



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2023 – 11:03 PM EDT

PDB ID : 7RFM  
Title : CamA Adenine Methyltransferase Complexed to Cognate Substrate DNA and Inhibitor EPZ004777  
Authors : Horton, J.R.; Cheng, X.; Zhou, J.  
Deposited on : 2021-07-14  
Resolution : 2.68 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.

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 : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

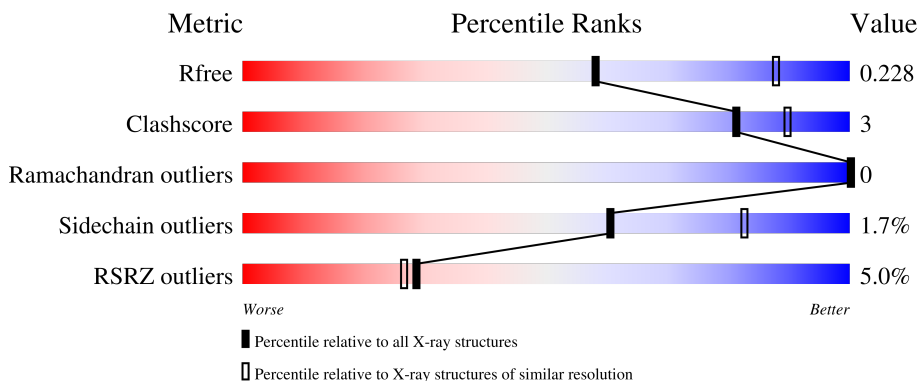
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.68 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.



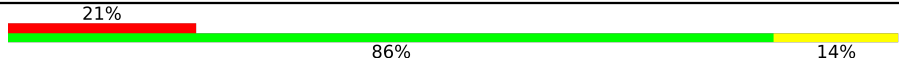
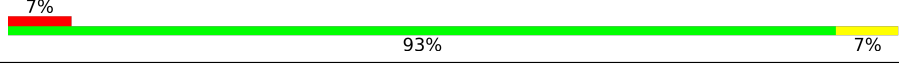
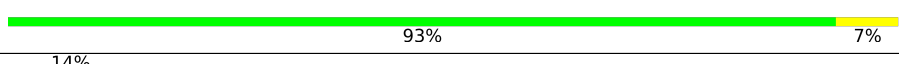

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)

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	578	 2% 88% 7% 5%
1	B	578	 4% 89% 7% .
1	C	578	 8% 84% 8% 7%
2	E	14	 7% 79% 14% 7%
2	G	14	 100%

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Mol	Chain	Length	Quality of chain
2	I	14	
3	D	14	
3	F	14	
3	H	14	

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 15441 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 Site-specific DNA-methyltransferase (adenine-specific).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	550	4502	2929	729	827	17	0	2	0
1	B	555	4547	2959	733	838	17	0	0	0
1	C	537	4270	2780	684	789	17	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	expression tag	UNP Q183J3
B	0	HIS	-	expression tag	UNP Q183J3
C	0	HIS	-	expression tag	UNP Q183J3

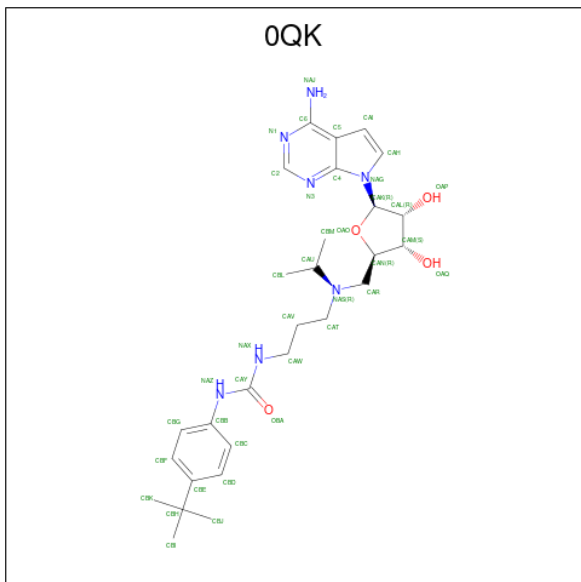
- Molecule 2 is a DNA chain called DNA Strand 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	E	13	269	129	45	82	13	0	0	0
2	G	14	287	139	50	85	13	0	0	0
2	I	14	287	139	50	85	13	0	0	0

- Molecule 3 is a DNA chain called DNA Strand 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	D	14	281	136	53	79	13	0	0	0
3	F	14	281	136	53	79	13	0	0	0
3	H	14	281	136	53	79	13	0	0	0

- Molecule 4 is 7-{5-[(3-[[[(4-tert-butylphenyl)carbamoyl]amino}propyl)(propan-2-yl)amino]-5-deoxy-beta-D-ribofuranosyl]-7H-pyrrolo[2,3-d]pyrimidin-4-amine (three-letter code: 0QK) (formula: C<sub>28</sub>H<sub>41</sub>N<sub>7</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
4	A	1	Total	C	N	O	0	0
			39	28	7	4		
4	B	1	Total	C	N	O	0	0
			39	28	7	4		
4	C	1	Total	C	N	O	0	0
			39	28	7	4		

