Full wwPDB X-ray Structure Validation 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 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:

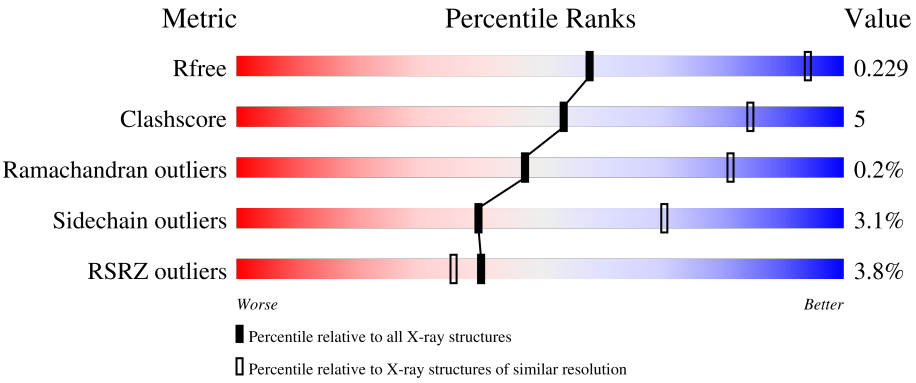
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 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
1	A	390	Total	C	N	O	S	0	0	0
			3002	1896	517	577	12			
1	B	346	Total	C	N	O	S	0	0	0
			2656	1685	457	505	9			
1	C	373	Total	C	N	O	S	0	0	0
			2872	1814	496	551	11			

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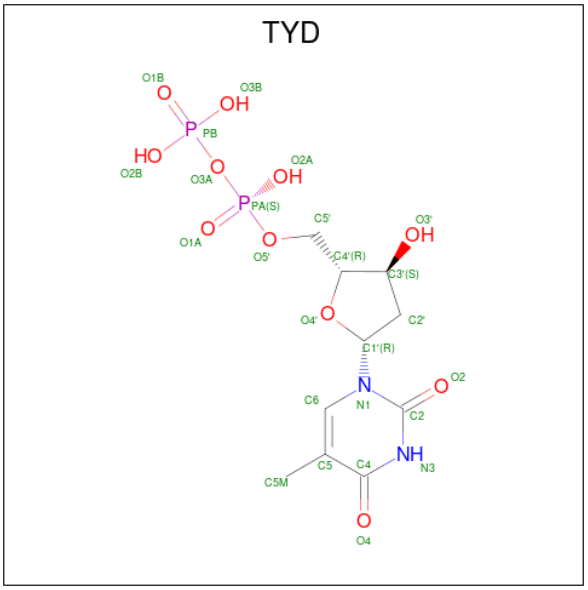
Chain	Residue	Modelled	Actual	Comment	Reference
C	432	LEU	PRO	conflict	UNP A0A0T7K9X0

- 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).

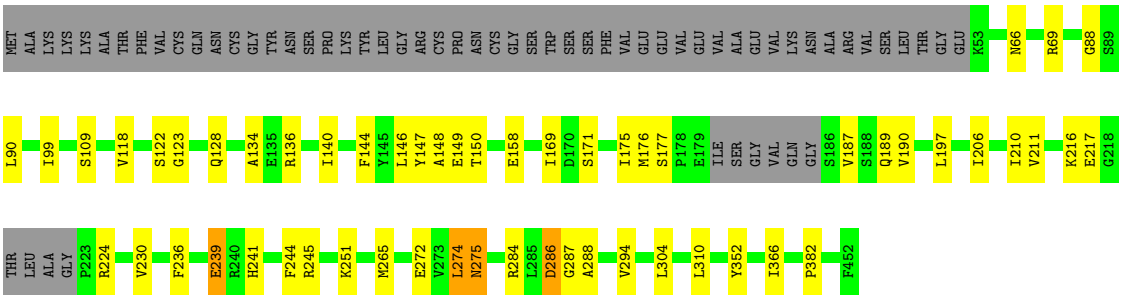
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

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.

