



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 11, 2021 – 02:03 PM EDT

PDB ID : 7K9Y
Title : GsI-IIC RT Template-Switching Complex (twinned)
Authors : Stamos, J.L.; Lentzsch, A.M.
Deposited on : 2020-09-29
Resolution : 3.20 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 ⓘ symbol.

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)
Xtriage (Phenix) : 1.13
EDS : 2.23.1
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) : 2.23.1

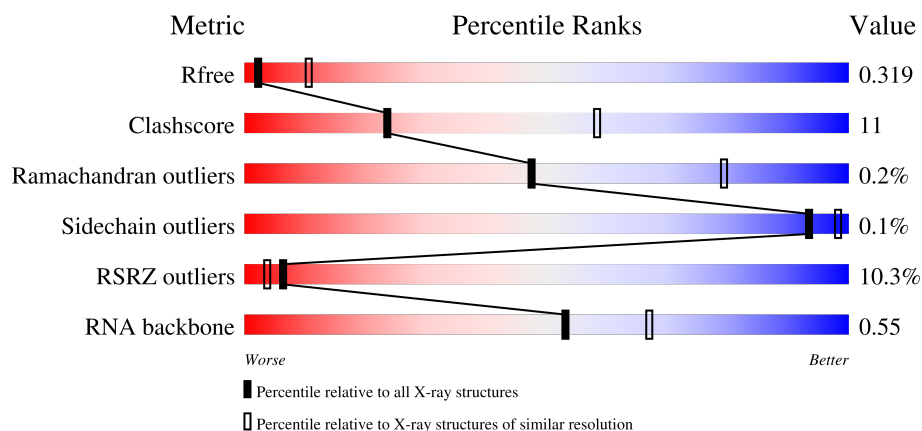
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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.





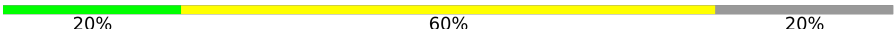
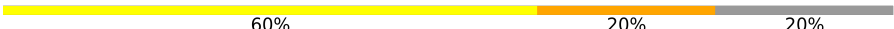
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)
RNA backbone	3102	1010 (3.50-2.90)

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 $\leq 5\%$. 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	428	<div> <div>10%</div> <div>78%</div> <div>21%</div> </div>
1	D	428	<div> <div>12%</div> <div>77%</div> <div>21%</div> </div>
2	B	11	<div> <div>73%</div> <div>27%</div> </div>
2	E	11	<div> <div>64%</div> <div>36%</div> </div>

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Mol	Chain	Length	Quality of chain
3	C	10	
3	F	10	
4	G	5	
4	H	5	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	SO4	A	502	-	-	X	-
6	SO4	D	502	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7991 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 Trt.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	425	Total	C	N	O	S	0	0	0
			3481	2204	670	598	9			
1	D	418	Total	C	N	O	S	0	0	0
			3417	2166	651	591	9			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	421	HIS	-	expression tag	UNP E2GM63
A	422	HIS	-	expression tag	UNP E2GM63
A	423	HIS	-	expression tag	UNP E2GM63
A	424	HIS	-	expression tag	UNP E2GM63
A	425	HIS	-	expression tag	UNP E2GM63
A	426	HIS	-	expression tag	UNP E2GM63
A	427	HIS	-	expression tag	UNP E2GM63
A	428	HIS	-	expression tag	UNP E2GM63
D	421	HIS	-	expression tag	UNP E2GM63
D	422	HIS	-	expression tag	UNP E2GM63
D	423	HIS	-	expression tag	UNP E2GM63
D	424	HIS	-	expression tag	UNP E2GM63
D	425	HIS	-	expression tag	UNP E2GM63
D	426	HIS	-	expression tag	UNP E2GM63
D	427	HIS	-	expression tag	UNP E2GM63
D	428	HIS	-	expression tag	UNP E2GM63

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	11	Total	C	N	O	P	0	0	0
			218	105	42	61	10			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	11	Total	C	N	O	P	0	0	0
			218	105	42	61	10			

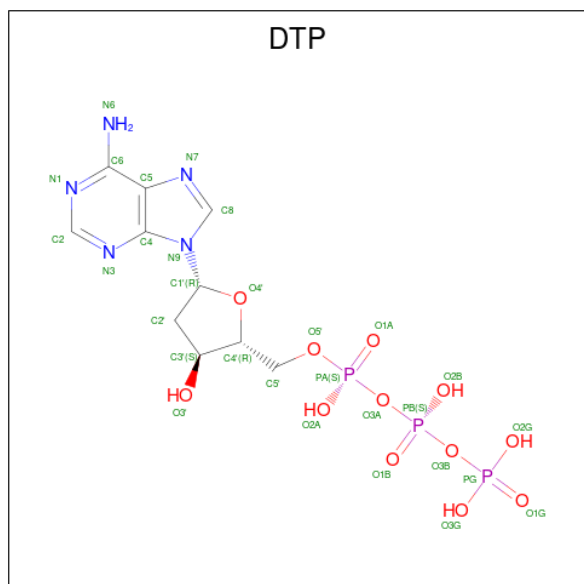
- Molecule 3 is a RNA chain called RNA (5'-R(*UP*UP*GP*CP*CP*UP*GP*GP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	10	Total	C	N	O	P	0	0	0
			211	95	37	70	9			
3	F	10	Total	C	N	O	P	0	0	0
			211	95	37	70	9			

- Molecule 4 is a RNA chain called RNA (5'-R(*U*UP*UP*UP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	4	Total	C	N	O	P	0	0	0
			78	36	11	28	3			
4	H	4	Total	C	N	O	P	0	0	0
			80	37	11	29	3			

- Molecule 5 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula: C₁₀H₁₆N₅O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	D	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		