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	K	0	0
			2	2		
5	B	2	Total	K	0	0
			2	2		
5	C	1	Total	K	0	0
			1	1		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	98	Total O 98 98	0	0
7	B	90	Total O 90 90	0	0
7	C	38	Total O 38 38	0	0
7	E	8	Total O 8 8	0	0
7	D	17	Total O 17 17	0	0
7	F	14	Total O 14 14	0	0
7	G	15	Total O 15 15	0	0

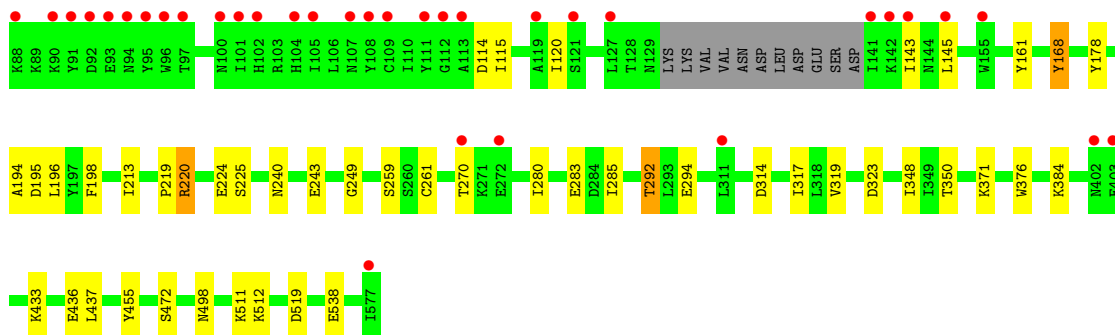
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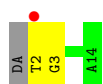
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
7	H	8	Total O 8 8	0	0
7	I	6	Total O 6 6	0	0







• Molecule 2: DNA Strand 2

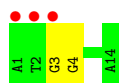
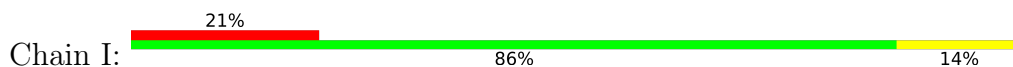


• Molecule 2: DNA Strand 2

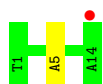
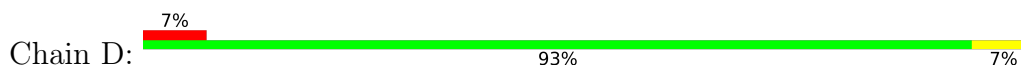


There are no outlier residues recorded for this chain.

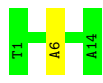
• Molecule 2: DNA Strand 2



• Molecule 3: DNA Strand 1

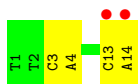


• Molecule 3: DNA Strand 1



• Molecule 3: DNA Strand 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.70Å 161.17Å 230.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.89 – 2.68 46.89 – 2.68	Depositor EDS
% Data completeness (in resolution range)	97.4 (46.89-2.68) 97.4 (46.89-2.68)	Depositor EDS
$R_{merge}$	0.49	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.58 (at 2.69Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.182 , 0.229 0.182 , 0.228	Depositor DCC
$R_{free}$ test set	1998 reflections (2.38%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.4	Xtrriage
Anisotropy	0.526	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 50.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	15441	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, OQK, K

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	0.28	0/4597	0.48	0/6194
1	B	0.28	0/4641	0.48	0/6252
1	C	0.26	0/4359	0.45	0/5894
2	E	0.62	0/300	1.02	0/462
2	G	0.66	0/321	0.99	0/495
2	I	0.59	0/321	0.99	0/495
3	D	0.56	0/315	0.88	0/483
3	F	0.60	0/315	0.84	0/483
3	H	0.48	0/315	0.80	0/483
All	All	0.33	0/15484	0.55	0/21241

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	A	4502	0	4438	21	0
1	B	4547	0	4500	19	0
1	C	4270	0	4082	25	0
2	E	269	0	150	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	287	0	162	0	0
2	I	287	0	162	1	0
3	D	281	0	159	1	0
3	F	281	0	159	1	0
3	H	281	0	159	2	0
4	A	39	0	41	2	0
4	B	39	0	41	4	0
4	C	39	0	41	2	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	1	0	0	0	0
6	A	8	0	12	0	0
6	B	4	0	6	0	0
6	C	4	0	6	0	0
6	F	4	0	6	0	0
7	A	98	0	0	1	0
7	B	90	0	0	1	0
7	C	38	0	0	0	0
7	D	17	0	0	0	0
7	E	8	0	0	0	0
7	F	14	0	0	0	0
7	G	15	0	0	0	0
7	H	8	0	0	0	0
7	I	6	0	0	0	0
All	All	15441	0	14124	75	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 3.