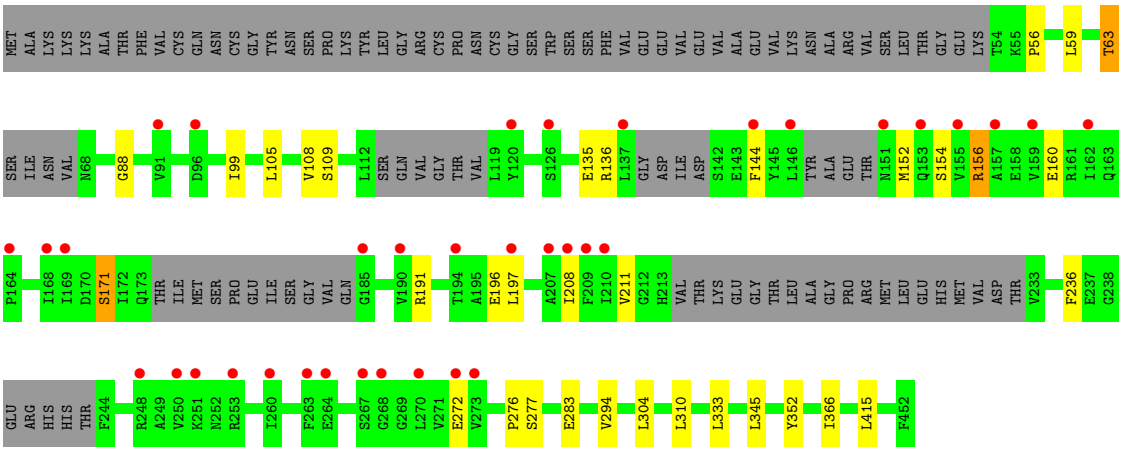
• Molecule 1: DNA repair protein RadA

Chain A:



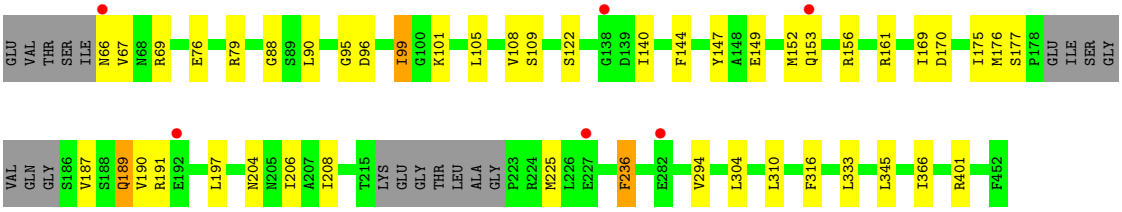
• Molecule 1: DNA repair protein RadA

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

5.1 Standard geometry

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.

All (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
1	C	161	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	A	224	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	A	286	ASP	CB-CG-OD1	6.03	123.73	118.30
1	B	136	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	A	286	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	C	99	ILE	CB-CA-C	-5.74	100.12	111.60
1	C	161	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	B	156	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	251	LYS	CB-CA-C	-5.27	99.86	110.40
1	A	69	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	A	244	PHE	N-CA-C	5.17	124.95	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
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.