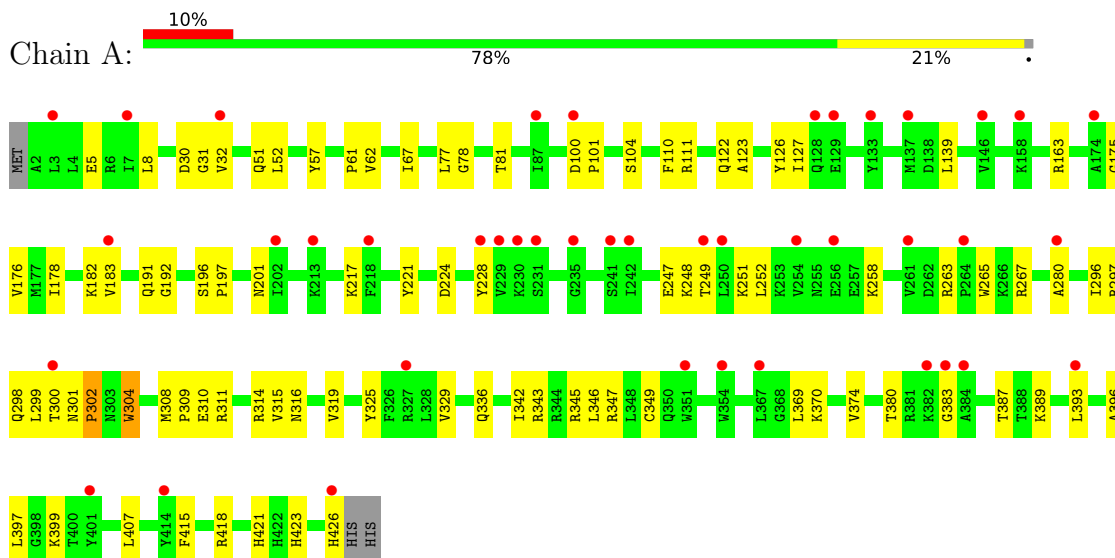
- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Mg	0	0
			1	1		
7	D	1	Total	Mg	0	0
			1	1		

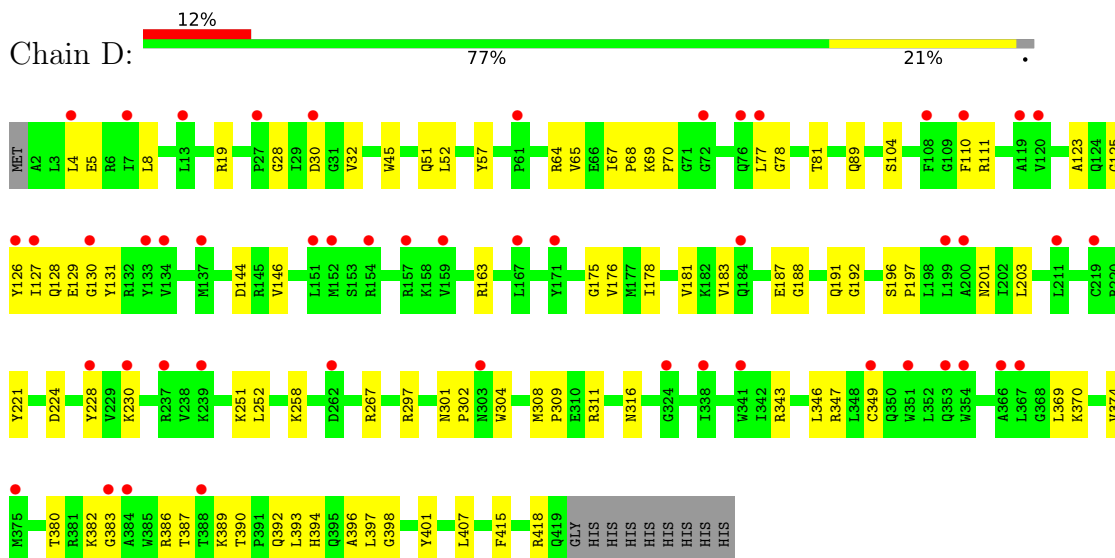
3 Residue-property plots [i](#)

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: Trt

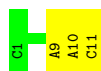


- Molecule 1: Trt

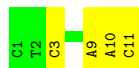


- Molecule 2: DNA (5'-D(*CP*TP*CP*CP*AP*GP*GP*CP*AP*AP*C)-3')

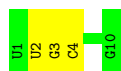




- Molecule 2: DNA (5'-D(*CP*TP*CP*CP*AP*GP*GP*CP*AP*AP*C)-3')



- Molecule 3: RNA (5'-R(*UP*UP*GP*CP*CP*UP*GP*GP*AP*G)-3')



- Molecule 3: RNA (5'-R(*UP*UP*GP*CP*CP*UP*GP*GP*AP*G)-3')



- Molecule 4: RNA (5'-R(*U*UP*UP*UP*G)-3')



- Molecule 4: RNA (5'-R(*U*UP*UP*UP*G)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	179.38Å 107.42Å 71.97Å 90.00° 113.65° 90.00°	Depositor
Resolution (Å)	48.79 – 3.20 48.79 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.79-3.20) 99.7 (48.79-3.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.271 , 0.324 0.270 , 0.319	Depositor DCC
R_{free} test set	2074 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å ²)	91.8	Xtriage
Anisotropy	0.637	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 87.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.460 for -h-2*1,-k,l	Xtriage
Reported twinning fraction	0.500 for H, K, L 0.500 for H+4/2L, -K, -L	Depositor
Outliers	0 of 20705 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7991	wwPDB-VP
Average B, all atoms (Å ²)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: DTP, SO4, 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	0.68	0/3554	0.75	0/4794
1	D	0.67	0/3484	0.74	0/4699
2	B	0.45	0/244	0.69	0/373
2	E	0.38	0/244	0.68	0/373
3	C	0.34	0/235	0.72	0/365
3	F	0.35	0/235	0.70	0/365
4	G	0.72	0/86	0.80	0/132
4	H	0.35	0/88	0.81	0/135
All	All	0.65	0/8170	0.74	0/11236

