Full wwPDB X-ray Structure Validation Report (i)

Dec 17, 2023 – 03:46 am GMT

PDB ID	:	4BWJ
Title	:	KlenTaq mutant in complex with DNA and ddCTP
Authors	:	Blatter, N.; Bergen, K.; Welte, W.; Diederichs, K.; Marx, A.
Deposited on	:	2013-07-03
Resolution	:	1.55 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

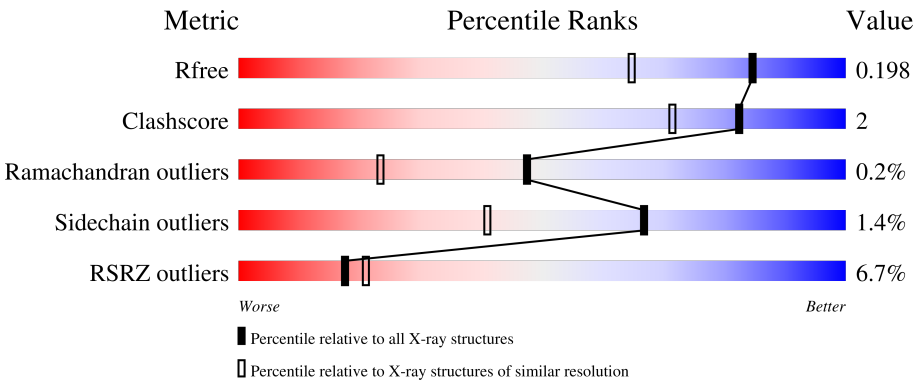
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.55 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	1483 (1.56-1.56)
Clashscore	141614	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)
RSRZ outliers	127900	1465 (1.56-1.56)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	540	7% / 93% / 7%
2	B	12	8% / 83% / 8%
3	C	16	38% / 44% / 6% / 12%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 10124 atoms, of which 4730 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 I, THERMOSTABLE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	539	8777	2768	4427	787	782	13	0	11	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	459	MET	LEU	engineered mutation	UNP P19821
A	515	ARG	SER	engineered mutation	UNP P19821
A	638	PHE	ILE	engineered mutation	UNP P19821
A	747	LYS	MET	engineered mutation	UNP P19821

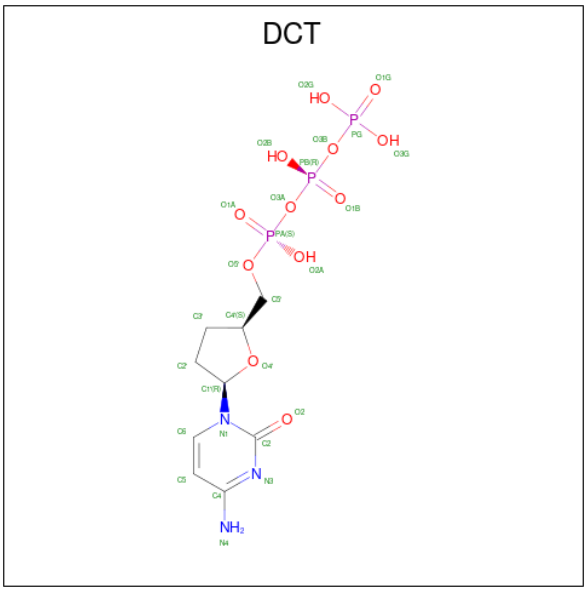
- Molecule 2 is a DNA chain called 5'-D(*GP*AP*CP*CP*AP*CP*GP*GP*CP*GP*CP*DOCP)-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	P			
2	B	12	374	114	134	48	67	11	0	0	0

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	P			
3	C	14	448	136	157	56	85	14	0	0	0

- Molecule 4 is 2',3'-DIDEOXYCYTIDINE 5'-TRIPHOSPHATE (three-letter code: DCT) (formula: $C_9H_{16}N_3O_{12}P_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
4	A	1	39	9	12	3	12	3	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
5	A	3	3	3	0	0
5	B	2	2	2	0	0

- Molecule 6 is water.