All (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
1:C:122:SER:CB	1:C:170:ASP:HB3	2.07	0.84
1:A:286:ASP:OD1	1:A:287:GLY:N	2.10	0.83
1:C:177:SER:O	1:C:189:GLN:NE2	2.17	0.78
1:C:191:ARG:HH21	1:C:225:MET:CE	1.97	0.77
1:A:140:ILE:HG21	1:B:59:LEU:HB3	1.67	0.77
1:A:90:LEU:HD23	1:A:230:VAL:HG12	1.66	0.76
1:B:277:SER:HB2	1:B:415:LEU:O	1.86	0.74
1:C:187:VAL:O	1:C:190:VAL:HB	1.87	0.74
1:C:99:ILE:HD12	1:C:236:PHE:HB3	1.71	0.72
1:A:146:LEU:HD22	1:B:59:LEU:CD1	2.20	0.71
1:A:90:LEU:HD23	1:A:230:VAL:CB	2.22	0.68
1:C:90:LEU:HD23	1:C:208:ILE:HB	1.75	0.68
1:A:187:VAL:O	1:A:190:VAL:HG22	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:LEU:HD22	1:B:59:LEU:HD11	1.76	0.67
1:A:90:LEU:HD23	1:A:230:VAL:CG1	2.25	0.66
1:C:191:ARG:HH21	1:C:225:MET:HE3	1.60	0.66
1:A:140:ILE:HD13	1:B:59:LEU:HD23	1.80	0.64
1:C:96:ASP:O	1:C:101:LYS:NZ	2.31	0.64
1:C:176:MET:HA	1:C:189:GLN:OE1	1.98	0.64
1:A:274:LEU:O	1:A:275:ASN:OD1	2.16	0.63
1:C:90:LEU:CD2	1:C:208:ILE:HB	2.29	0.63
1:B:276:PRO:HG2	1:B:415:LEU:HG	1.80	0.63
1:B:156:ARG:HH22	1:B:196:GLU:HB3	1.65	0.61
1:A:122:SER:O	1:A:148:ALA:HA	2.00	0.61
1:A:90:LEU:CD2	1:A:230:VAL:CG1	2.73	0.61
1:C:176:MET:O	1:C:176:MET:HG3	2.00	0.60
1:C:191:ARG:HH21	1:C:225:MET:HE1	1.65	0.59
1:A:288:ALA:O	1:A:382:PRO:HB3	2.00	0.59
1:C:177:SER:N	1:C:189:GLN:OE1	2.35	0.59
1:A:99:ILE:HG13	1:A:245:ARG:HD3	1.85	0.59
1:C:140:ILE:O	1:C:140:ILE:CG2	2.41	0.59
1:A:245:ARG:NH1	1:A:265:MET:HB3	2.18	0.58
1:B:152:MET:O	1:B:156:ARG:HG3	2.03	0.58
1:B:197:LEU:HD12	1:B:208:ILE:HG21	1.85	0.57
1:C:152:MET:HG3	1:C:153:GLN:N	2.18	0.57
1:A:140:ILE:HD13	1:B:59:LEU:CD2	2.35	0.56
1:C:147:TYR:OH	1:C:149:GLU:HG3	2.04	0.56
1:A:177:SER:O	1:A:189:GLN:NE2	2.39	0.56
1:C:197:LEU:HD12	1:C:208:ILE:HG21	1.86	0.55
1:A:128:GLN:HE21	1:B:63:THR:C	2.09	0.55
1:C:152:MET:SD	1:C:177:SER:CB	2.94	0.55
1:C:95:GLY:HA3	1:C:99:ILE:HD11	1.89	0.53
1:A:90:LEU:HD23	1:A:230:VAL:HB	1.90	0.53
1:C:152:MET:SD	1:C:177:SER:HB3	2.49	0.53
1:C:147:TYR:CE1	1:C:149:GLU:HG3	2.39	0.53
1:C:169:ILE:HG23	1:C:175:ILE:HD12	1.89	0.53
1:C:76:GLU:OE2	1:C:79:ARG:NH2	2.42	0.52
1:B:105:LEU:HA	1:B:108:VAL:HG22	1.92	0.51
1:A:171:SER:H	1:A:211:VAL:HB	1.75	0.51
1:C:105:LEU:HA	1:C:108:VAL:HG22	1.92	0.50
1:C:152:MET:SD	1:C:177:SER:HB2	2.52	0.49
1:A:189:GLN:O	1:A:189:GLN:HG2	2.12	0.49
1:C:99:ILE:HD13	1:C:236:PHE:O	2.13	0.48
1:A:134:ALA:HB1	1:A:140:ILE:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:TYR:HB3	1:C:333:LEU:CD2	2.44	0.47
1:B:109:SER:HB3	1:B:144:PHE:HE1	1.80	0.47
1:C:88:GLY:H	1:C:206:ILE:C	2.18	0.47
1:C:147:TYR:CE2	1:C:149:GLU:HB2	2.49	0.47
1:C:169:ILE:CG2	1:C:175:ILE:HD12	2.44	0.47
1:C:147:TYR:CZ	1:C:149:GLU:CG	2.78	0.47
1:C:66:ASN:O	1:C:67:VAL:HG23	2.15	0.47
1:B:294:VAL:HG21	1:B:366:ILE:HA	1.98	0.46
1:B:352:TYR:HB3	1:C:333:LEU:HD22	1.96	0.46
1:A:88:GLY:H	1:A:206:ILE:C	2.19	0.46
1:A:109:SER:HB3	1:A:144:PHE:HE1	1.81	0.46
1:B:171:SER:H	1:B:211:VAL:HB	1.80	0.45
1:A:197:LEU:HD13	1:A:210:ILE:HD11	1.96	0.45
1:A:245:ARG:NH1	1:A:265:MET:CB	2.79	0.45
1:C:109:SER:HB3	1:C:144:PHE:HE1	1.82	0.44
1:A:90:LEU:HD23	1:A:230:VAL:HA	2.00	0.44
1:A:140:ILE:HG22	1:A:140:ILE:O	2.17	0.44
1:A:294:VAL:HG21	1:A:366:ILE:HA	1.99	0.44
1:A:352:TYR:HB3	1:B:333:LEU:CD2	2.48	0.43
1:C:294:VAL:HG21	1:C:366:ILE:HA	2.01	0.43
1:A:147:TYR:CE2	1:A:149:GLU:HB3	2.54	0.43
1:A:239:GLU:HB3	1:A:241:HIS:CD2	2.54	0.43
1:B:156:ARG:NH2	1:B:196:GLU:HB3	2.30	0.42
1:A:109:SER:HB3	1:A:118:VAL:HG11	2.02	0.42
1:A:169:ILE:HG23	1:A:175:ILE:HD13	2.01	0.42
1:A:284:ARG:HD2	1:A:288:ALA:CB	2.49	0.42
1:A:216:LYS:C	1:A:217:GLU:HG2	2.39	0.42
1:C:191:ARG:NH2	1:C:225:MET:HE1	2.33	0.42
1:C:88:GLY:HA2	1:C:206:ILE:O	2.19	0.42
1:A:158:GLU:HG3	1:B:56:PRO:HD3	2.02	0.41
1:A:123:GLY:HA3	1:A:150:THR:HG22	2.02	0.40
1:C:169:ILE:HG23	1:C:175:ILE:CD1	2.50	0.40
1:A:245:ARG:HH12	1:A:265:MET:HB3	1.83	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	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