All (75) 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)
4:A:701:0QK:H29	4:A:701:0QK:H34	1.75	0.69
1:C:58:ILE:HG13	1:C:161:TYR:HB2	1.79	0.64
1:C:220:ARG:NH2	1:C:224:GLU:OE1	2.31	0.64
1:A:319:VAL:HG11	1:A:508:ILE:HG23	1.84	0.60
1:A:168:TYR:CE1	1:A:219:PRO:HD3	2.36	0.60
1:B:66:GLY:HA3	1:B:123:LEU:HD13	1.83	0.59
1:C:143:ILE:HB	1:C:145:LEU:HD13	1.84	0.58
1:C:39:TYR:OH	1:C:243:GLU:OE2	2.14	0.57
1:B:168:TYR:CE1	1:B:219:PRO:HD3	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:496:ILE:HD11	1:B:530:ILE:HD12	1.87	0.56
1:C:384:LYS:O	1:C:498:ASN:ND2	2.39	0.56
1:A:66:GLY:HA3	1:A:123:LEU:HD13	1.90	0.54
4:B:601:OQK:H34	4:B:601:OQK:H26	1.89	0.54
1:C:283:GLU:OE2	1:C:512:LYS:NZ	2.37	0.53
1:A:35:ILE:HD12	1:A:35:ILE:H	1.73	0.52
1:B:227:SER:OG	3:F:6:DA:OP1	2.17	0.52
1:C:168:TYR:CE1	1:C:219:PRO:HD3	2.44	0.52
1:C:294:GLU:OE1	1:C:294:GLU:N	2.35	0.52
1:C:280:ILE:HD11	1:C:285:ILE:HG12	1.92	0.52
1:B:26:ALA:HA	4:B:601:OQK:H9	1.90	0.51
1:B:51:ILE:HD11	1:B:83:ASN:HB3	1.92	0.51
1:A:281:LYS:HE3	1:A:303:GLU:HB3	1.93	0.50
1:C:249:GLY:HA2	1:C:259:SER:OG	2.12	0.50
1:C:64:GLY:HA3	4:C:601:OQK:H16	1.76	0.50
1:B:100:ASN:OD1	1:B:103:ARG:NH1	2.44	0.49
1:B:162:ILE:HG21	1:B:204:ILE:HG12	1.94	0.48
1:B:280:ILE:HD11	1:B:285:ILE:HG12	1.94	0.48
1:B:69:LEU:HD12	1:B:123:LEU:HD21	1.96	0.48
1:C:114:ASP:OD1	1:C:115:ILE:N	2.47	0.48
1:A:195:ASP:OD1	1:A:196:LEU:N	2.47	0.47
1:B:319:VAL:HB	1:B:323:ASP:HB2	1.96	0.47
1:C:240:ASN:HD21	1:C:270:THR:HG22	1.80	0.46
1:A:42:LYS:O	1:A:46:LYS:HB2	2.16	0.46
1:A:406:ASN:HB3	1:A:409:ILE:HD12	1.98	0.46
1:B:194:ALA:HB1	1:B:198:PHE:CD2	2.50	0.46
1:A:86:GLU:OE1	1:A:86:GLU:N	2.48	0.45
1:C:195:ASP:OD1	1:C:196:LEU:N	2.49	0.45
1:C:225:SER:HB3	1:C:511:LYS:HE3	1.98	0.45
1:C:433:LYS:HB2	1:C:436:GLU:HG3	1.99	0.45
1:A:191:LYS:HG2	7:A:863:HOH:O	2.16	0.45
1:C:44:THR:HG22	1:C:213:ILE:HG22	1.99	0.45
1:B:195:ASP:OD1	1:B:196:LEU:N	2.50	0.45
1:A:103:ARG:NH2	1:A:139:SER:OG	2.50	0.45
1:C:350:THR:HG22	1:C:437:LEU:HD22	1.99	0.44
1:A:143:ILE:HG22	1:A:145:LEU:HG	1.98	0.44
4:B:601:OQK:H31	4:B:601:OQK:H30	1.70	0.44
1:B:461:ARG:NH1	7:B:710:HOH:O	2.50	0.44
1:C:317:ILE:HG22	1:C:319:VAL:HG22	1.99	0.44
1:B:58:ILE:HG13	1:B:161:TYR:HB2	1.99	0.44
1:A:51:ILE:HD11	1:A:83:ASN:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:13:DC:H2''	3:H:14:DA:C8	2.53	0.44
2:I:3:DG:H2''	2:I:4:DG:C8	2.53	0.43
1:C:194:ALA:HB1	1:C:198:PHE:CD2	2.53	0.43
4:A:701:0QK:H27	4:A:701:0QK:H31	1.70	0.43
2:E:2:DT:H2''	2:E:3:DG:C8	2.54	0.43
4:C:601:0QK:H33	4:C:601:0QK:H21	1.65	0.43
1:C:292:THR:OG1	1:C:294:GLU:OE1	2.36	0.42
1:A:194:ALA:HB1	1:A:198:PHE:CD2	2.55	0.42
1:C:376:TRP:CZ2	1:C:472:SER:HB2	2.55	0.42
1:C:319:VAL:HB	1:C:323:ASP:HB2	2.02	0.41
1:C:348:ILE:O	1:C:472:SER:HA	2.20	0.41
1:A:168:TYR:CZ	1:A:219:PRO:HD3	2.55	0.41
1:A:326:PHE:HE1	1:A:577:ILE:HD12	1.82	0.41
1:B:418:LYS:HE3	1:B:434:TRP:CE2	2.56	0.41
1:A:450:LYS:NZ	1:A:465:ASP:OD2	2.51	0.41
1:A:193:LYS:HE2	3:D:5:DA:C2	2.56	0.41
1:A:348:ILE:O	1:A:472:SER:HA	2.21	0.41
1:B:143:ILE:HG22	1:B:145:LEU:HG	2.01	0.41
1:C:120:ILE:HG23	1:C:145:LEU:HD23	2.03	0.41
1:A:494:VAL:O	1:A:498:ASN:ND2	2.54	0.40
1:B:378:LYS:HE2	1:B:378:LYS:HA	2.03	0.40
4:B:601:0QK:H15	4:B:601:0QK:H18	1.68	0.40
1:A:330:ILE:HG12	1:A:575:LEU:HD13	2.04	0.40
1:B:131:LYS:HG3	1:B:133:VAL:H	1.87	0.40
3:H:3:DC:H2'	3:H:4:DA:C8	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	548/578 (95%)	530 (97%)	18 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	553/578 (96%)	535 (97%)	18 (3%)	0	100	100
1	C	533/578 (92%)	521 (98%)	12 (2%)	0	100	100
All	All	1634/1734 (94%)	1586 (97%)	48 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	483/548 (88%)	477 (99%)	6 (1%)	71	87
1	B	492/548 (90%)	485 (99%)	7 (1%)	67	85
1	C	442/548 (81%)	431 (98%)	11 (2%)	47	74
All	All	1417/1644 (86%)	1393 (98%)	24 (2%)	60	82