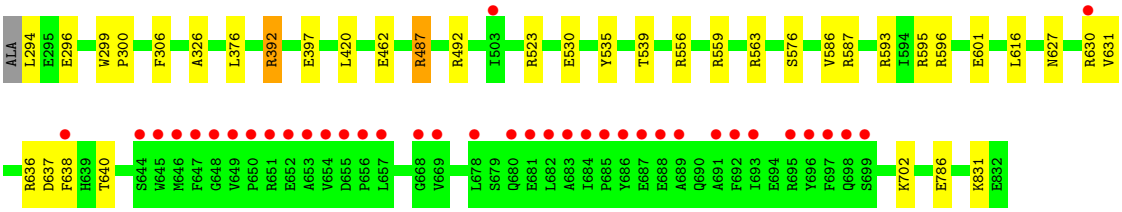
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	408	408	408	0	0
6	B	37	37	37	0	0
6	C	36	36	36	0	0

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 I, THERMOSTABLE

Chain A: 7% 93% 7%



• Molecule 2: 5'-D(*GP*AP*CP*CP*AP*CP*GP*GP*CP*GP*CP*DOCP)-3'

Chain B: 8% 83% 8%

• Molecule 3: 5'-D(*AP*GP*GP*GP*CP*GP*CP*CP*GP*TP*GP*GP*TP*CP)-3'

Chain C: 38% 44% 6% 12%

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	108.14Å 108.14Å 89.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.83 – 1.55 46.83 – 1.55	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.83-1.55) 100.0 (46.83-1.55)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.50 (at 1.55Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.158 , 0.201 0.165 , 0.198	Depositor DCC
R_{free} test set	4377 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	29.2	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 41.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	10124	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: MG, DCT, DOC

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	0.54	0/4482	0.67	4/6063 (0.1%)
2	B	1.24	1/249 (0.4%)	2.11	14/382 (3.7%)
3	C	1.34	2/326 (0.6%)	2.00	11/502 (2.2%)
All	All	0.67	3/5057 (0.1%)	0.96	29/6947 (0.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	208	DG	C8-N7	-7.19	1.26	1.30
2	B	102	DA	C3'-O3'	-6.14	1.35	1.44
3	C	204	DG	C3'-O3'	-5.36	1.36	1.44

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	210	DC	O5'-P-OP2	-12.20	94.72	105.70
2	B	109	DC	O4'-C1'-N1	10.09	115.06	108.00
3	C	212	DT	O5'-P-OP2	-9.12	97.50	105.70
2	B	108	DG	O4'-C1'-N9	7.52	113.27	108.00
3	C	212	DT	O4'-C1'-N1	-7.34	102.86	108.00
1	A	559	ARG	NE-CZ-NH2	-6.98	116.81	120.30
2	B	110	DG	N7-C8-N9	6.93	116.56	113.10
2	B	110	DG	C8-N9-C4	-6.45	103.82	106.40
2	B	110	DG	C4'-C3'-C2'	-6.04	97.67	103.10
3	C	210	DC	OP1-P-OP2	6.02	128.63	119.60
2	B	102	DA	O4'-C1'-C2'	5.99	110.69	105.90
3	C	209	DC	O4'-C1'-N1	-5.94	103.84	108.00
2	B	111	DC	C6-N1-C2	-5.90	117.94	120.30
2	B	105	DA	N1-C2-N3	5.85	132.22	129.30
3	C	208	DG	C8-N9-C4	-5.80	104.08	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	487	ARG	NE-CZ-NH2	-5.59	117.50	120.30
2	B	103	DC	O4'-C1'-C2'	5.59	110.38	105.90
2	B	106	DC	O5'-P-OP2	-5.58	100.67	105.70
1	A	487	ARG	NE-CZ-NH1	5.55	123.08	120.30
2	B	110	DG	C6-N1-C2	5.55	128.43	125.10
1	A	559	ARG	NE-CZ-NH1	5.50	123.05	120.30
3	C	210	DC	O4'-C1'-N1	-5.23	104.34	108.00
3	C	210	DC	O4'-C1'-C2'	5.17	110.03	105.90
3	C	206	DG	N3-C4-C5	5.17	131.18	128.60
2	B	107	DG	O5'-P-OP2	-5.12	101.09	105.70
2	B	111	DC	C5-C6-N1	5.12	123.56	121.00
2	B	107	DG	C2-N3-C4	-5.07	109.37	111.90
3	C	215	DT	C1'-O4'-C4'	-5.06	105.04	110.10
3	C	206	DG	O4'-C4'-C3'	-5.05	102.48	104.50

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	4350	4427	4397	22	0
2	B	240	134	134	1	0
3	C	291	157	157	1	0
4	A	27	12	12	0	0
5	A	3	0	0	0	0
5	B	2	0	0	0	0
6	A	408	0	0	6	1
6	B	37	0	0	0	0
6	C	36	0	0	0	0
All	All	5394	4730	4700	24	1

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 2.

