wwPDB X-ray Structure Validation Summary Report (i)

Jan 3, 2024 – 03:54 am GMT

PDB ID	:	5LKM
Title	:	RadA bound to dTDP
Authors	:	Rapisarda, C.; Remaut, H.; Fornzes, R.
Deposited on	:	2016-07-22
Resolution	:	3.50 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*
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:

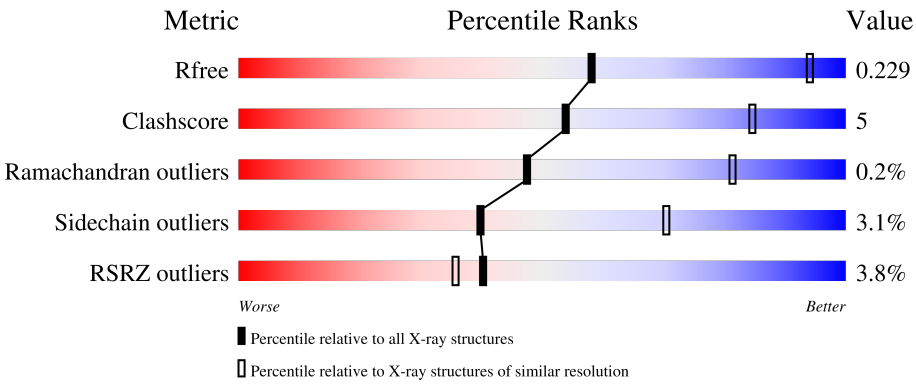
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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	452	74% 12% • 14%
1	B	452	8% 69% 7% • 23%
1	C	452	% 72% 10% • 17%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8608 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 repair protein RadA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	390	3002	1896	517	577	12	0	0	0
1	B	346	2656	1685	457	505	9	0	0	0
1	C	373	2872	1814	496	551	11	0	0	0

