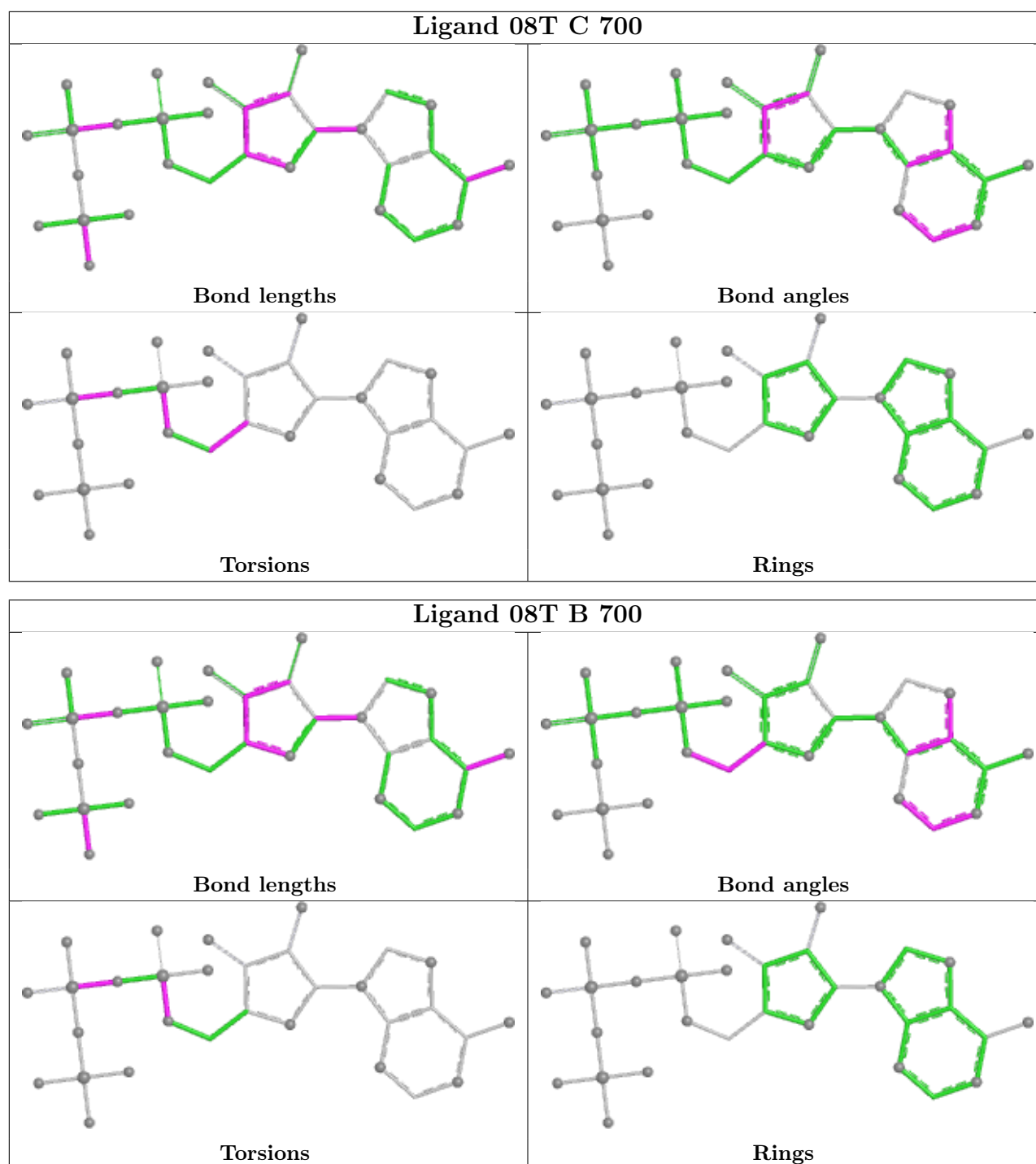
There are no ring outliers.

