



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 02:11 am BST

PDB ID : 3AUO
Title : DNA polymerase X from *Thermus thermophilus* HB8 ternary complex with 1-nt gapped DNA and ddGTP
Authors : Nakane, S.; Nakagawa, N.; Masui, R.; Kuramitsu, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2011-02-11
Resolution : 2.70 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 : 2.11
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) : 2.11

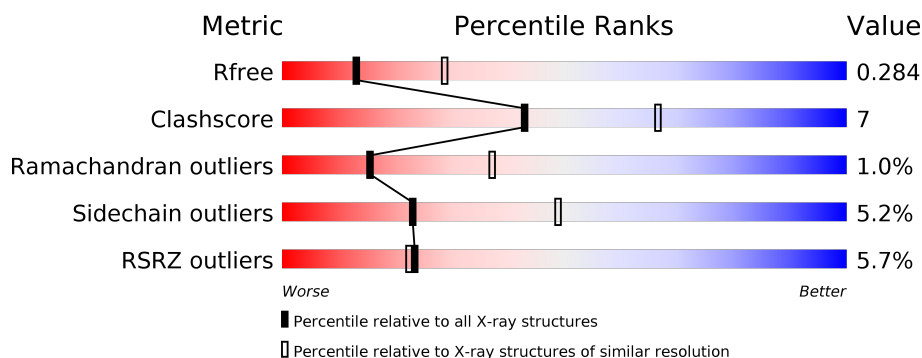
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 on 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	575	<div> <div>6%</div> <div>81%</div> <div>17%</div> <div>..</div> </div>
1	B	575	<div> <div>4%</div> <div>85%</div> <div>14%</div> <div>..</div> </div>
2	D	29	<div> <div>21%</div> <div>59%</div> <div>24%</div> <div>17%</div> </div>
2	E	29	<div> <div>10%</div> <div>66%</div> <div>21%</div> <div>14%</div> </div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 10378 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.

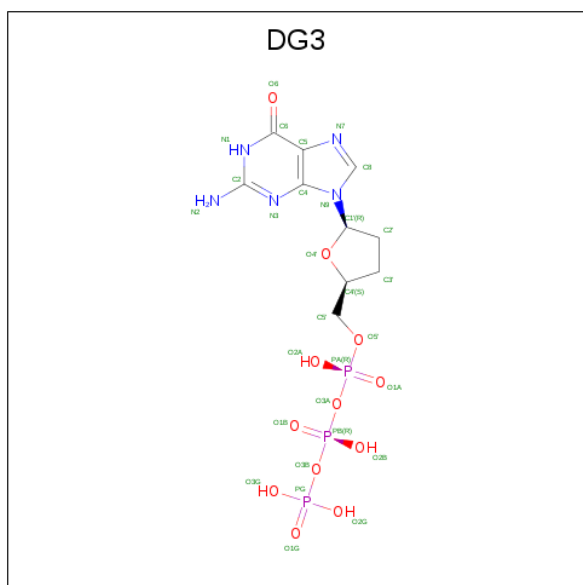
- Molecule 1 is a protein called DNA polymerase beta family (X family).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	572	Total	C	N	O	S	0	0	0
			4500	2852	808	830	10			
1	B	572	Total	C	N	O	S	0	0	0
			4500	2852	808	830	10			

- Molecule 2 is a DNA chain called 1-nt gapped DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	29	Total	C	N	O	P	0	0	0
			589	281	97	182	29			
2	E	29	Total	C	N	O	P	0	0	0
			589	281	97	182	29			

- Molecule 3 is 2'-3'-DIDEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DG3) (formula: $C_{10}H_{16}N_5O_{12}P_3$).



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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Zn	0	0
			1	1		
5	A	1	Total	Zn	0	0
			1	1		