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A0T7K9X0
A	2	ALA	-	expression tag	UNP A0A0T7K9X0
A	3	LYS	-	expression tag	UNP A0A0T7K9X0
A	4	LYS	-	expression tag	UNP A0A0T7K9X0
A	5	LYS	-	expression tag	UNP A0A0T7K9X0
A	6	ALA	-	expression tag	UNP A0A0T7K9X0
A	7	THR	-	expression tag	UNP A0A0T7K9X0
A	8	PHE	-	expression tag	UNP A0A0T7K9X0
A	9	VAL	-	expression tag	UNP A0A0T7K9X0
A	10	CYS	-	expression tag	UNP A0A0T7K9X0
A	11	GLN	-	expression tag	UNP A0A0T7K9X0
A	12	ASN	-	expression tag	UNP A0A0T7K9X0
A	13	CYS	-	expression tag	UNP A0A0T7K9X0
A	14	GLY	-	expression tag	UNP A0A0T7K9X0
A	15	TYR	-	expression tag	UNP A0A0T7K9X0
A	16	ASN	-	expression tag	UNP A0A0T7K9X0
A	17	SER	-	expression tag	UNP A0A0T7K9X0
A	18	PRO	-	expression tag	UNP A0A0T7K9X0
A	19	LYS	-	expression tag	UNP A0A0T7K9X0
A	20	TYR	-	expression tag	UNP A0A0T7K9X0
A	21	LEU	-	expression tag	UNP A0A0T7K9X0
A	432	LEU	PRO	conflict	UNP A0A0T7K9X0
B	1	MET	-	initiating methionine	UNP A0A0T7K9X0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	2	ALA	-	expression tag	UNP A0A0T7K9X0
B	3	LYS	-	expression tag	UNP A0A0T7K9X0
B	4	LYS	-	expression tag	UNP A0A0T7K9X0
B	5	LYS	-	expression tag	UNP A0A0T7K9X0
B	6	ALA	-	expression tag	UNP A0A0T7K9X0
B	7	THR	-	expression tag	UNP A0A0T7K9X0
B	8	PHE	-	expression tag	UNP A0A0T7K9X0
B	9	VAL	-	expression tag	UNP A0A0T7K9X0
B	10	CYS	-	expression tag	UNP A0A0T7K9X0
B	11	GLN	-	expression tag	UNP A0A0T7K9X0
B	12	ASN	-	expression tag	UNP A0A0T7K9X0
B	13	CYS	-	expression tag	UNP A0A0T7K9X0
B	14	GLY	-	expression tag	UNP A0A0T7K9X0
B	15	TYR	-	expression tag	UNP A0A0T7K9X0
B	16	ASN	-	expression tag	UNP A0A0T7K9X0
B	17	SER	-	expression tag	UNP A0A0T7K9X0
B	18	PRO	-	expression tag	UNP A0A0T7K9X0
B	19	LYS	-	expression tag	UNP A0A0T7K9X0
B	20	TYR	-	expression tag	UNP A0A0T7K9X0
B	21	LEU	-	expression tag	UNP A0A0T7K9X0
B	432	LEU	PRO	conflict	UNP A0A0T7K9X0
C	1	MET	-	initiating methionine	UNP A0A0T7K9X0
C	2	ALA	-	expression tag	UNP A0A0T7K9X0
C	3	LYS	-	expression tag	UNP A0A0T7K9X0
C	4	LYS	-	expression tag	UNP A0A0T7K9X0
C	5	LYS	-	expression tag	UNP A0A0T7K9X0
C	6	ALA	-	expression tag	UNP A0A0T7K9X0
C	7	THR	-	expression tag	UNP A0A0T7K9X0
C	8	PHE	-	expression tag	UNP A0A0T7K9X0
C	9	VAL	-	expression tag	UNP A0A0T7K9X0
C	10	CYS	-	expression tag	UNP A0A0T7K9X0
C	11	GLN	-	expression tag	UNP A0A0T7K9X0
C	12	ASN	-	expression tag	UNP A0A0T7K9X0
C	13	CYS	-	expression tag	UNP A0A0T7K9X0
C	14	GLY	-	expression tag	UNP A0A0T7K9X0
C	15	TYR	-	expression tag	UNP A0A0T7K9X0
C	16	ASN	-	expression tag	UNP A0A0T7K9X0
C	17	SER	-	expression tag	UNP A0A0T7K9X0
C	18	PRO	-	expression tag	UNP A0A0T7K9X0
C	19	LYS	-	expression tag	UNP A0A0T7K9X0
C	20	TYR	-	expression tag	UNP A0A0T7K9X0
C	21	LEU	-	expression tag	UNP A0A0T7K9X0

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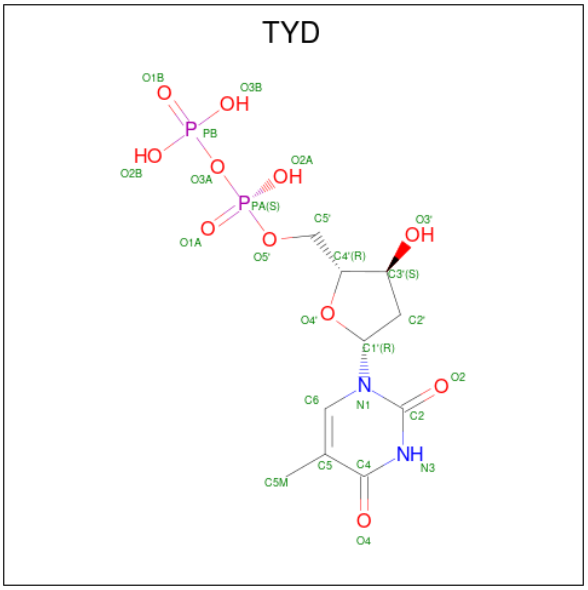
Chain	Residue	Modelled	Actual	Comment	Reference
C	432	LEU	PRO	conflict	UNP A0A0T7K9X0

- Molecule 2 is THYMIDINE-5'-DIPHOSPHATE (three-letter code: TYD) (formula: $C_{10}H_{16}N_2O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			25	10	2	11	2		
2	B	1	Total	C	N	O	P	0	0
			25	10	2	11	2		
2	C	1	Total	C	N	O	P	0	0
			25	10	2	11	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