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	3481	0	3585	91	0
1	D	3417	0	3540	80	0
2	B	218	0	122	3	0
2	E	218	0	122	3	0
3	C	211	0	109	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	211	0	109	3	0
4	G	78	0	39	5	0
4	H	80	0	43	6	0
5	A	30	0	12	3	0
5	D	30	0	12	1	0
6	A	10	0	0	6	0
6	D	5	0	0	2	0
7	A	1	0	0	0	0
7	D	1	0	0	0	0
All	All	7991	0	7693	175	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 11.

All (175) 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:D:127:ILE:HA	1:D:131:TYR:O	1.47	1.09
1:A:126:TYR:CE1	1:A:217:LYS:HB3	1.93	1.04
1:D:175:GLY:HA2	1:D:183:VAL:O	1.61	1.00
1:D:369:LEU:HD13	1:D:396:ALA:HB2	1.44	0.97
1:A:316:ASN:HD21	1:A:407:LEU:HA	1.37	0.89
1:D:175:GLY:CA	1:D:183:VAL:O	2.24	0.86
1:A:61:PRO:HB3	1:A:175:GLY:O	1.78	0.84
1:A:61:PRO:CB	1:A:175:GLY:O	2.25	0.84
1:A:311:ARG:O	1:A:315:VAL:HG23	1.79	0.82
1:A:30:ASP:CG	1:A:32:VAL:HG12	2.00	0.82
1:A:316:ASN:OD1	1:A:407:LEU:HD12	1.82	0.79
1:D:347:ARG:HD3	1:D:393:LEU:HB3	1.64	0.78
1:A:298:GLN:N	1:A:298:GLN:OE1	2.19	0.76
1:A:301:ASN:OD1	1:A:304:TRP:N	2.20	0.75
6:A:502:SO4:O2	1:D:178:ILE:HD13	1.86	0.74
1:D:64:ARG:HG2	1:D:176:VAL:HG21	1.71	0.73
3:F:1:U:C6	4:H:5:G:H2'	2.24	0.73
1:A:336:GLN:HE22	1:D:65:VAL:HA	1.55	0.72
1:A:139:LEU:HD23	1:A:252:LEU:HD23	1.71	0.70
6:A:502:SO4:O2	1:D:178:ILE:CD1	2.41	0.69
1:A:192:GLY:HA2	4:G:5:G:H1'	1.76	0.68
1:D:129:GLU:O	1:D:129:GLU:HG3	1.94	0.68
1:D:192:GLY:HA2	4:H:5:G:H1'	1.75	0.68
1:D:369:LEU:CD1	1:D:396:ALA:HB2	2.23	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:343:ARG:NE	6:D:502:SO4:O1	2.22	0.67
1:A:67:ILE:HD13	1:A:77:LEU:HD11	1.78	0.66
1:D:8:LEU:HD21	1:D:52:LEU:HD11	1.78	0.66
1:A:51:GLN:HE21	1:A:57:TYR:HD1	1.44	0.66
1:A:192:GLY:HA2	4:G:5:G:C1'	2.27	0.64
1:A:247:GLU:O	1:A:251:LYS:HA	1.96	0.64
1:A:8:LEU:HD21	1:A:52:LEU:HD11	1.76	0.64
1:A:399:LYS:N	6:A:502:SO4:O1	2.30	0.64
1:D:67:ILE:HD13	1:D:77:LEU:HD11	1.79	0.63
1:D:176:VAL:O	1:D:183:VAL:N	2.32	0.63
1:D:52:LEU:HB3	1:D:57:TYR:CB	2.29	0.63
1:D:369:LEU:HD13	1:D:396:ALA:CB	2.24	0.63
1:A:380:THR:HG21	1:A:387:THR:HG22	1.81	0.62
1:A:389:LYS:O	1:D:181:VAL:HG21	2.00	0.61
5:D:501:DTP:H8	2:E:11:DC:H2'	1.81	0.61
1:A:421:HIS:NE2	6:A:504:SO4:O1	2.34	0.60
1:A:52:LEU:HB3	1:A:57:TYR:CB	2.31	0.60
1:D:382:LYS:HE3	1:D:386:ARG:HG2	1.84	0.60
1:D:51:GLN:HE21	1:D:57:TYR:HD1	1.48	0.59
1:A:126:TYR:HE1	1:A:217:LYS:HB3	1.61	0.59
1:A:126:TYR:CD1	1:A:217:LYS:HB3	2.38	0.58
1:A:110:PHE:HB2	1:A:201:ASN:HD21	1.68	0.58
1:D:144:ASP:O	1:D:187:GLU:HG3	2.04	0.57
1:A:347:ARG:NH1	6:A:502:SO4:O4	2.38	0.56
1:A:62:VAL:CG2	1:A:176:VAL:HG12	2.36	0.56
1:D:301:ASN:OD1	1:D:304:TRP:N	2.37	0.56
2:E:9:DA:H2'	2:E:10:DA:C8	2.40	0.56
2:B:9:DA:H2'	2:B:10:DA:C8	2.41	0.56
1:A:380:THR:HG21	1:A:387:THR:CG2	2.36	0.56
1:A:393:LEU:O	1:A:397:LEU:O	2.23	0.56
1:D:110:PHE:HB2	1:D:201:ASN:HD21	1.71	0.55
1:A:329:VAL:O	1:A:418:ARG:NH2	2.39	0.55
1:A:178:ILE:HD13	1:A:183:VAL:HG21	1.89	0.55
1:A:300:THR:HG21	1:A:345:ARG:HG3	1.87	0.55
1:D:415:PHE:O	1:D:418:ARG:HB3	2.07	0.55
1:A:30:ASP:OD1	1:A:31:GLY:N	2.40	0.54
1:A:296:ILE:HD13	1:A:299:LEU:HD12	1.89	0.54
1:D:392:GLN:O	1:D:396:ALA:CB	2.56	0.54
1:D:389:LYS:HA	1:D:394:HIS:NE2	2.23	0.53
1:A:336:GLN:HE22	1:D:65:VAL:CA	2.21	0.53
1:A:30:ASP:OD2	1:A:32:VAL:HG12	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:PRO:CA	1:A:175:GLY:O	2.57	0.52
5:A:501:DTP:C8	2:B:11:DC:H2'	2.39	0.52
1:D:380:THR:HG21	1:D:387:THR:HG22	1.91	0.51
1:D:380:THR:HG21	1:D:387:THR:CG2	2.40	0.51
2:E:3:DC:O2	3:F:8:G:N2	2.34	0.51
1:A:62:VAL:HG23	1:A:176:VAL:HG12	1.91	0.51
1:D:369:LEU:HD23	1:D:374:VAL:HG23	1.92	0.51
5:A:501:DTP:H8	2:B:11:DC:H2'	1.93	0.51
4:H:4:U:C2	4:H:5:G:C8	2.98	0.51
1:A:123:ALA:HB1	1:A:228:TYR:OH	2.10	0.51
1:A:221:TYR:O	1:A:224:ASP:O	2.29	0.50
4:G:4:U:C2	4:G:5:G:C8	2.99	0.50
1:A:258:LYS:NZ	5:A:501:DTP:O3G	2.45	0.50
1:A:67:ILE:CD1	1:A:77:LEU:HD11	2.42	0.50
1:D:196:SER:N	1:D:197:PRO:HD2	2.27	0.50
1:D:398:GLY:O	1:D:401:TYR:N	2.44	0.49
1:A:196:SER:N	1:A:197:PRO:HD2	2.27	0.49
1:D:347:ARG:NH2	6:D:502:SO4:O3	2.45	0.49
1:A:325:TYR:O	1:A:325:TYR:CG	2.66	0.49
1:D:369:LEU:HD23	1:D:374:VAL:CG2	2.42	0.49
1:A:383:GLY:O	1:A:387:THR:HG23	2.12	0.49
1:A:300:THR:HG21	1:A:345:ARG:CG	2.43	0.48
1:D:123:ALA:HB1	1:D:228:TYR:OH	2.12	0.48
1:D:370:LYS:O	1:D:374:VAL:HG23	2.13	0.48