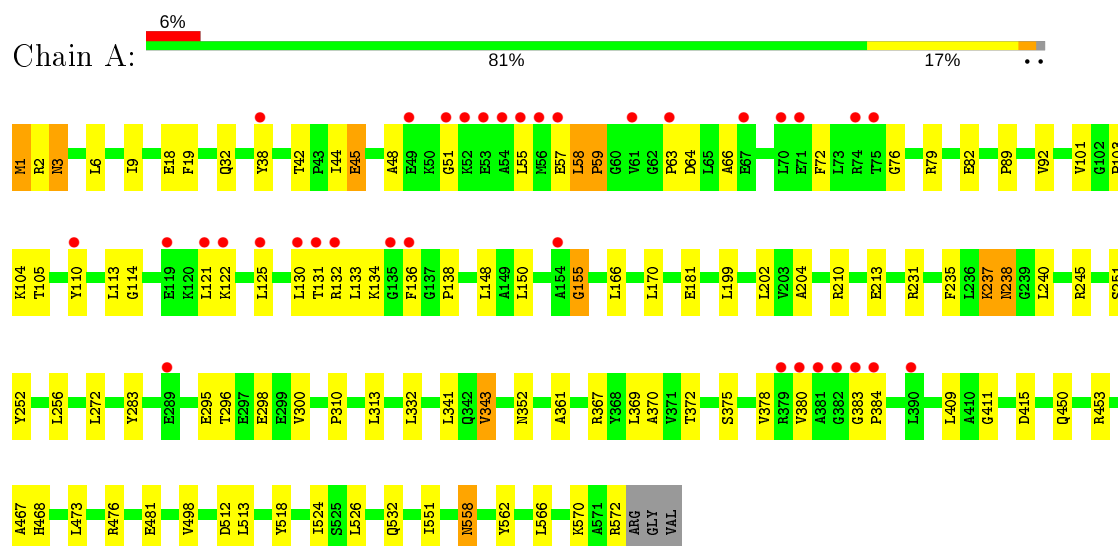
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	53	Total	O	0	0
			53	53		
6	B	70	Total	O	0	0
			70	70		
6	D	7	Total	O	0	0
			7	7		
6	E	4	Total	O	0	0
			4	4		

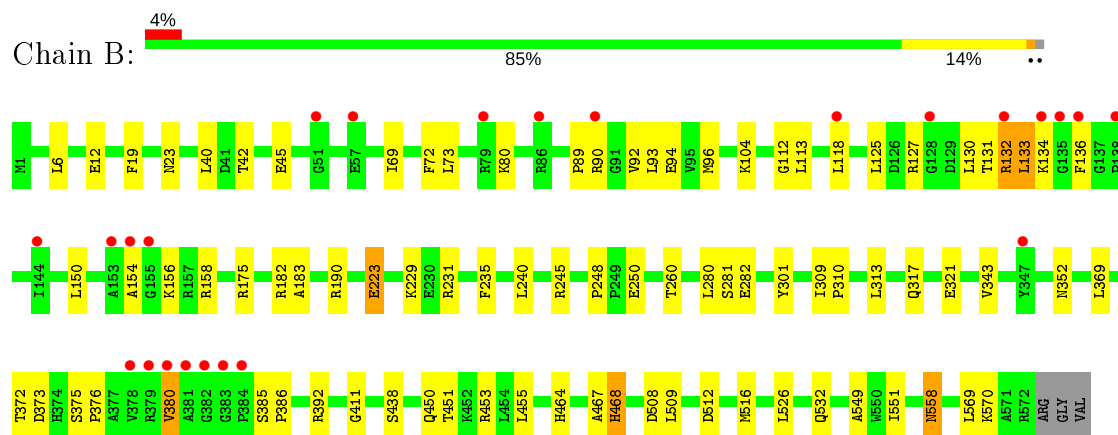
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

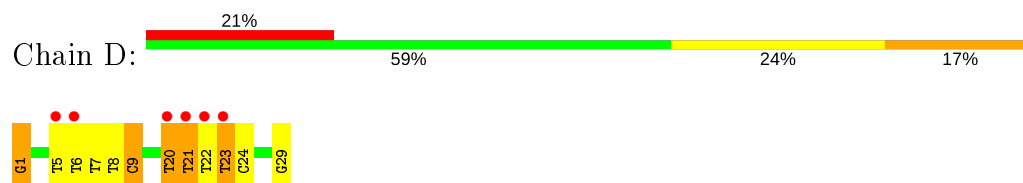
- Molecule 1: DNA polymerase beta family (X family)