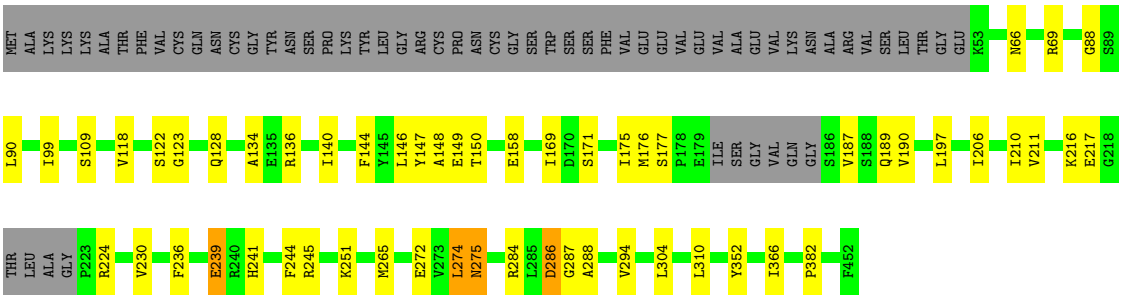
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

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.

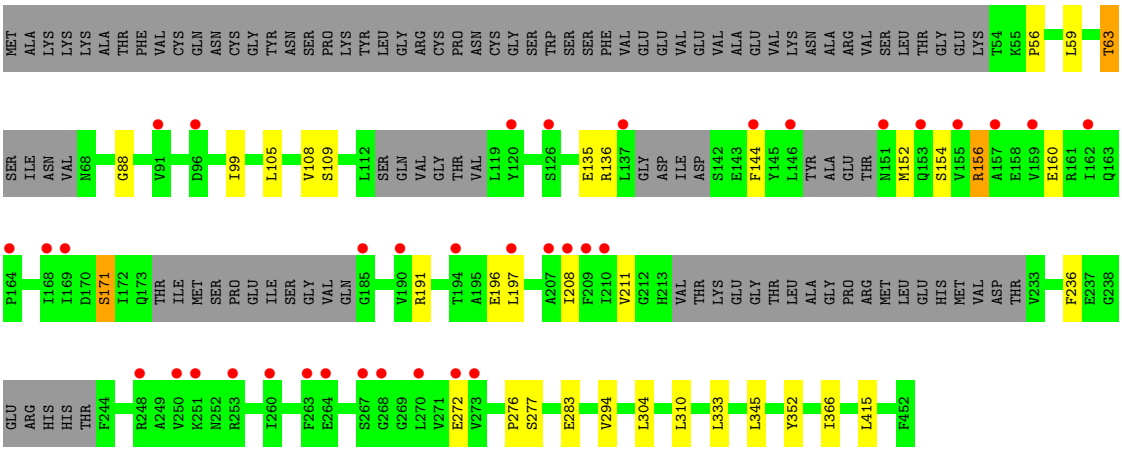
• Molecule 1: DNA repair protein RadA

Chain A:



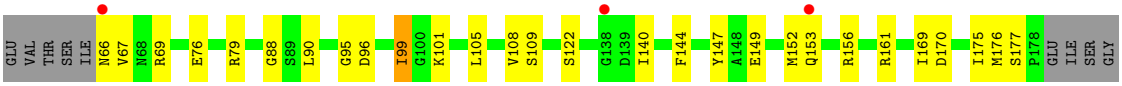
• Molecule 1: DNA repair protein RadA

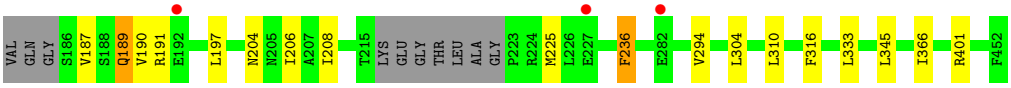
Chain B:



• Molecule 1: DNA repair protein RadA

Chain C:


GLU
VAL
THR
SER
ILE
N66
V67
N68
R69
E76
R79
G88
S89
L90
G95
D96
I99
G100
K101
L105
V108
S109
S122
G138
D139
I140
F144
Y147
A148
E149
M152
Q153
R156
R161
I169
D170
I175
M176
S177
P178
GLU
ILE
SER
GLY