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	168	TYR
1	A	263	LEU
1	A	390	SER
1	A	420	LYS
1	A	455	TYR
1	A	519	ASP
1	B	168	TYR
1	B	188	GLU
1	B	263	LEU
1	B	314	ASP
1	B	401	ASP
1	B	432	ARG
1	B	455	TYR
1	C	35	ILE
1	C	168	TYR
1	C	178	TYR

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Mol	Chain	Res	Type
1	C	220	ARG
1	C	261	CYS
1	C	292	THR
1	C	314	ASP
1	C	371	LYS
1	C	455	TYR
1	C	519	ASP
1	C	538	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 5 are monoatomic - leaving 8 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	0QK	B	601	-	39,42,42	0.64	0	49,61,61	0.66	0
4	0QK	C	601	-	39,42,42	0.67	0	49,61,61	0.73	0
6	EDO	C	603	-	3,3,3	0.49	0	2,2,2	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	EDO	F	101	-	3,3,3	0.53	0	2,2,2	0.26	0
6	EDO	A	705	5	3,3,3	0.52	0	2,2,2	0.25	0
4	0QK	A	701	-	39,42,42	0.65	0	49,61,61	0.65	0
6	EDO	B	604	-	3,3,3	0.50	0	2,2,2	0.17	0
6	EDO	A	704	-	3,3,3	0.53	0	2,2,2	0.25	0

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	0QK	B	601	-	-	9/25/45/45	0/4/4/4
4	0QK	C	601	-	-	7/25/45/45	0/4/4/4
6	EDO	C	603	-	-	0/1/1/1	-
6	EDO	F	101	-	-	1/1/1/1	-
6	EDO	A	705	5	-	1/1/1/1	-
4	0QK	A	701	-	-	6/25/45/45	0/4/4/4
6	EDO	B	604	-	-	0/1/1/1	-
6	EDO	A	704	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	701	0QK	CBM-CAU-NAS-CAT
4	A	701	0QK	CBL-CAU-NAS-CAT
4	A	701	0QK	CBL-CAU-NAS-CAR
4	B	601	0QK	CBM-CAU-NAS-CAT
4	B	601	0QK	CBL-CAU-NAS-CAT
4	C	601	0QK	CAN-CAR-NAS-CAT
4	C	601	0QK	OAO-CAN-CAR-NAS
4	C	601	0QK	CAM-CAN-CAR-NAS
4	B	601	0QK	OBA-CAY-NAX-CAW
4	B	601	0QK	NAZ-CAY-NAX-CAW
4	A	701	0QK	CBM-CAU-NAS-CAR
4	B	601	0QK	CBL-CAU-NAS-CAR
4	B	601	0QK	NAS-CAT-CAV-CAW