1:A:299:LEU:HD13	1:A:315:VAL:HA	1.95	0.48
1:A:369:LEU:HD23	1:A:374:VAL:HG23	1.94	0.48
1:A:370:LYS:O	1:A:374:VAL:HG23	2.13	0.48
1:D:192:GLY:HA2	4:H:5:G:C1'	2.43	0.48
1:D:67:ILE:CD1	1:D:77:LEU:HD11	2.43	0.48
1:A:192:GLY:O	4:G:5:G:C4'	2.62	0.48
1:A:302:PRO:HD2	1:A:304:TRP:HB2	1.96	0.48
1:A:263:ARG:HD3	1:A:265:TRP:CH2	2.49	0.47
1:D:146:VAL:HB	1:D:188:GLY:HA2	1.95	0.47
3:C:3:G:H2'	3:C:4:C:O4'	2.14	0.47
1:A:315:VAL:O	1:A:319:VAL:HG23	2.14	0.47
1:D:203:LEU:HD21	1:D:252:LEU:HD11	1.96	0.47
1:D:69:LYS:HB2	1:D:70:PRO:CD	2.45	0.47
1:D:221:TYR:O	1:D:224:ASP:O	2.33	0.47
1:A:346:LEU:O	1:A:349:CYS:SG	2.73	0.46
1:A:369:LEU:HD23	1:A:374:VAL:CG2	2.46	0.46
1:D:130:GLY:O	1:D:230:LYS:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:52:LEU:HB3	1:D:57:TYR:HB3	1.98	0.46
1:A:296:ILE:HG21	1:A:342:ILE:HG12	1.96	0.46
1:D:383:GLY:O	1:D:387:THR:HG23	2.15	0.46
1:A:299:LEU:HB3	1:A:315:VAL:HG22	1.98	0.46
1:A:308:MET:HB3	1:A:309:PRO:HD3	1.97	0.46
1:D:30:ASP:HB2	1:D:32:VAL:HG12	1.98	0.46
1:D:127:ILE:CA	1:D:131:TYR:O	2.39	0.46
1:D:316:ASN:HD21	1:D:407:LEU:HA	1.81	0.46
1:A:389:LYS:O	1:D:181:VAL:HG11	2.16	0.46
1:D:308:MET:HB3	1:D:309:PRO:HD3	1.99	0.46
1:D:67:ILE:HG22	4:H:3:U:C4	2.51	0.45
1:D:392:GLN:O	1:D:396:ALA:HB2	2.17	0.45
1:A:316:ASN:ND2	1:A:407:LEU:HA	2.18	0.45
1:D:347:ARG:HD3	1:D:393:LEU:HD23	1.98	0.45
1:A:310:GLU:OE2	1:A:314:ARG:NE	2.50	0.45
1:A:30:ASP:OD2	1:A:81:THR:HG23	2.17	0.45
1:D:386:ARG:HD2	1:D:389:LYS:HE2	1.99	0.45
1:A:343:ARG:NH2	6:A:502:SO4:O3	2.46	0.44
4:H:2:U:H4'	4:H:3:U:OP2	2.17	0.44
1:A:30:ASP:OD1	1:A:32:VAL:HG12	2.18	0.44
1:A:297:ARG:O	1:A:300:THR:OG1	2.33	0.44
1:D:346:LEU:O	1:D:349:CYS:SG	2.74	0.44
1:D:397:LEU:HD12	1:D:397:LEU:N	2.32	0.44
1:A:127:ILE:CD1	1:A:280:ALA:HB3	2.48	0.44
1:A:176:VAL:O	1:A:182:LYS:HA	2.17	0.44
1:A:139:LEU:HD23	1:A:252:LEU:CD2	2.45	0.44
1:A:5:GLU:OE1	1:A:163:ARG:NH2	2.51	0.44
1:A:78:GLY:O	1:A:191:GLN:O	2.35	0.43
1:D:52:LEU:HB3	1:D:57:TYR:CG	2.53	0.43
1:A:176:VAL:HG23	1:A:178:ILE:CD1	2.48	0.43
1:D:69:LYS:HB2	1:D:70:PRO:HD2	2.00	0.43
1:D:104:SER:O	1:D:111:ARG:NH1	2.52	0.43
1:D:5:GLU:OE1	1:D:163:ARG:NH2	2.51	0.43
1:A:296:ILE:O	1:A:300:THR:HG23	2.18	0.43
1:A:389:LYS:O	1:D:181:VAL:CG2	2.66	0.43
1:A:415:PHE:CZ	1:D:68:PRO:HD3	2.54	0.42
1:D:301:ASN:HB2	1:D:311:ARG:NH2	2.34	0.42
1:A:248:LYS:HG3	1:A:249:THR:N	2.35	0.42
1:D:390:THR:O	1:D:394:HIS:CD2	2.73	0.42
1:A:415:PHE:CG	1:D:68:PRO:HB3	2.55	0.42
1:A:52:LEU:C	1:A:52:LEU:HD12	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:LYS:CG	1:A:249:THR:N	2.83	0.42
1:D:51:GLN:HG3	1:D:57:TYR:HB2	2.01	0.42
1:A:258:LYS:O	1:A:267:ARG:NH2	2.53	0.42
1:A:301:ASN:HB3	1:A:349:CYS:CB	2.50	0.41
1:A:52:LEU:HB3	1:A:57:TYR:CG	2.54	0.41
1:A:104:SER:O	1:A:111:ARG:NH1	2.52	0.41
1:A:316:ASN:OD1	1:A:407:LEU:CD1	2.63	0.41
1:A:122:GLN:HG2	1:A:126:TYR:CE2	2.56	0.41
1:D:45:TRP:CE3	1:D:45:TRP:HA	2.55	0.41
1:A:175:GLY:HA3	1:A:182:LYS:HG2	2.02	0.41
1:A:426:HIS:HB3	1:D:297:ARG:HB3	2.01	0.41
1:D:176:VAL:CG1	1:D:183:VAL:HB	2.51	0.41
1:D:258:LYS:O	1:D:267:ARG:NH2	2.52	0.41
1:A:100:ASP:N	1:A:101:PRO:CD	2.84	0.41
1:A:369:LEU:HD13	1:A:396:ALA:HB2	2.02	0.41
1:D:19:ARG:HG2	1:D:89:GLN:NE2	2.35	0.41
1:A:192:GLY:O	4:G:5:G:H4'	2.21	0.41
1:A:423:HIS:O	1:D:297:ARG:NH1	2.53	0.41
1:D:78:GLY:O	1:D:191:GLN:O	2.38	0.41
1:D:389:LYS:HA	1:D:394:HIS:CE1	2.56	0.41
1:D:28:GLY:HA3	1:D:81:THR:HA	2.01	0.41
3:C:2:U:C2	3:C:3:G:C8	3.09	0.41
1:D:4:LEU:HD22	1:D:163:ARG:HB3	2.03	0.40
3:F:3:G:H2'	3:F:4:C:O4'	2.21	0.40
1:D:125:GLY:O	1:D:128:GLN:HG2	2.21	0.40
1:D:251:LYS:CG	1:D:251:LYS:O	2.70	0.40
1:A:62:VAL:HG22	1:A:176:VAL:HG12	2.02	0.40
1:D:126:TYR:O	1:D:131:TYR:HB2	2.22	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	423/428 (99%)	417 (99%)	5 (1%)	1 (0%)	47	79
1	D	416/428 (97%)	410 (99%)	5 (1%)	1 (0%)	47	79
All	All	839/856 (98%)	827 (99%)	10 (1%)	2 (0%)	47	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	302	PRO
1	D	302	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	368/371 (99%)	367 (100%)	1 (0%)	92	96
1	D	362/371 (98%)	362 (100%)	0	100	100
All	All	730/742 (98%)	729 (100%)	1 (0%)	93	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	304	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	24	GLN
1	A	93	GLN
1	A	201	ASN
1	A	353	GLN
1	D	12	ASN
1	D	89	GLN
1	D	93	GLN