VAL
GLN
GLY
S186
V187
S188
Q189
V190
R191
E192
L197
N204
N205
I206
A207
I208
T215
LYS
GLU
GLY
THR
LEU
ALA
GLY
P223
R224
M225
L226
E227
F236
E282
V294
L304
L310
F316
L333
L345
I366
R401
F452

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	99.40Å 169.90Å 187.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.21 – 3.50 49.70 – 3.19	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.21-3.50) 99.9 (49.70-3.19)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0124, BUSTER, PHENIX	Depositor
R, R_{free}	0.183 , 0.224 0.184 , 0.229	Depositor DCC
R_{free} test set	1339 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	131.3	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 103.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8608	wwPDB-VP
Average B, all atoms (Å^2)	149.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.84% 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: TYD, MG

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	0.71	0/3038	0.93	9/4102 (0.2%)
1	B	0.67	0/2681	0.89	3/3610 (0.1%)
1	C	0.71	0/2906	0.92	4/3925 (0.1%)
All	All	0.70	0/8625	0.92	16/11637 (0.1%)

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	69	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	C	69	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	B	156	ARG	NE-CZ-NH2	-6.63	116.98	120.30
1	A	136	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	A	274	LEU	N-CA-C	-6.44	93.62	111.00

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	3002	0	3098	41	0
1	B	2656	0	2756	20	0
1	C	2872	0	2953	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	25	0	13	0	0
2	B	25	0	13	0	0
2	C	25	0	13	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
All	All	8608	0	8846	92	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 5.

The worst 5 of 92 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:C:147:TYR:CZ	1:C:149:GLU:HG3	1.88	1.09
1:A:90:LEU:CD2	1:A:230:VAL:HG12	1.91	1.00
1:C:122:SER:HB2	1:C:170:ASP:HB3	1.45	0.97
1:C:140:ILE:O	1:C:140:ILE:HG22	1.65	0.95
1:A:90:LEU:HD21	1:A:230:VAL:HG12	1.51	0.92

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	384/452 (85%)	359 (94%)	25 (6%)	0	100 100
1	B	330/452 (73%)	318 (96%)	10 (3%)	2 (1%)	25 64
1	C	365/452 (81%)	346 (95%)	19 (5%)	0	100 100
All	All	1079/1356 (80%)	1023 (95%)	54 (5%)	2 (0%)	47 81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	88	GLY
1	B	171	SER

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	333/383 (87%)	325 (98%)	8 (2%)	49	76
1	B	292/383 (76%)	280 (96%)	12 (4%)	30	63
1	C	318/383 (83%)	309 (97%)	9 (3%)	43	72
All	All	943/1149 (82%)	914 (97%)	29 (3%)	40	70

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	236	PHE
1	C	345	LEU
1	B	304	LEU
1	C	304	LEU
1	B	283	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	425	ASN
1	C	129	GLN
1	C	386	GLN
1	C	242	HIS
1	C	349	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
2	TYD	A	500	3	21,26,26	0.99	1 (4%)	27,40,40	1.69	1 (3%)
2	TYD	C	500	3	21,26,26	1.07	1 (4%)	27,40,40	1.78	4 (14%)
2	TYD	B	500	3	21,26,26	0.93	1 (4%)	27,40,40	1.78	4 (14%)

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	TYD	A	500	3	-	5/13/28/28	0/2/2/2
2	TYD	C	500	3	-	5/13/28/28	0/2/2/2
2	TYD	B	500	3	-	4/13/28/28	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	TYD	C5-C4	3.55	1.49	1.41
2	A	500	TYD	C5-C4	3.26	1.48	1.41
2	B	500	TYD	C5-C4	3.16	1.48	1.41

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	500	TYD	C2-N3-C4	7.44	121.43	115.14
2	B	500	TYD	C2-N3-C4	7.44	121.42	115.14
2	A	500	TYD	C2-N3-C4	7.07	121.11	115.14
2	B	500	TYD	C5M-C5-C6	2.46	123.87	118.68
2	C	500	TYD	C4'-O4'-C1'	-2.38	103.70	109.45