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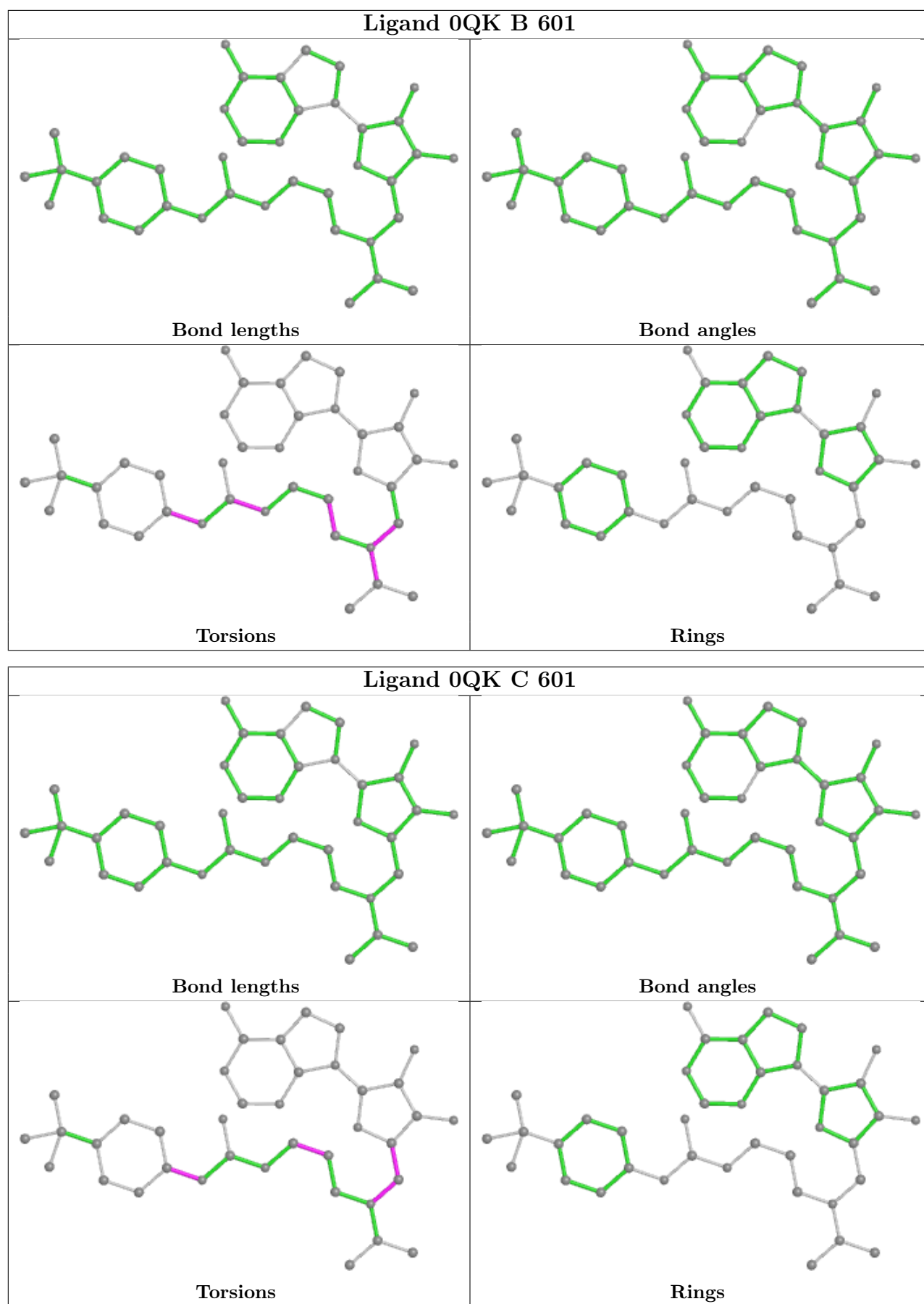
Mol	Chain	Res	Type	Atoms
4	A	701	0QK	CAN-CAR-NAS-CAU
4	B	601	0QK	CBM-CAU-NAS-CAR
6	A	705	EDO	O1-C1-C2-O2
4	C	601	0QK	CAT-CAV-CAW-NAX
4	A	701	0QK	CAN-CAR-NAS-CAT
4	B	601	0QK	CAN-CAR-NAS-CAU
4	C	601	0QK	CAN-CAR-NAS-CAU
4	C	601	0QK	CBG-CBB-NAZ-CAY
6	F	101	EDO	O1-C1-C2-O2
4	B	601	0QK	CBG-CBB-NAZ-CAY
4	C	601	0QK	CBC-CBB-NAZ-CAY