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	ASN

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Mol	Chain	Res	Type
1	A	176	MET
1	A	236	PHE
1	A	239	GLU
1	A	272	GLU
1	A	275	ASN
1	A	304	LEU
1	A	310	LEU
1	B	63	THR
1	B	99	ILE
1	B	135	GLU
1	B	154	SER
1	B	160	GLU
1	B	191	ARG
1	B	236	PHE
1	B	272	GLU
1	B	283	GLU
1	B	304	LEU
1	B	310	LEU
1	B	345	LEU
1	C	156	ARG
1	C	189	GLN
1	C	204	ASN
1	C	236	PHE
1	C	304	LEU
1	C	310	LEU
1	C	316	PHE
1	C	345	LEU
1	C	401	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	GLN
1	A	241	HIS
1	A	437	GLN
1	B	68	ASN
1	B	129	GLN
1	B	204	ASN
1	B	213	HIS
1	B	425	ASN
1	C	129	GLN
1	C	241	HIS

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Mol	Chain	Res	Type
1	C	242	HIS
1	C	349	GLN
1	C	386	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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

All (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
2	C	500	TYD	PA-O3A-PB	-2.16	125.40	132.83
2	B	500	TYD	C5-C6-N1	-2.07	119.96	122.19
2	C	500	TYD	O2B-PB-O1B	2.06	118.74	110.68
2	B	500	TYD	PA-O3A-PB	-2.03	125.87	132.83

There are no chirality outliers.