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Mol	Chain	Res	Type
1	D	201	ASN
1	D	353	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	C	9/10 (90%)	0	0
3	F	9/10 (90%)	1 (11%)	0
4	G	3/5 (60%)	0	1 (33%)
4	H	3/5 (60%)	1 (33%)	0
All	All	24/30 (80%)	2 (8%)	1 (4%)

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	F	7	G
4	H	3	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	G	2	U

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 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	$\# Z > 2$
5	DTP	A	501	7	26,32,32	0.70	0	30,50,50	0.90	1 (3%)
6	SO4	A	502	-	4,4,4	0.44	0	6,6,6	0.14	0
5	DTP	D	501	7	26,32,32	0.68	0	30,50,50	0.81	1 (3%)
6	SO4	D	502	-	4,4,4	0.41	0	6,6,6	0.11	0
6	SO4	A	504	-	4,4,4	0.37	0	6,6,6	0.07	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
5	DTP	A	501	7	-	1/18/34/34	0/3/3/3
5	DTP	D	501	7	-	2/18/34/34	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	501	DTP	C5-C6-N6	2.17	123.65	120.35
5	A	501	DTP	PB-O3B-PG	-2.03	125.86	132.83

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	DTP	PB-O3B-PG-O3G
5	D	501	DTP	PB-O3A-PA-O2A
5	D	501	DTP	PB-O3A-PA-O1A

There are no ring outliers.