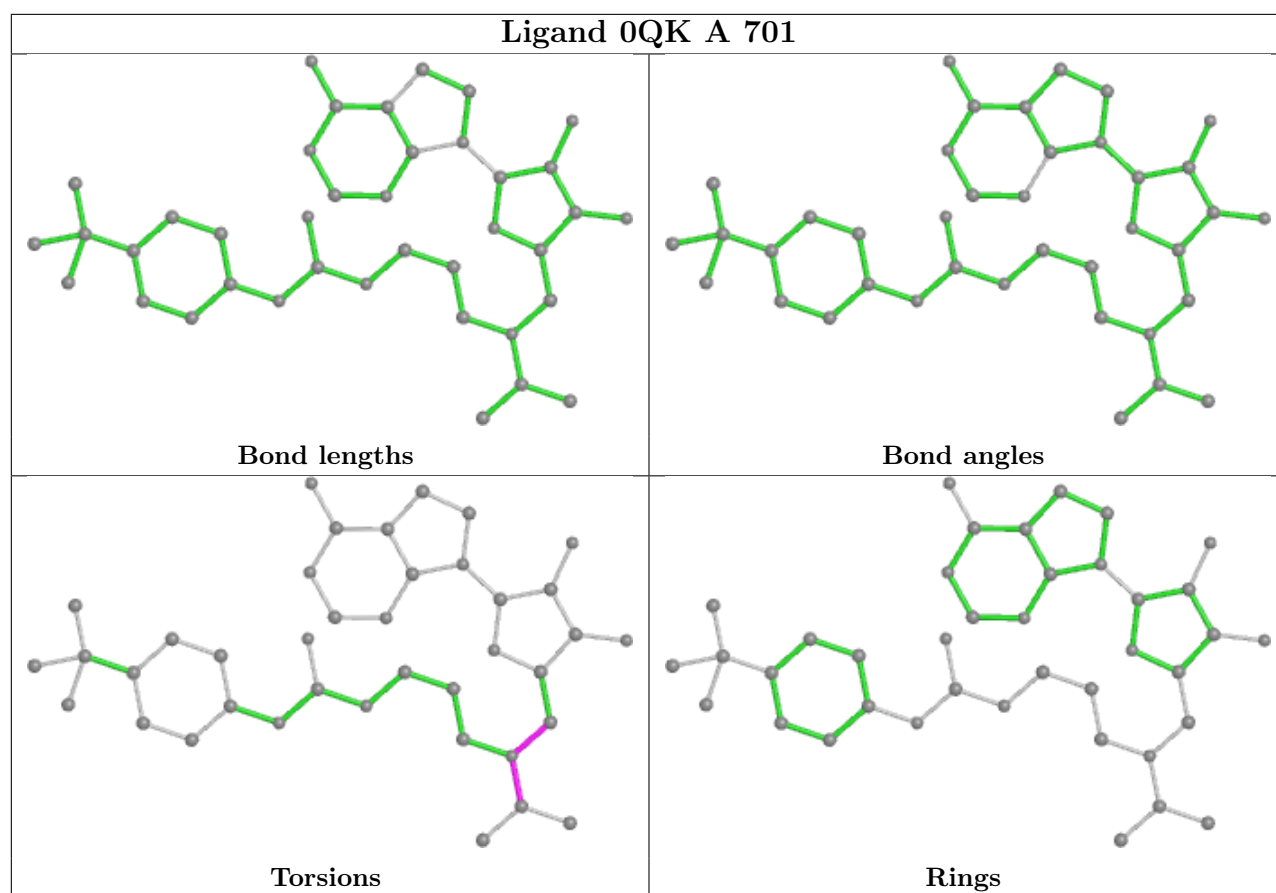
There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	601	0QK	4	0
4	C	601	0QK	2	0
4	A	701	0QK	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 [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	550/578 (95%)	-0.16	11 (2%) 65 65	32, 58, 104, 168	0
1	B	555/578 (96%)	-0.08	21 (3%) 40 38	32, 56, 102, 200	0
1	C	537/578 (92%)	0.29	47 (8%) 10 8	49, 80, 137, 168	0
2	E	13/14 (92%)	-0.34	1 (7%) 13 11	48, 51, 143, 176	0
2	G	14/14 (100%)	-0.74	0 100 100	45, 51, 82, 83	0
2	I	14/14 (100%)	0.83	3 (21%) 0 0	54, 66, 190, 210	0
3	D	14/14 (100%)	0.00	1 (7%) 16 13	42, 50, 167, 186	0
3	F	14/14 (100%)	-0.24	0 100 100	39, 48, 95, 96	0
3	H	14/14 (100%)	0.35	2 (14%) 2 1	56, 73, 170, 194	0
All	All	1725/1818 (94%)	0.01	86 (4%) 28 26	32, 63, 130, 210	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	28	GLY	11.2
2	I	1	DA	8.8
1	A	29	ILE	6.9
3	H	14	DA	6.3
1	A	26	ALA	5.6
1	A	27	SER	5.5
1	C	96	TRP	5.4
1	C	95	TYR	5.3
1	B	28	GLY	5.2
1	B	26	ALA	5.1
1	C	91	TYR	4.9
1	C	113	ALA	4.9
1	C	94	ASN	4.8
1	C	51	ILE	4.4
2	I	2	DT	4.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	30	TYR	4.3
1	C	87	LEU	4.2
1	C	80	PHE	4.1
1	B	27	SER	3.9
1	C	73	TYR	3.7
1	C	105	ILE	3.7
1	C	108	TYR	3.6
1	C	112	GLY	3.5
1	C	101	ILE	3.4
1	C	97	THR	3.4
2	I	3	DG	3.2
1	C	109	CYS	3.2
1	B	29	ILE	3.2
1	B	412	GLU	3.0
3	D	14	DA	3.0
1	C	143	ILE	2.9
1	C	30	TYR	2.9
2	E	2	DT	2.9
1	C	56	PRO	2.9
1	B	577	ILE	2.8
3	H	13	DC	2.8
1	B	135	ASP	2.8
1	B	25	LYS	2.7
1	C	107	ASN	2.7
1	C	104	HIS	2.7
1	C	272	GLU	2.6
1	C	577	ILE	2.6
1	C	100	ASN	2.6
1	B	132	VAL	2.6
1	B	290	PHE	2.6
1	C	66	GLY	2.6
1	C	77	TYR	2.5
1	C	403	GLU	2.5
1	C	76	LEU	2.5
1	C	92	ASP	2.5
1	A	288	ASN	2.5
1	B	358	LEU	2.4
1	C	121	SER	2.4
1	C	141	ILE	2.4
1	C	145	LEU	2.3
1	C	270	THR	2.3
1	A	555	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	90	LYS	2.3
1	B	404	ASN	2.3
1	B	133	VAL	2.3
1	B	411	ASP	2.3
1	A	409	ILE	2.2
1	C	155	TRP	2.2
1	B	139	SER	2.2
1	A	370	ASP	2.2
1	C	88	LYS	2.2
1	B	136	LEU	2.2
1	C	127	LEU	2.2
1	C	119	ALA	2.2
1	C	142	LYS	2.1
1	B	30	TYR	2.1
1	B	24	LYS	2.1
1	C	311	LEU	2.1
1	B	23	THR	2.1
1	C	93	GLU	2.1
1	C	402	ASN	2.1
1	C	65	CYS	2.1
1	C	111	TYR	2.1
1	B	410	LEU	2.1
1	C	59	LEU	2.1
1	C	31	TYR	2.1
1	A	137	ASP	2.1
1	A	372	PHE	2.0
1	C	102	HIS	2.0
1	C	54	PRO	2.0
1	B	406	ASN	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.