All (14) torsion outliers are listed below:

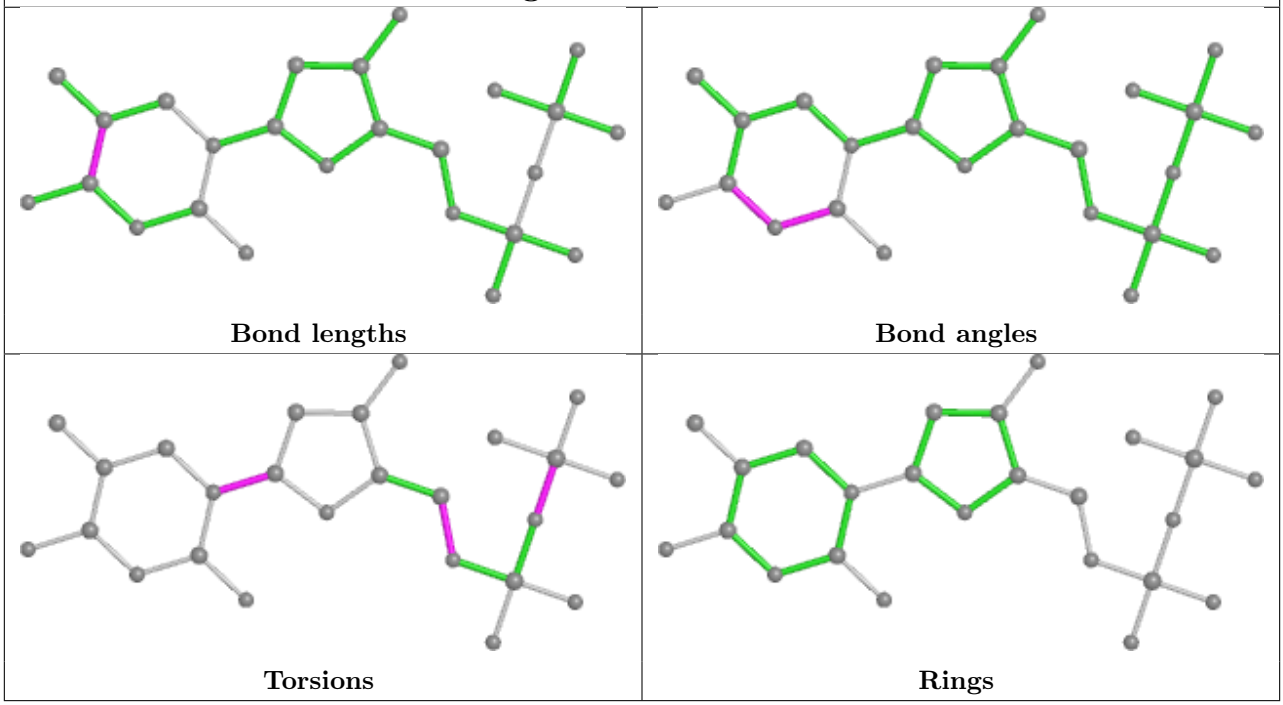
Mol	Chain	Res	Type	Atoms
2	A	500	TYD	O4'-C1'-N1-C6
2	C	500	TYD	O4'-C1'-N1-C6
2	A	500	TYD	PA-O3A-PB-O1B
2	B	500	TYD	PA-O3A-PB-O1B
2	C	500	TYD	PA-O3A-PB-O1B
2	A	500	TYD	C4'-C5'-O5'-PA
2	C	500	TYD	C4'-C5'-O5'-PA
2	A	500	TYD	PA-O3A-PB-O2B
2	A	500	TYD	PA-O3A-PB-O3B
2	B	500	TYD	PA-O3A-PB-O2B
2	B	500	TYD	PA-O3A-PB-O3B
2	C	500	TYD	PA-O3A-PB-O2B
2	C	500	TYD	PA-O3A-PB-O3B
2	B	500	TYD	C5'-O5'-PA-O1A

There are no ring outliers.