All (24) 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:A:601:GLU:OE1	6:A:2265:HOH:O	1.97	0.81
1:A:631:VAL:HG11	1:A:638[B]:PHE:CE1	2.23	0.73
1:A:523:ARG:NH2	1:A:530:GLU:OE1	2.24	0.71
1:A:587:ARG:NH2	6:A:2295:HOH:O	2.28	0.64
2:B:101:DG:H2"	2:B:102:DA:H5"	1.82	0.62
1:A:294:LEU:N	6:A:2001:HOH:O	2.33	0.61
1:A:786[B]:GLU:OE2	1:A:831:LYS:NZ	2.34	0.61
1:A:616:LEU:HD13	1:A:638[B]:PHE:HD2	1.69	0.58
1:A:492:ARG:NH1	6:A:2224:HOH:O	2.38	0.56
1:A:376:LEU:HD22	1:A:420:LEU:HD12	1.91	0.52
1:A:462:GLU:OE2	1:A:593[B]:ARG:NH2	2.42	0.51
1:A:631:VAL:HG13	1:A:636:ARG:HB2	1.93	0.50
1:A:397:GLU:OE1	6:A:2093:HOH:O	2.20	0.50
1:A:631:VAL:HG11	1:A:638[B]:PHE:CZ	2.48	0.48
1:A:631:VAL:HG21	1:A:638[B]:PHE:CZ	2.50	0.47
1:A:596:ARG:NH1	6:A:2300:HOH:O	2.38	0.45
1:A:637:ASP:OD2	1:A:640:THR:OG1	2.34	0.44
1:A:627:ASN:OD1	1:A:630:ARG:NH1	2.48	0.44
3:C:210:DC:H2'	3:C:211:DG:C8	2.53	0.43
1:A:392[A]:ARG:HH22	1:A:397:GLU:HB2	1.84	0.43
1:A:299:TRP:CG	1:A:300:PRO:HA	2.55	0.42
1:A:535:TYR:CZ	1:A:539:THR:HG21	2.54	0.42
1:A:306:PHE:O	1:A:326:ALA:HA	2.21	0.40
1:A:563:ARG:O	1:A:576:SER:HA	2.21	0.40

All (1) 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)
6:A:2230:HOH:O	6:A:2343:HOH:O[6_555]	2.14	0.06

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	548/540 (102%)	535 (98%)	12 (2%)	1 (0%)	47 23

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	586	VAL

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	450/441 (102%)	443 (98%)	7 (2%)	62 35

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	296	GLU
1	A	392[A]	ARG
1	A	392[B]	ARG
1	A	487	ARG
1	A	556	ARG
1	A	595	ARG
1	A	702	LYS

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)

1 non-standard protein/DNA/RNA residue is 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	DOC	B	112	3,2	16,19,20	1.99	6 (37%)	20,26,29	1.08	1 (5%)