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

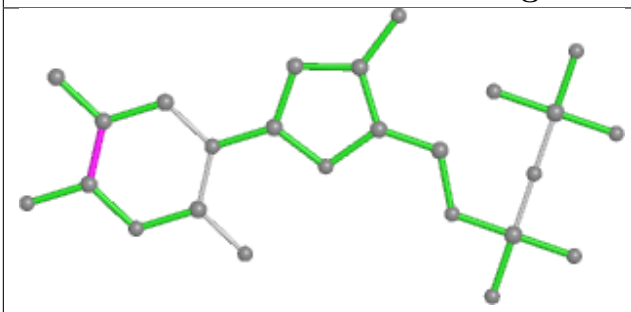
Mol	Chain	Res	Type	Atoms
2	A	500	TYD	O4'-C1'-N1-C6
2	C	500	TYD	O4'-C1'-N1-C6
2	A	500	TYD	PA-O3A-PB-O1B
2	B	500	TYD	PA-O3A-PB-O1B
2	C	500	TYD	PA-O3A-PB-O1B

There are no ring outliers.

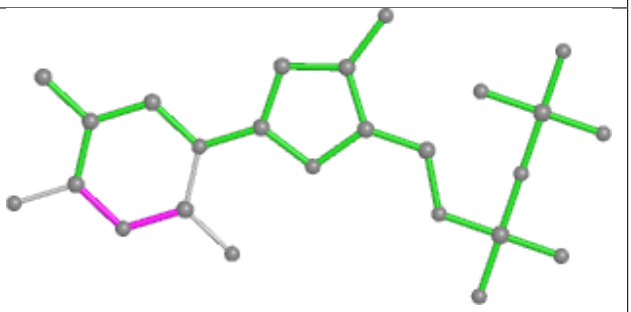
No monomer is involved in short contacts.

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.