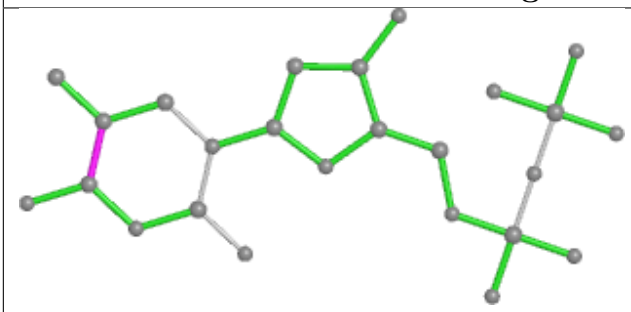
No monomer is involved in short contacts.

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.

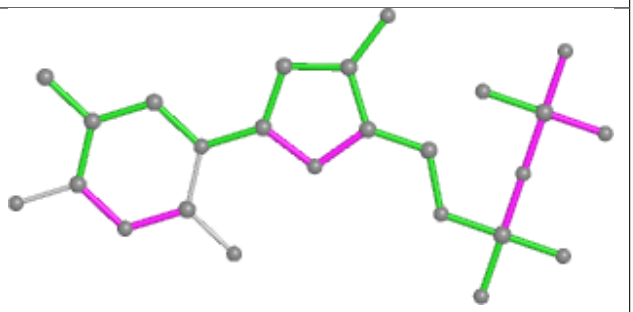
Ligand TYD A 500



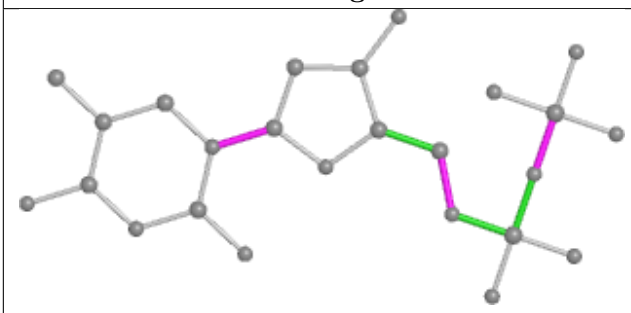
Ligand TYD C 500



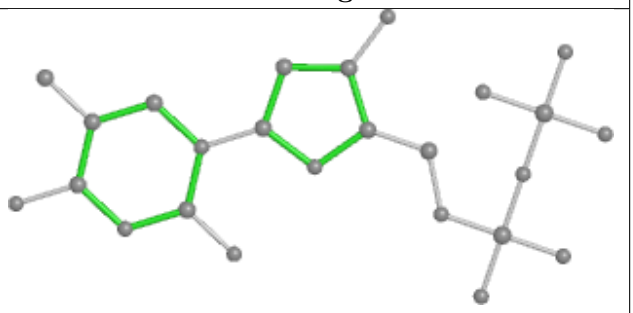
Bond lengths



Bond angles

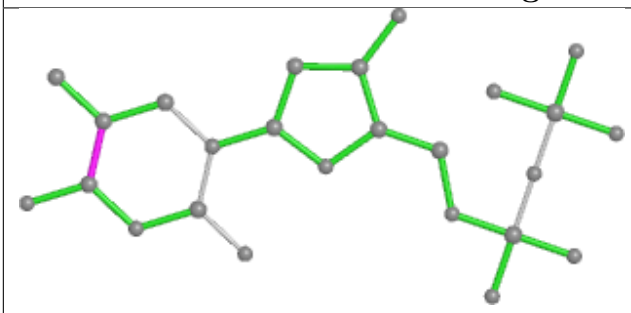


Torsions

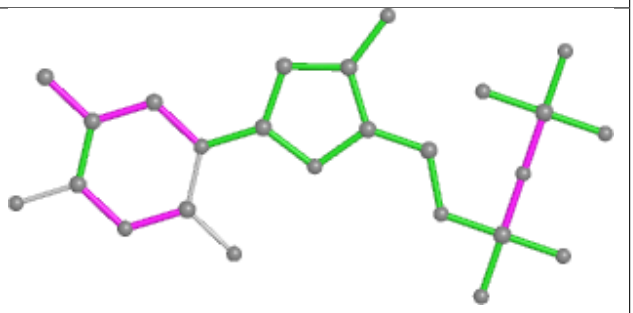


Rings

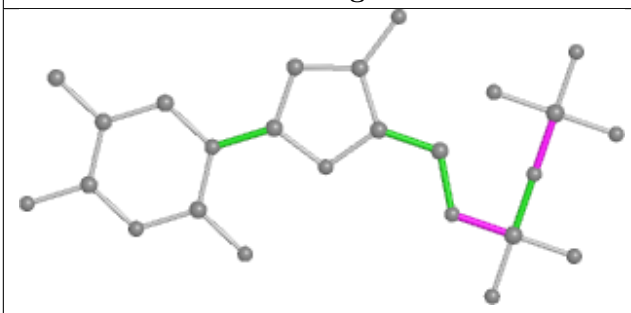
Ligand TYD B 500



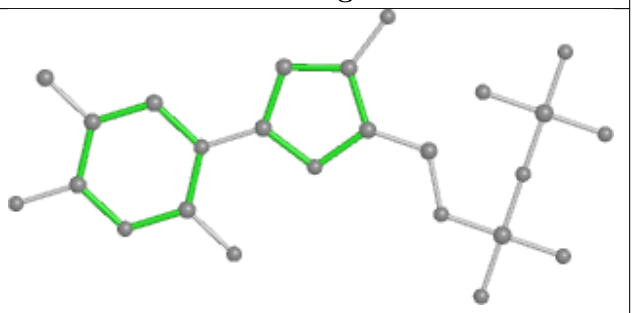
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

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

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^{th} 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

All (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
1	B	146	LEU	4.6
1	B	209	PHE	4.5
1	B	164	PRO	4.4
1	C	138	GLY	4.2
1	B	185	GLY	3.8
1	B	273	VAL	3.7
1	B	153	GLN	3.7
1	B	120	TYR	3.7