5 monomers are involved in 12 short contacts:

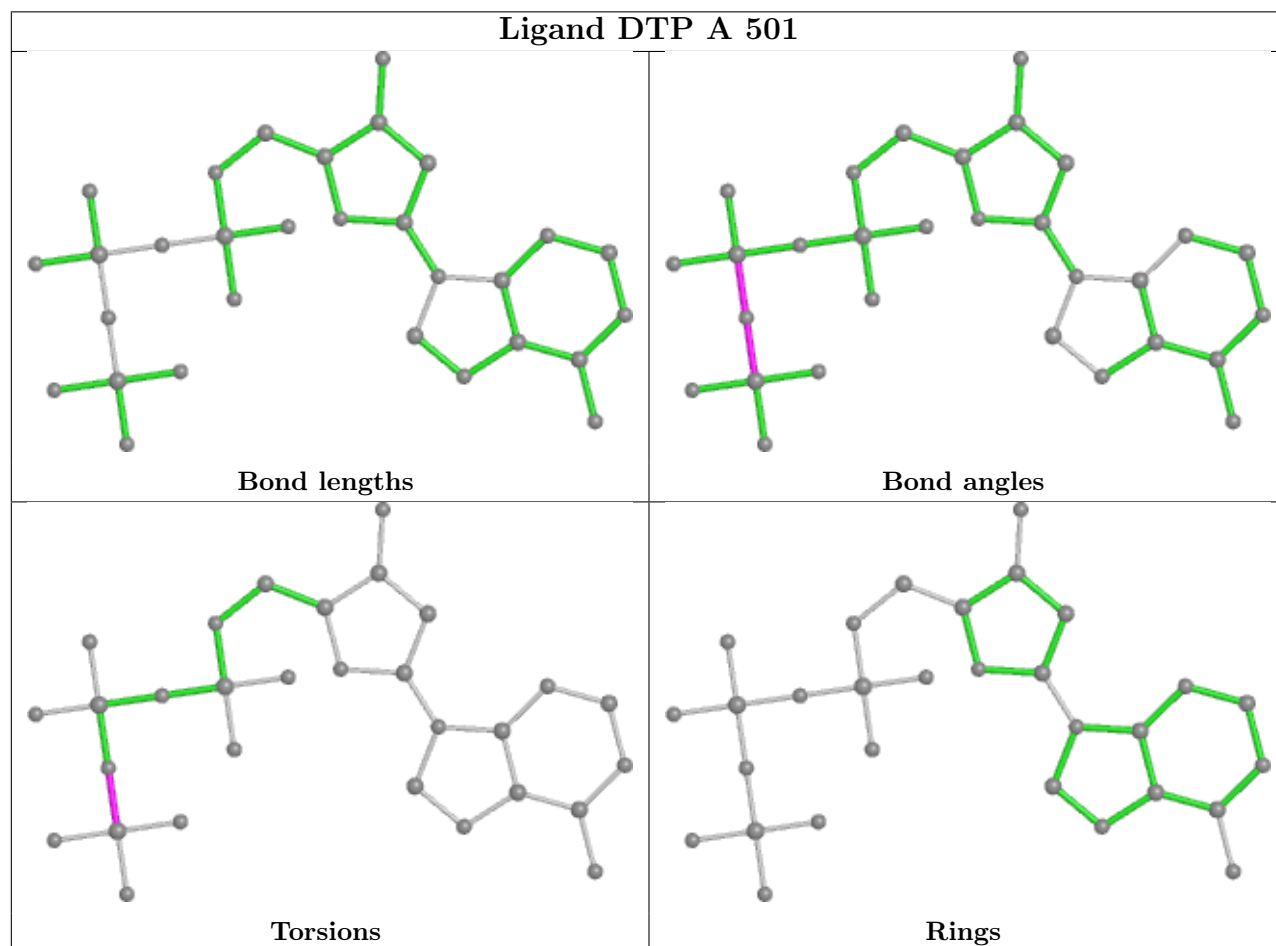
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	DTP	3	0
6	A	502	SO4	5	0