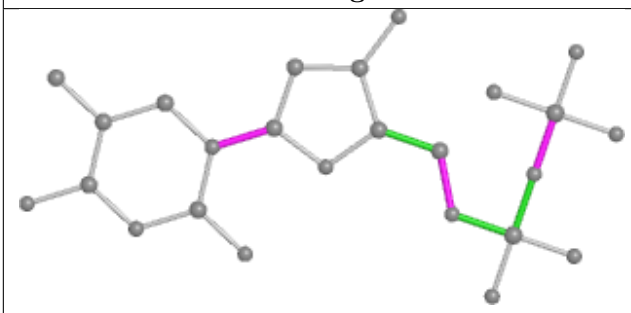
Ligand TYD A 500



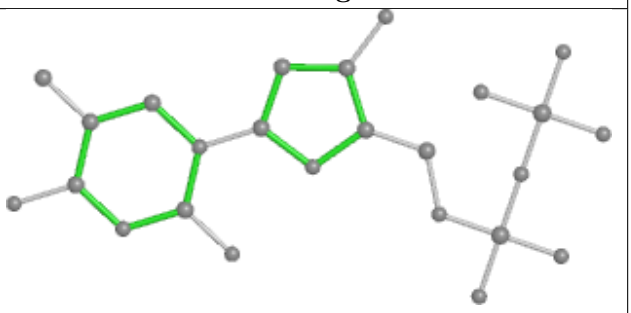
Bond lengths



Bond angles

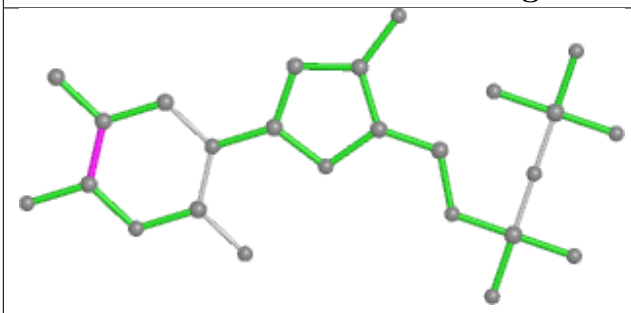


Torsions

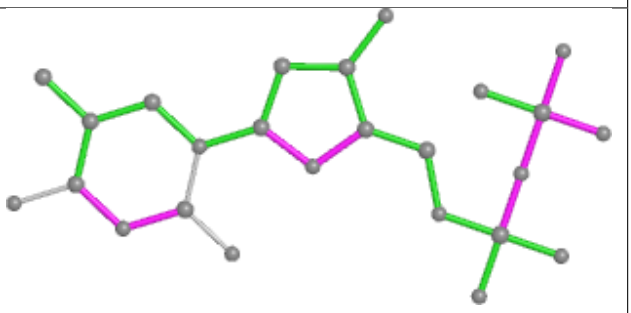


Rings

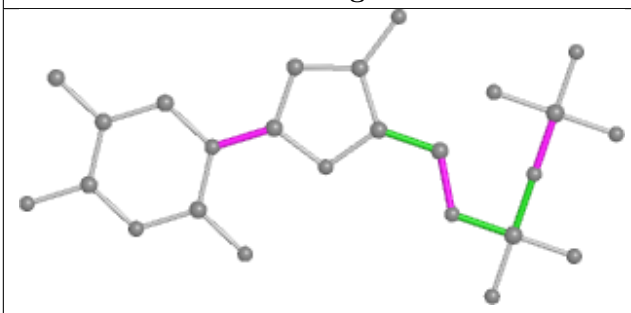
Ligand TYD C 500



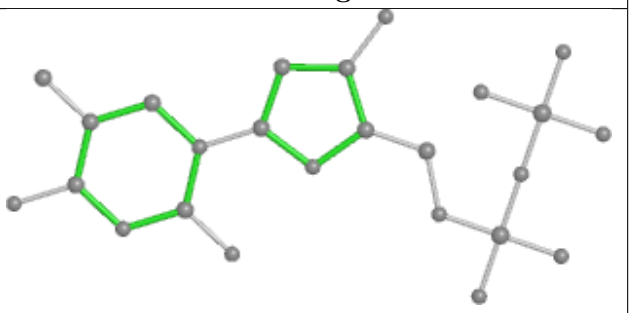
Bond lengths



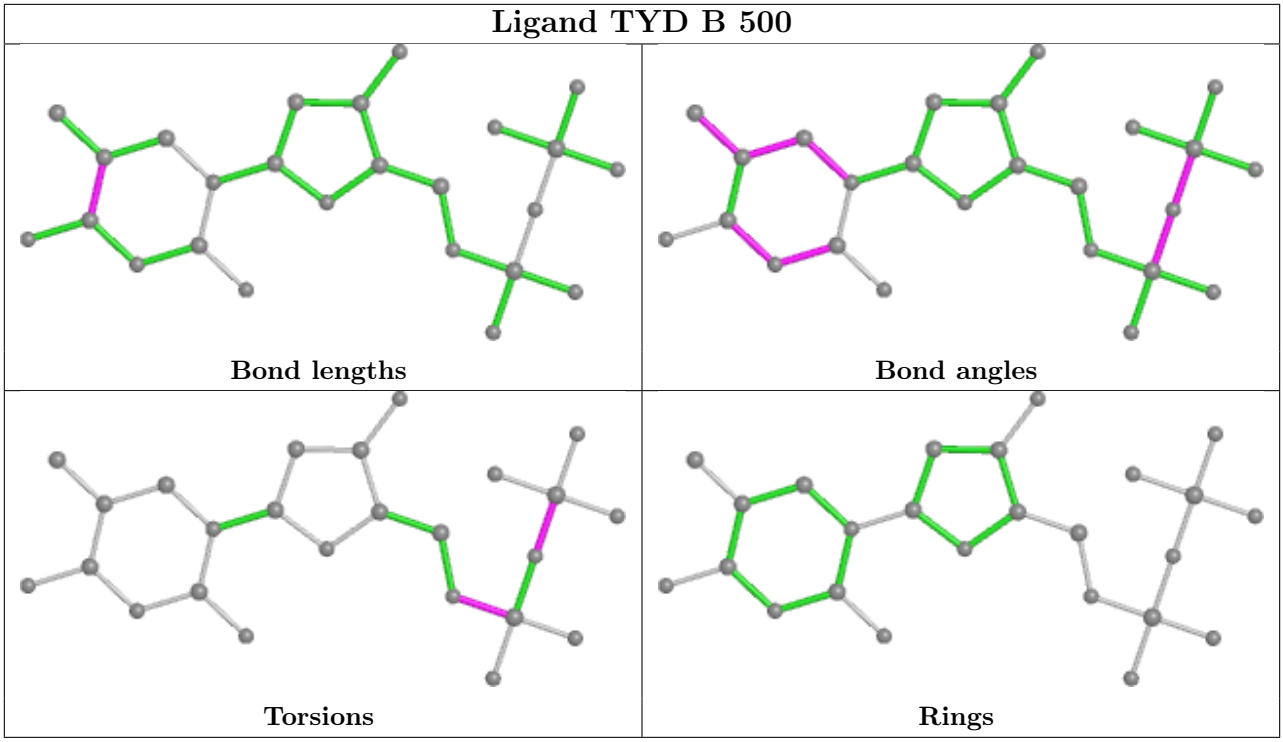
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	281:LEU	C	282:GLU	N	2.83