4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	E	700	ADP	8	0
6	D	700	08T	4	0
6	C	700	08T	2	0
6	B	700	08T	3	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	B	319/324 (98%)	0.26	15 (4%) 37 29	24, 54, 94, 158	0
1	C	320/324 (98%)	0.01	5 (1%) 70 58	26, 45, 82, 131	0
1	D	319/324 (98%)	0.01	10 (3%) 51 39	25, 48, 95, 170	0
1	E	305/324 (94%)	0.52	27 (8%) 17 16	31, 63, 110, 185	0
2	I	24/30 (80%)	-0.02	1 (4%) 41 31	35, 66, 216, 261	0
3	J	20/20 (100%)	0.26	0 100 100	54, 92, 235, 258	0
4	A	186/195 (95%)	0.11	5 (2%) 56 43	29, 70, 122, 157	0
5	F	222/228 (97%)	0.69	9 (4%) 42 31	76, 129, 172, 202	0
5	G	222/228 (97%)	0.60	8 (3%) 46 35	54, 80, 121, 136	0
5	H	222/228 (97%)	0.89	17 (7%) 21 18	67, 99, 147, 185	0
All	All	2159/2225 (97%)	0.35	97 (4%) 39 30	24, 66, 146, 261	0

The worst 5 of 97 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	G	5036	GLY	5.9
1	E	112	SER	5.5
1	B	120	HIS	5.4
1	E	110	ASP	5.3
1	E	214	TYR	4.3

### 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 monosaccharides in this entry.

### 6.4 Ligands [i](#)

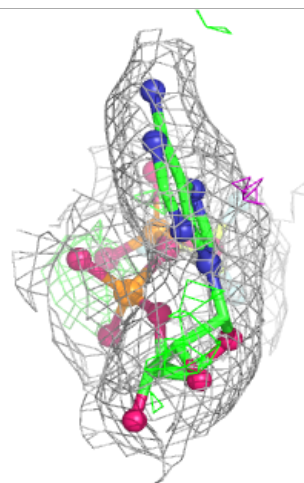
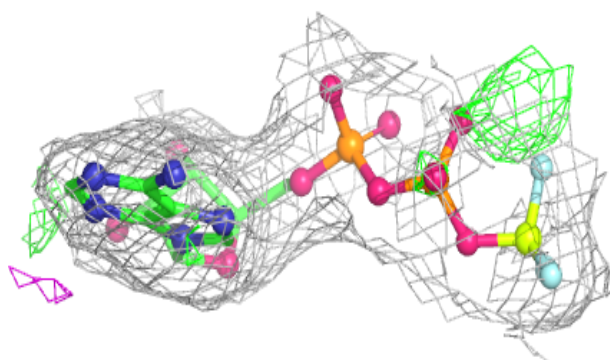
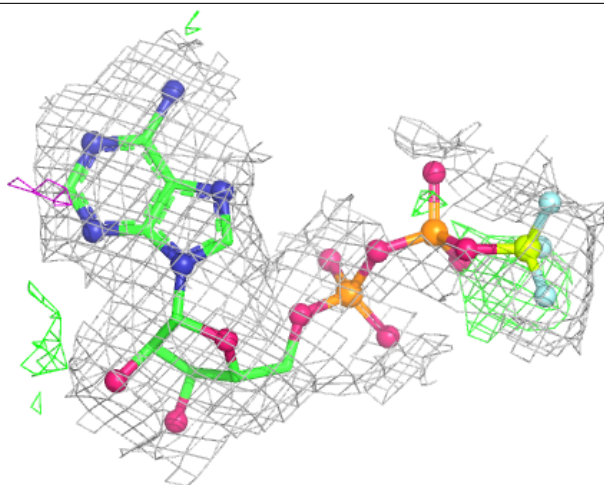
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
7	MG	E	801	1/1	0.86	0.23	47,47,47,47	0
7	MG	D	800	1/1	0.87	0.24	47,47,47,47	0
7	MG	C	800	1/1	0.88	0.23	47,47,47,47	0
7	MG	B	800	1/1	0.93	0.19	47,47,47,47	0
6	08T	C	700	31/31	0.96	0.08	47,47,48,48	0
6	08T	D	700	31/31	0.96	0.08	47,47,48,48	0
6	08T	B	700	31/31	0.96	0.07	47,47,48,48	0
8	ADP	E	700	27/27	0.96	0.08	47,47,48,48	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 08T C 700:**