## 6.4 Ligands

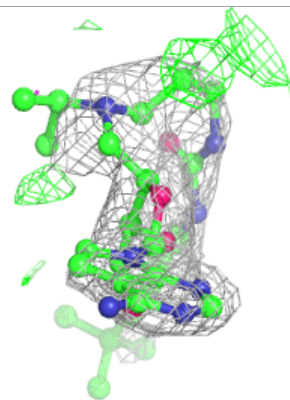
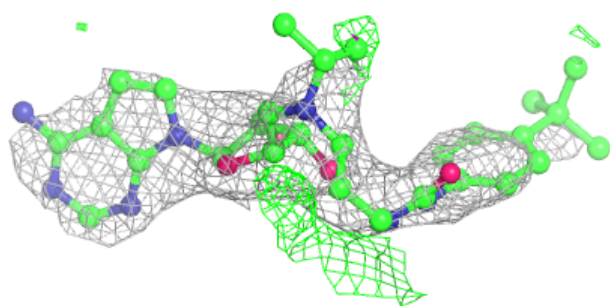
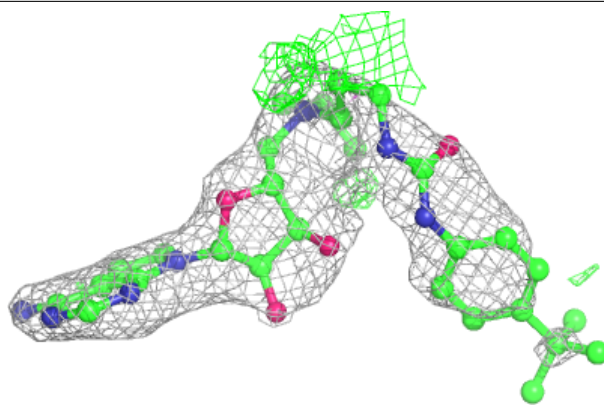
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	0QK	C	601	39/39	0.81	0.37	100,120,135,140	0
6	EDO	C	603	4/4	0.86	0.29	86,87,89,101	0
6	EDO	A	705	4/4	0.87	0.19	61,63,69,79	0
6	EDO	A	704	4/4	0.88	0.19	74,75,75,83	0
4	0QK	A	701	39/39	0.92	0.19	56,72,96,102	0
6	EDO	F	101	4/4	0.92	0.29	38,60,61,67	0
4	0QK	B	601	39/39	0.93	0.21	48,69,95,101	0
5	K	A	702	1/1	0.94	0.09	58,58,58,58	0
6	EDO	B	604	4/4	0.94	0.28	48,49,51,57	0
5	K	B	603	1/1	0.95	0.09	72,72,72,72	0
5	K	A	703	1/1	0.97	0.09	76,76,76,76	0
5	K	B	602	1/1	0.97	0.07	66,66,66,66	0
5	K	C	602	1/1	0.98	0.09	79,79,79,79	0