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	DOC	B	112	3,2	-	0/7/18/19	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	112	DOC	O2-C2	4.52	1.32	1.23
2	B	112	DOC	O5'-C5'	-2.80	1.37	1.44
2	B	112	DOC	C2-N3	2.75	1.41	1.36
2	B	112	DOC	C4-N4	2.74	1.40	1.33
2	B	112	DOC	O4'-C4'	-2.58	1.39	1.44
2	B	112	DOC	C2'-C1'	-2.35	1.46	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	112	DOC	O4'-C1'-C2'	2.77	109.67	106.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 5 are monoatomic - leaving 1 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	DCT	A	1833	5	24,28,28	2.61	8 (33%)	33,43,43	2.56	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	DCT	A	1833	5	-	3/22/31/31	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1833	DCT	O4'-C4'	-6.53	1.31	1.44
4	A	1833	DCT	O2-C2	6.03	1.34	1.23
4	A	1833	DCT	O4'-C1'	-5.51	1.30	1.42
4	A	1833	DCT	C4-N4	3.40	1.41	1.33
4	A	1833	DCT	C2-N3	3.09	1.42	1.36
4	A	1833	DCT	C4-N3	-2.94	1.28	1.34
4	A	1833	DCT	C3'-C2'	2.65	1.61	1.54
4	A	1833	DCT	C6-N1	2.46	1.43	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1833	DCT	C4'-O4'-C1'	11.63	120.78	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1833	DCT	C2'-C1'-N1	-4.07	104.69	112.40
4	A	1833	DCT	O4'-C4'-C5'	3.69	115.59	109.52
4	A	1833	DCT	PB-O3A-PA	-2.47	124.34	132.83
4	A	1833	DCT	O3G-PG-O3B	2.28	112.28	104.64
4	A	1833	DCT	O4'-C1'-N1	2.20	111.80	107.86
4	A	1833	DCT	C6-C5-C4	2.17	121.00	117.50

There are no chirality outliers.

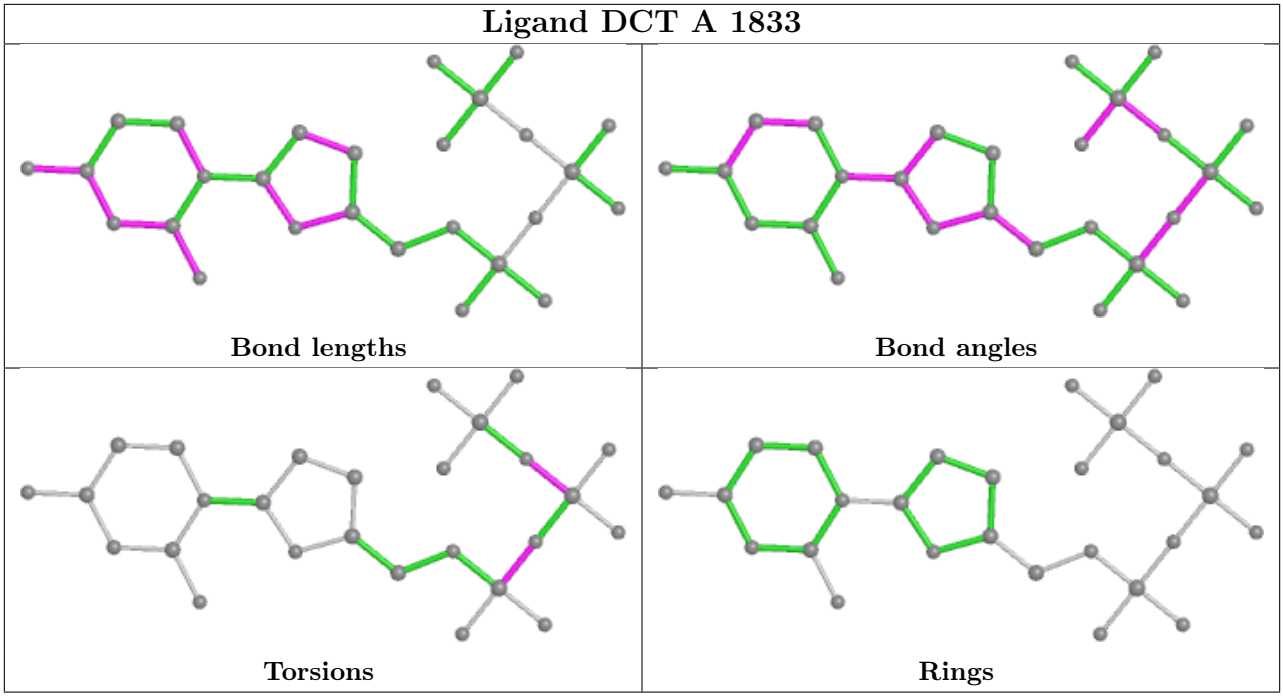
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1833	DCT	PB-O3A-PA-O2A
4	A	1833	DCT	PG-O3B-PB-O2B
4	A	1833	DCT	PG-O3B-PB-O1B

There are no ring outliers.

No monomer is involved in short contacts.