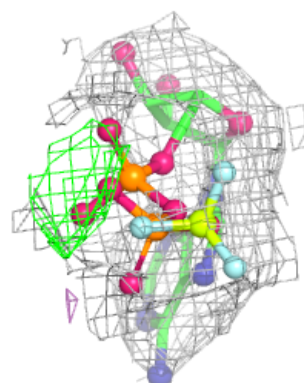
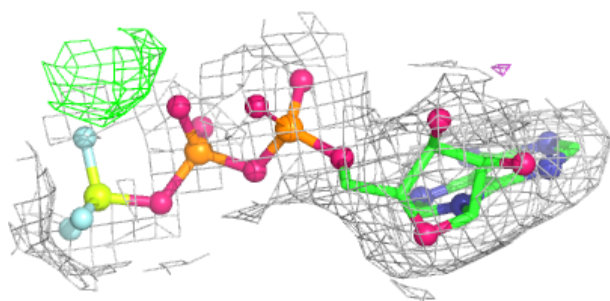
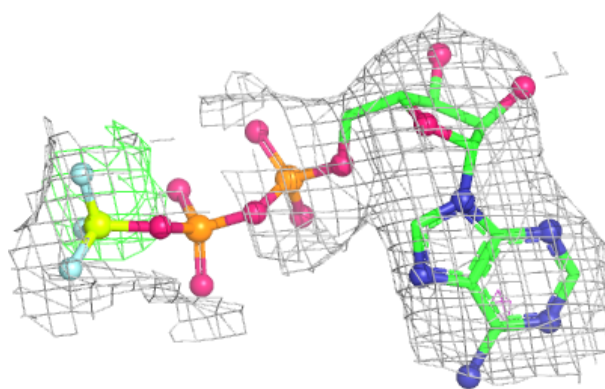
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



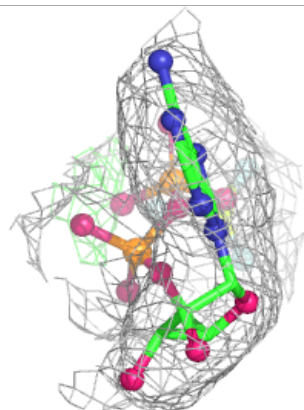
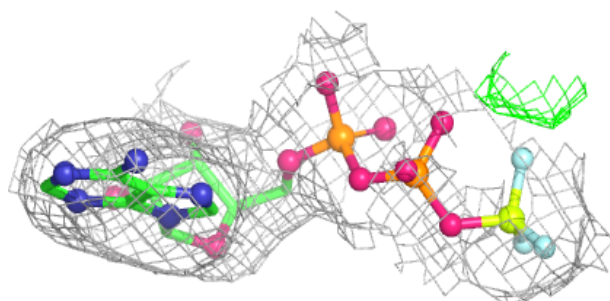
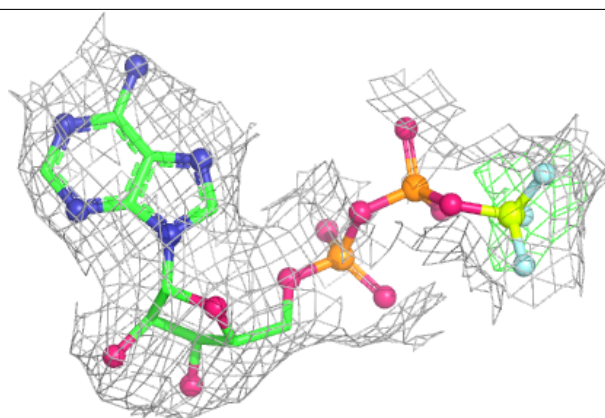