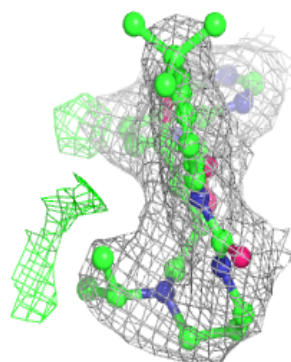
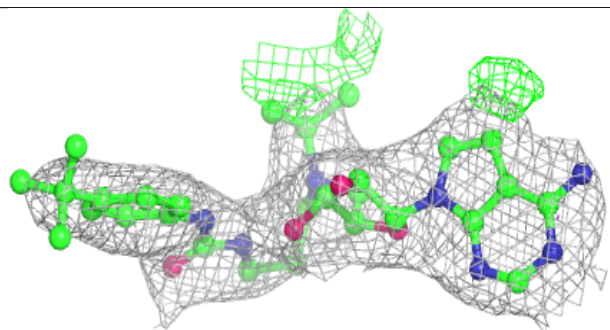
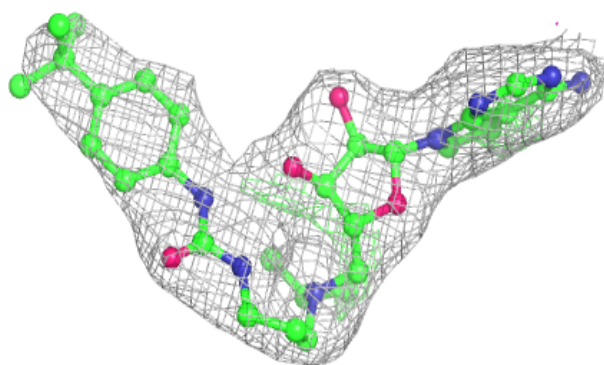
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

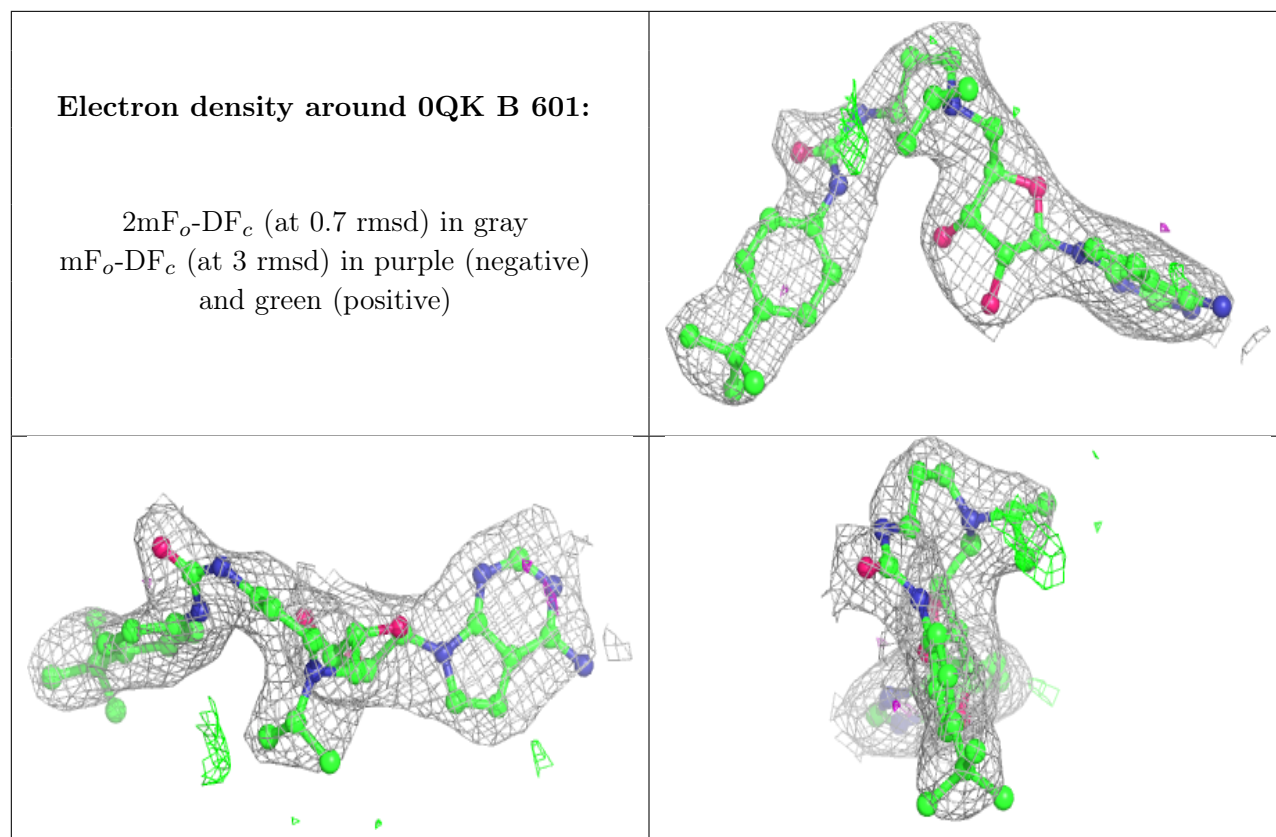
**Electron density around 0QK C 601:**

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

**Electron density around 0QK A 701:**

$2mF_o-DF_c$  (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.