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 then 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	539/540 (99%)	0.05	38 (7%) 16 18	23, 36, 73, 89	0
2	B	11/12 (91%)	-0.48	0 100 100	26, 28, 54, 56	0
3	C	14/16 (87%)	-0.48	0 100 100	24, 30, 46, 63	0
All	All	564/568 (99%)	0.03	38 (6%) 17 21	23, 36, 73, 89	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	683	ALA	15.2
1	A	657	LEU	7.1
1	A	649	VAL	6.9
1	A	645	TRP	6.9
1	A	693	ILE	6.8
1	A	692	PHE	6.6
1	A	648	GLY	6.4
1	A	647	PHE	5.8
1	A	684	ILE	5.6
1	A	696	TYR	5.4
1	A	653	ALA	5.3
1	A	695	ARG	5.2
1	A	686	TYR	5.0
1	A	691	ALA	5.0
1	A	650	PRO	5.0
1	A	638[A]	PHE	4.7
1	A	697	PHE	4.4
1	A	651	ARG	4.2
1	A	644	SER	4.2
1	A	688	GLU	4.0
1	A	682	LEU	4.0
1	A	689	ALA	4.0
1	A	698	GLN	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	503	ILE	3.6
1	A	681	GLU	3.5
1	A	680	GLN	3.4
1	A	646	MET	2.8
1	A	652	GLU	2.7
1	A	685	PRO	2.6
1	A	678	LEU	2.6
1	A	656	PRO	2.4
1	A	655	ASP	2.4
1	A	668	GLY	2.3
1	A	654	VAL	2.2
1	A	687	GLU	2.2
1	A	630	ARG	2.2
1	A	669	VAL	2.2
1	A	699	SER	2.1

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	DOC	B	112	18/19	0.98	0.08	22,28,34,36	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MG	B	1113	1/1	0.84	0.11	60,60,60,60	0
5	MG	B	1112	1/1	0.96	0.04	54,54,54,54	0

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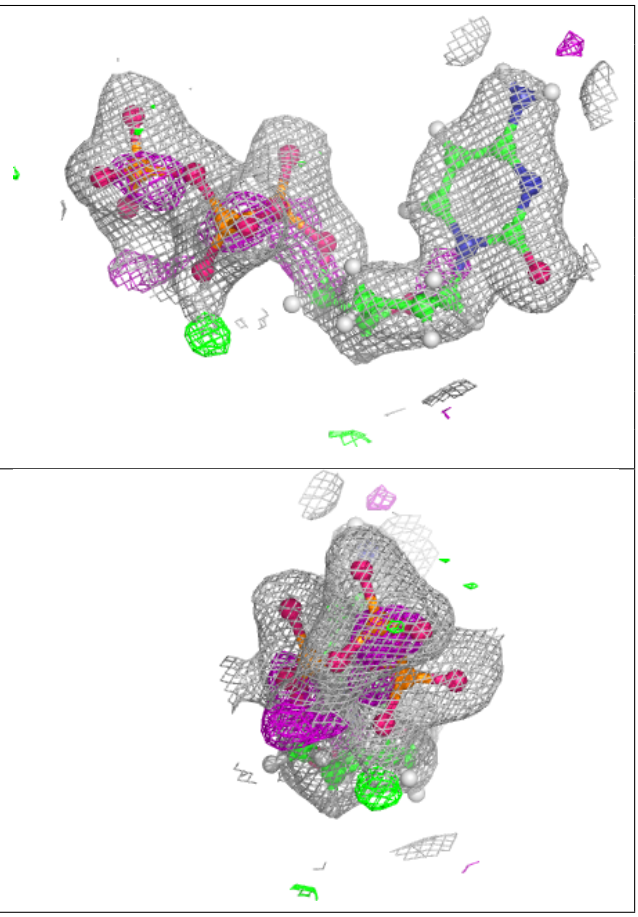
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	DCT	A	1833	27/27	0.96	0.07	27,34,43,47	0
5	MG	A	1836	1/1	0.97	0.03	37,37,37,37	0
5	MG	A	1835	1/1	0.98	0.03	34,34,34,34	0
5	MG	A	1834	1/1	0.99	0.08	32,32,32,32	0

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 DCT A 1833:

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.