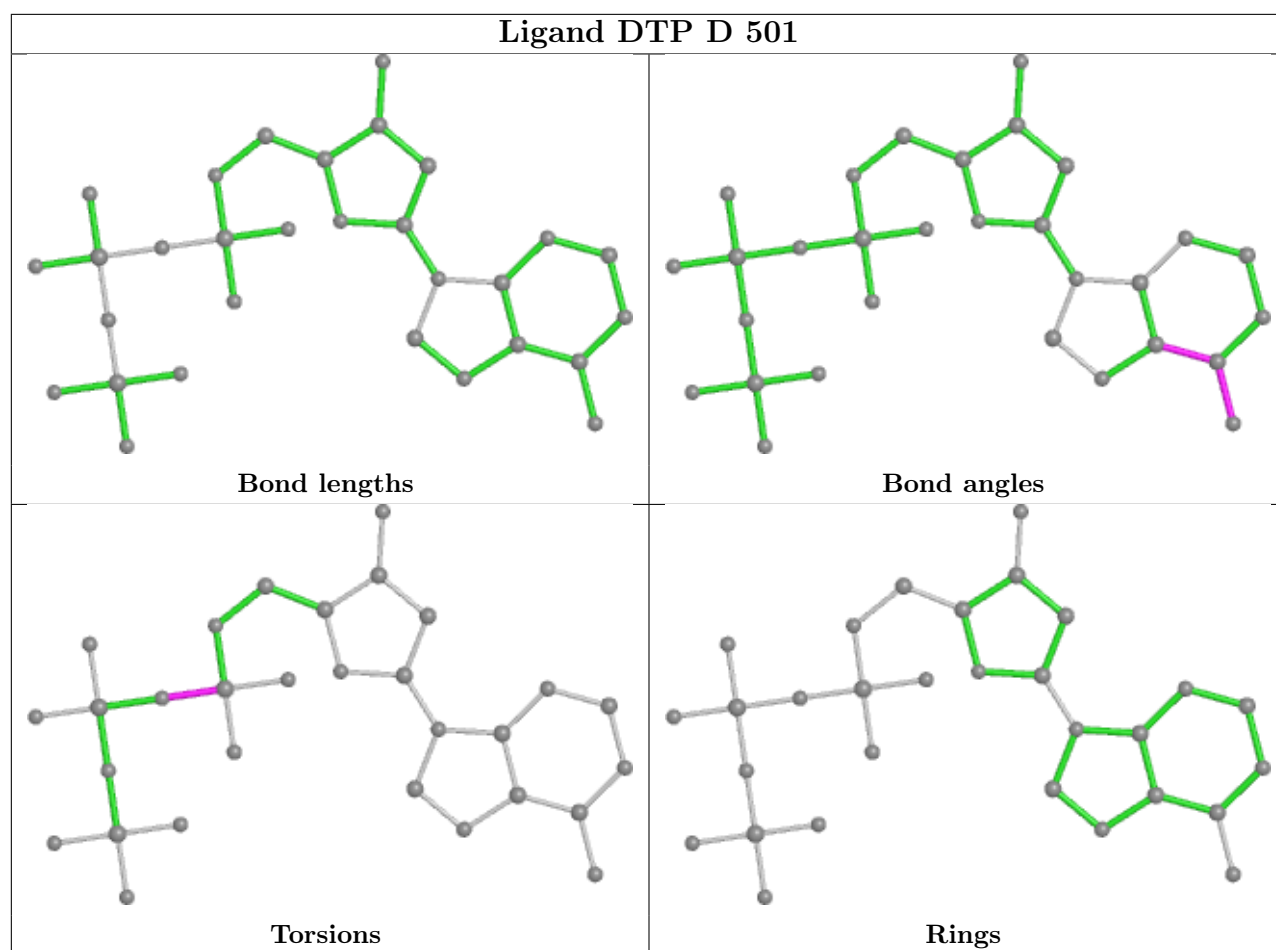
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	501	DTP	1	0
6	D	502	SO4	2	0
6	A	504	SO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	425/428 (99%)	0.70	42 (9%) 7 4	62, 116, 160, 228	0
1	D	418/428 (97%)	0.83	50 (11%) 4 2	64, 127, 174, 206	0
2	B	11/11 (100%)	-0.12	0 100 100	94, 106, 161, 170	0
2	E	11/11 (100%)	-0.13	0 100 100	109, 128, 170, 174	0
3	C	10/10 (100%)	-0.19	0 100 100	65, 111, 164, 189	0
3	F	10/10 (100%)	-0.23	0 100 100	94, 128, 139, 140	0
4	G	4/5 (80%)	0.38	0 100 100	54, 75, 76, 76	0
4	H	4/5 (80%)	0.56	0 100 100	94, 106, 115, 140	0
All	All	893/908 (98%)	0.72	92 (10%) 6 4	54, 122, 168, 228	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	384	ALA	10.5
1	D	262	ASP	5.6
1	D	199	LEU	5.1
1	D	354	TRP	5.0
1	D	126	TYR	4.9
1	A	213	LYS	4.3
1	A	230	LYS	4.1
1	A	228	TYR	4.0
1	A	218	PHE	3.9
1	D	7	ILE	3.8
1	D	303	ASN	3.7
1	D	366	ALA	3.6
1	D	239	LYS	3.6
1	D	119	ALA	3.6
1	A	133	TYR	3.4
1	D	133	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	134	VAL	3.4
1	A	242	ILE	3.4
1	D	76	GLN	3.4
1	D	388	THR	3.4
1	A	354	TRP	3.1
1	D	324	GLY	3.1
1	A	426	HIS	3.0
1	A	146	VAL	3.0
1	D	383	GLY	3.0
1	A	202	ILE	3.0
1	A	229	VAL	2.9
1	D	151	LEU	2.9
1	D	211	LEU	2.9
1	A	261	VAL	2.8
1	A	100	ASP	2.8
1	D	30	ASP	2.8
1	A	128	GLN	2.7
1	A	327	ARG	2.7
1	A	414	TYR	2.7
1	D	61	PRO	2.7
1	D	237	ARG	2.6
1	A	280	ALA	2.6
1	D	77	LEU	2.6
1	D	157	ARG	2.6
1	A	158	LYS	2.6
1	D	167	LEU	2.6
1	D	200	ALA	2.5
1	A	249	THR	2.5
1	D	375	MET	2.5
1	D	130	GLY	2.5
1	A	3	LEU	2.5
1	A	7	ILE	2.5
1	D	171	TYR	2.5
1	D	72	GLY	2.5
1	A	183	VAL	2.5
1	D	341	TRP	2.4
1	A	137	MET	2.4
1	D	367	LEU	2.4
1	A	351	TRP	2.4
1	A	401	TYR	2.4
1	D	184	GLN	2.4
1	D	230	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	241	SER	2.4
1	A	384	ALA	2.4
1	A	264	PRO	2.3
1	D	351	TRP	2.3
1	D	228	TYR	2.3
1	A	383	GLY	2.3
1	D	154	ARG	2.3
1	A	393	LEU	2.3
1	D	13	LEU	2.3
1	A	256	GLU	2.3
1	A	174	ALA	2.3
1	A	129	GLU	2.2
1	D	110	PHE	2.2
1	A	250	LEU	2.2
1	A	231	SER	2.2
1	A	367	LEU	2.2
1	D	4	LEU	2.2
1	D	108	PHE	2.2
1	D	353	GLN	2.2
1	D	127	ILE	2.2
1	D	152	MET	2.2
1	D	349	CYS	2.2
1	A	32	VAL	2.1
1	D	338	ILE	2.1
1	D	219	CYS	2.1
1	A	382	LYS	2.1
1	D	137	MET	2.1
1	D	159	VAL	2.1
1	A	300	THR	2.1
1	A	87	ILE	2.1
1	D	120	VAL	2.0
1	A	235	GLY	2.0
1	A	254	VAL	2.0
1	D	27	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