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	390/452 (86%)	-0.30	0 100 100	76, 129, 197, 230	0
1	B	346/452 (76%)	0.35	36 (10%) 6 7	81, 172, 275, 337	0
1	C	373/452 (82%)	-0.29	6 (1%) 72 66	80, 128, 198, 242	0
All	All	1109/1356 (81%)	-0.10	42 (3%) 40 36	76, 134, 245, 337	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	194	THR	6.8
1	B	264	GLU	5.3
1	B	207	ALA	4.8
1	B	197	LEU	4.8
1	B	190	VAL	4.6

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 (i)

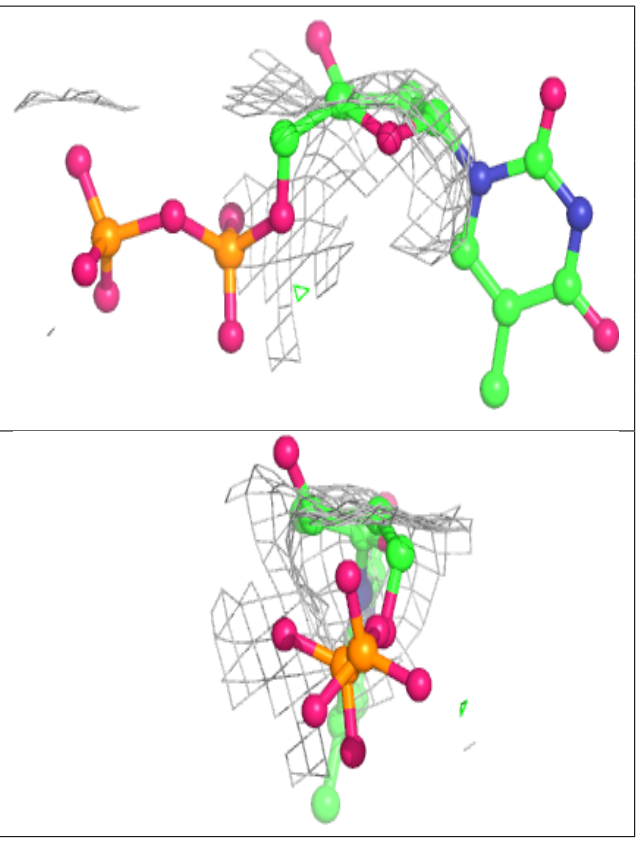
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	B	501	1/1	0.83	0.08	158,158,158,158	0
2	TYD	B	500	25/25	0.90	0.24	214,270,284,290	0
2	TYD	C	500	25/25	0.94	0.25	118,160,262,271	0
3	MG	C	501	1/1	0.94	0.23	98,98,98,98	0
2	TYD	A	500	25/25	0.96	0.20	119,171,224,235	0
3	MG	A	501	1/1	0.97	0.17	117,117,117,117	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.