1	B	268	GLY	3.6
1	B	260	ILE	3.5
1	B	270	LEU	3.3
1	B	137	LEU	3.2
1	B	155	VAL	3.2
1	B	250	VAL	3.1
1	B	126	SER	2.8
1	B	162	ILE	2.7
1	B	91	VAL	2.7
1	B	210	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	253	ARG	2.7
1	B	144	PHE	2.6
1	B	263	PHE	2.6
1	B	248	ARG	2.5
1	B	151	ASN	2.5
1	B	96	ASP	2.5
1	C	282	GLU	2.4
1	B	168	ILE	2.4
1	C	227	GLU	2.3
1	B	159	VAL	2.3
1	C	153	GLN	2.2
1	B	169	ILE	2.2
1	B	251	LYS	2.2
1	B	208	ILE	2.2
1	B	272	GLU	2.2
1	C	66	ASN	2.1
1	B	267	SER	2.1
1	C	192	GLU	2.1
1	B	157	ALA	2.1

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, 95^{th} 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

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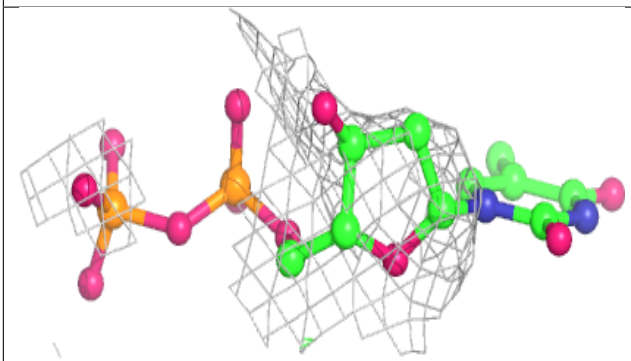
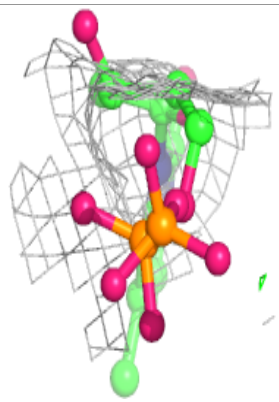
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	TYD	A	500	25/25	0.96	0.20	119,171,224,235	0
3	MG	A	501	1/1	0.97	0.17	117,117,117,117	0

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:

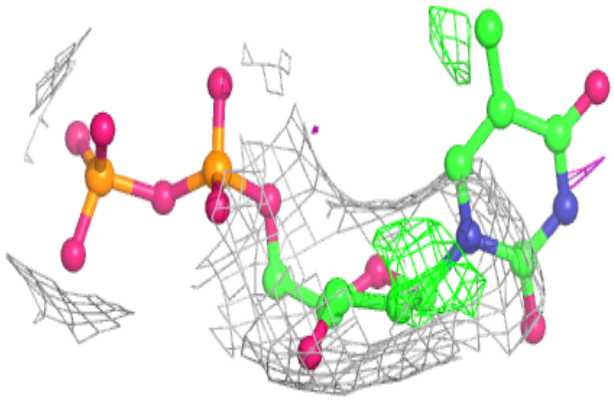
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

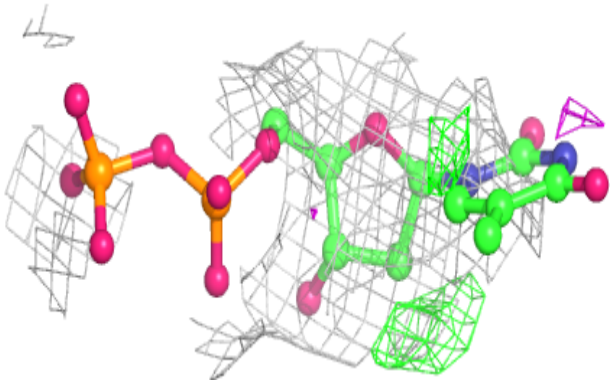


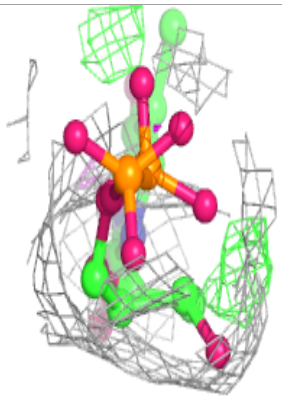


Electron density around TYD C 500:

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

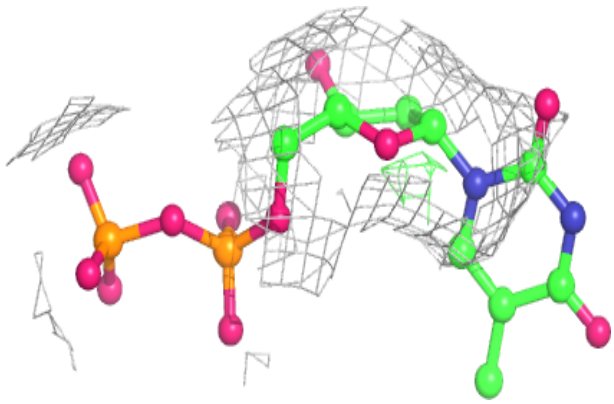


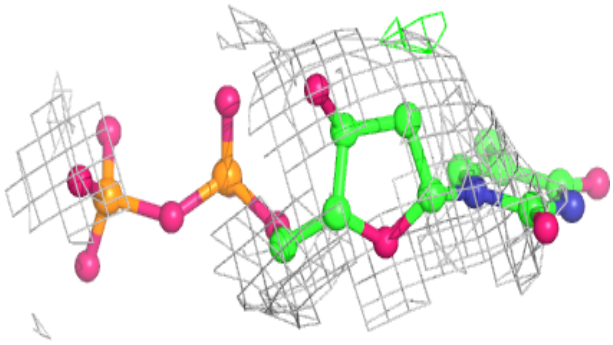


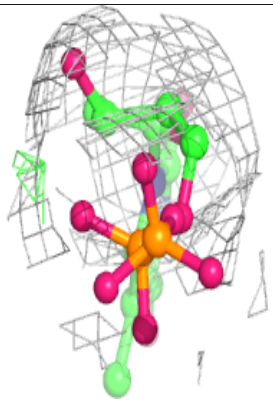


Electron density around TYD A 500:

$2mF_o$-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.