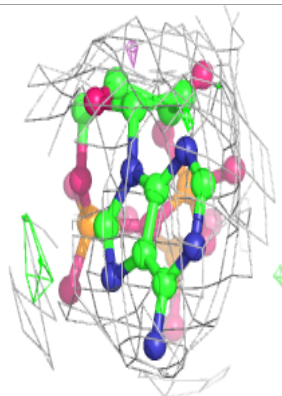
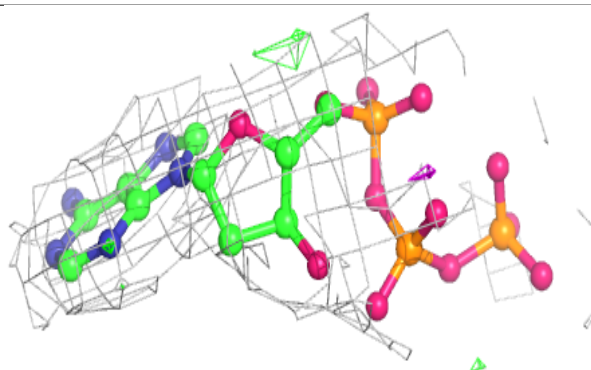
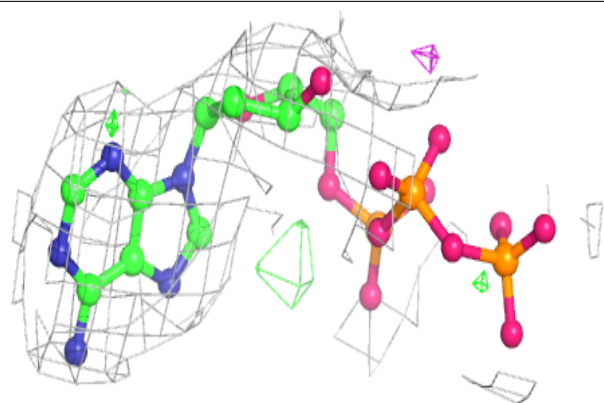
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	SO4	A	502	5/5	0.60	0.21	194,196,202,204	0
6	SO4	D	502	5/5	0.63	0.17	158,161,164,167	0
5	DTP	A	501	30/30	0.90	0.19	74,102,125,132	0
7	MG	D	503	1/1	0.92	0.14	131,131,131,131	0
5	DTP	D	501	30/30	0.93	0.24	109,122,128,131	0
7	MG	A	503	1/1	0.95	0.14	139,139,139,139	0
6	SO4	A	504	5/5	0.95	0.10	125,125,134,139	0

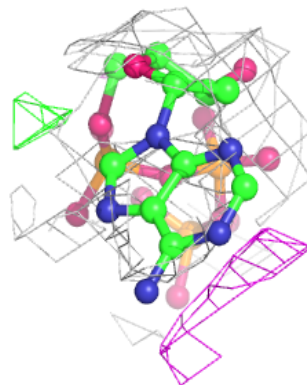
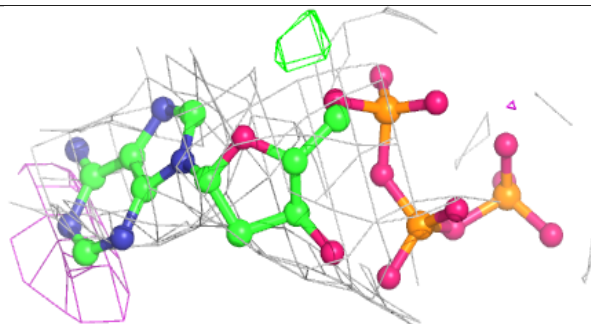
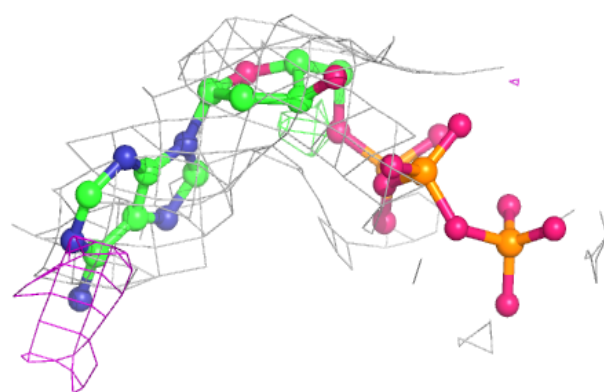
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DTP A 501:

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

**Electron density around DTP D 501:**

$2mF_o-DF_c$ (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.