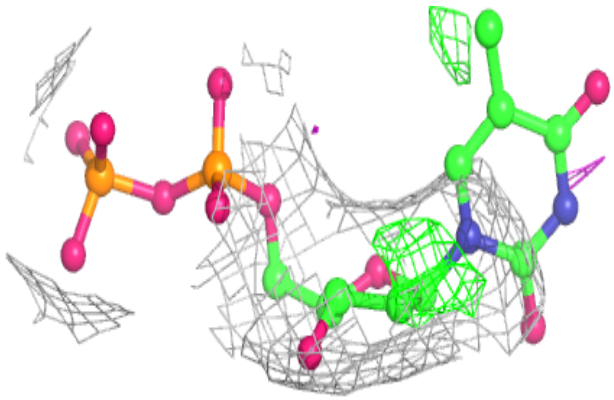
Electron density around TYD B 500:

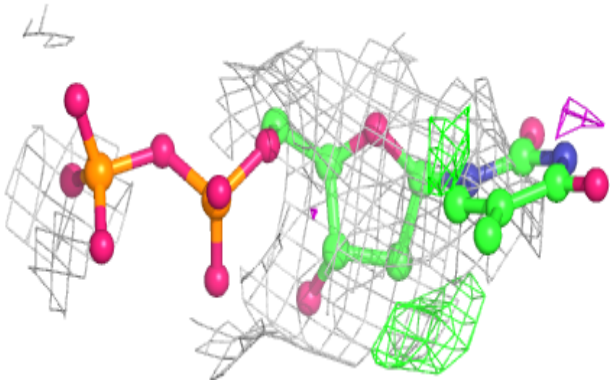
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

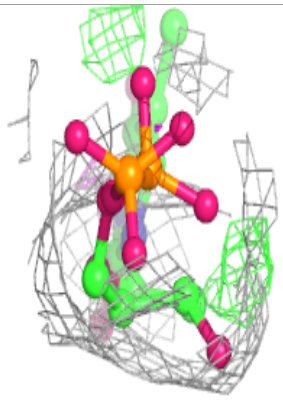


Electron density around TYD C 500:

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

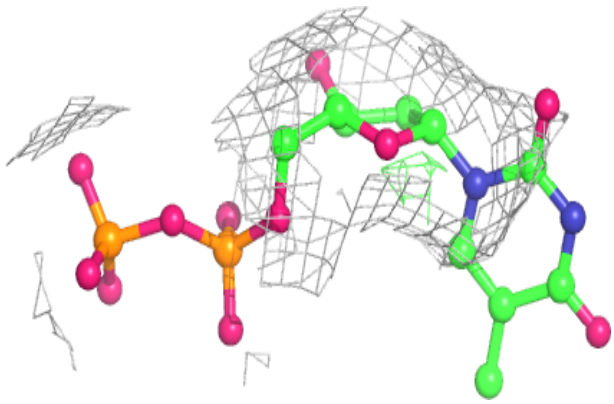


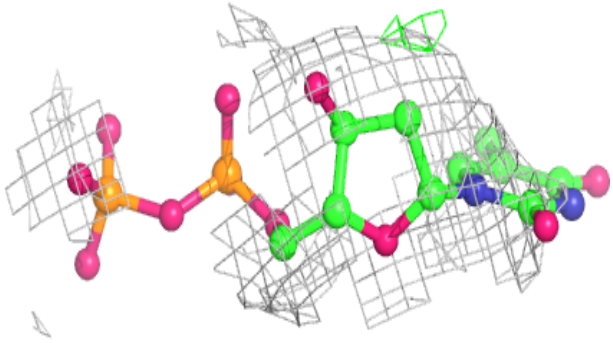


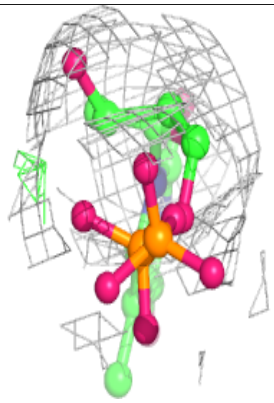


Electron density around TYD A 500:

$2mF_o$-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.