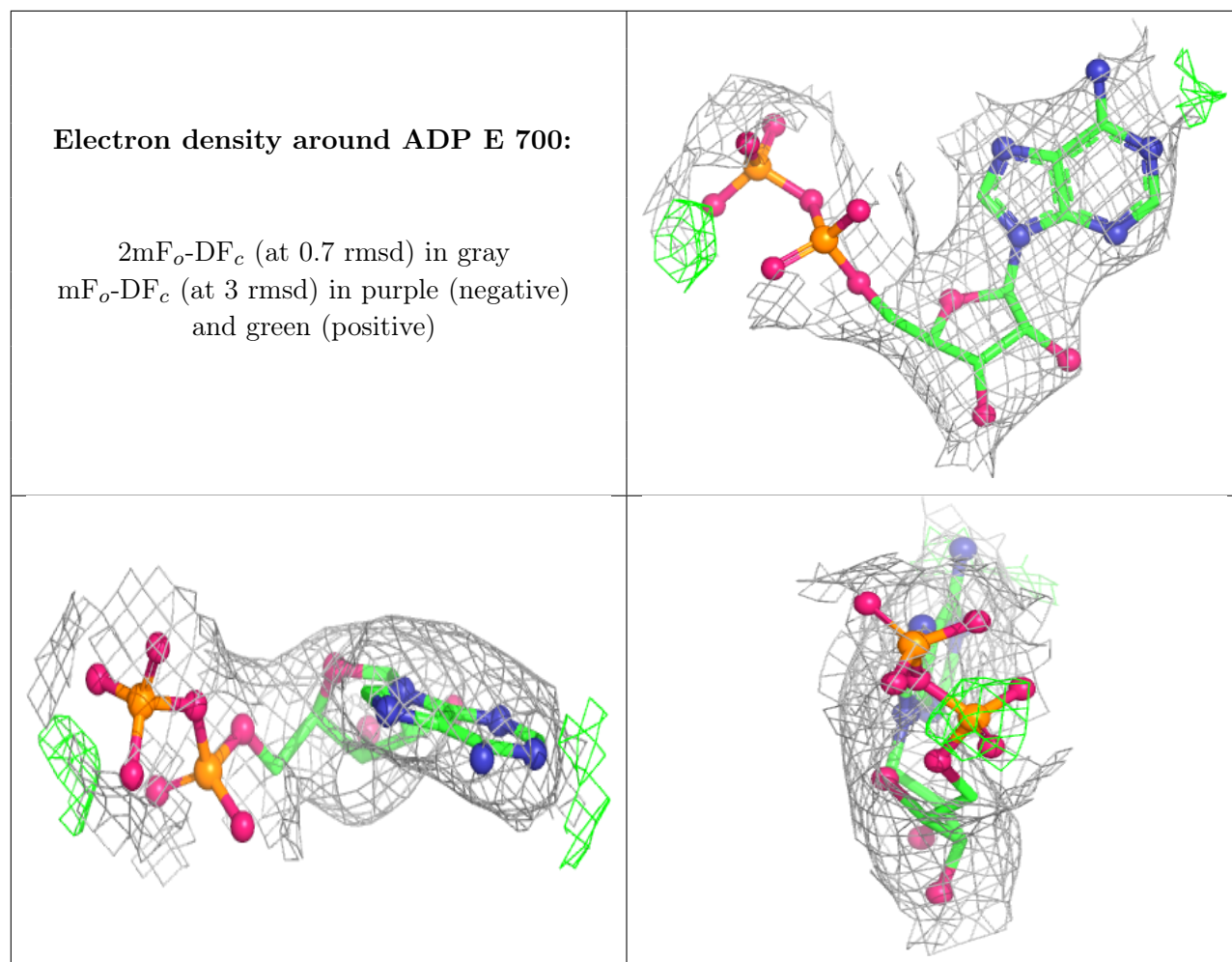
**Electron density around 08T D 700:**

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

**Electron density around 08T B 700:**

$2mF_o-DF_c$  (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.