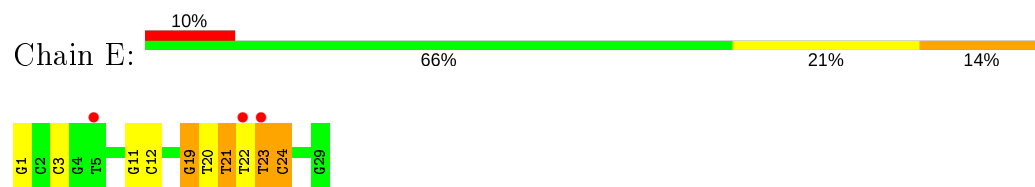
- Molecule 1: DNA polymerase beta family (X family)



- Molecule 2: 1-nt gapped DNA



- Molecule 2: 1-nt gapped DNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	95.44Å 96.94Å 143.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 39.11 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.00-2.70) 98.8 (39.11-2.69)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.42 (at 2.69Å)	Xtriage
Refinement program	REFMAC refmac _5.5.0110	Depositor
R, R_{free}	0.241 , 0.293 0.237 , 0.284	Depositor DCC
R_{free} test set	1874 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	37.4	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10378	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.88 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7059e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DG3, ZN, DDG, 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	0.33	0/4589	0.54	0/6205
1	B	0.33	0/4589	0.53	0/6205
2	D	0.86	1/632 (0.2%)	1.63	14/971 (1.4%)
2	E	0.81	1/632 (0.2%)	1.59	15/971 (1.5%)
All	All	0.42	2/10442 (0.0%)	0.77	29/14352 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	DG	OP3-P	-10.71	1.48	1.61
2	E	1	DG	OP3-P	-10.16	1.49	1.61

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	21	DT	O4'-C4'-C3'	-10.70	99.58	106.00
2	E	11	DG	O3'-P-O5'	-9.64	85.69	104.00
2	D	23	DT	O4'-C1'-N1	9.57	114.70	108.00
2	D	7	DT	O4'-C4'-C3'	-9.54	100.28	106.00
2	E	11	DG	OP1-P-O3'	-8.86	85.71	105.20
2	D	9	DC	O4'-C4'-C3'	-8.36	100.98	106.00
2	E	3	DC	P-O3'-C3'	8.25	129.60	119.70
2	D	23	DT	P-O3'-C3'	8.02	129.33	119.70
2	D	5	DT	P-O3'-C3'	7.73	128.98	119.70
2	E	11	DG	OP2-P-O3'	-7.63	88.42	105.20
2	D	21	DT	O4'-C1'-N1	7.52	113.26	108.00
2	E	23	DT	O4'-C1'-N1	7.19	113.04	108.00
2	E	24	DC	C1'-O4'-C4'	-7.13	102.97	110.10
2	D	23	DT	O4'-C1'-C2'	-6.79	100.47	105.90
2	E	23	DT	P-O3'-C3'	6.71	127.75	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	21	DT	C4'-C3'-C2'	-6.50	97.25	103.10
2	E	22	DT	O4'-C1'-N1	6.49	112.55	108.00
2	D	9	DC	O4'-C1'-N1	-6.41	103.52	108.00
2	D	22	DT	O4'-C4'-C3'	-6.34	101.97	104.50
2	D	20	DT	P-O3'-C3'	6.17	127.11	119.70
2	E	19	DG	P-O3'-C3'	5.95	126.84	119.70
2	E	21	DT	C4'-C3'-C2'	-5.93	97.76	103.10
2	E	11	DG	P-O3'-C3'	5.80	126.66	119.70
2	E	21	DT	O4'-C4'-C3'	-5.69	102.22	104.50
2	E	21	DT	N3-C2-O2	-5.54	118.97	122.30
2	D	22	DT	P-O3'-C3'	5.49	126.29	119.70
2	D	6	DT	O4'-C1'-N1	5.45	111.81	108.00
2	E	22	DT	P-O3'-C3'	5.18	125.91	119.70
2	E	12	DC	OP1-P-OP2	5.10	127.25	119.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	4500	0	4566	58	0
1	B	4500	0	4566	64	0
2	D	589	0	330	6	0
2	E	589	0	330	9	0
3	A	30	0	12	1	0
3	B	30	0	12	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	53	0	0	2	0
6	B	70	0	0	1	0
6	D	7	0	0	0	0
6	E	4	0	0	0	0
All	All	10378	0	9816	136	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 7.

All (136) 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:125:LEU:HD11	1:A:130:LEU:HD12	1.44	0.98
1:B:549:ALA:HB3	1:B:551:ILE:HD13	1.56	0.87
1:B:549:ALA:HB3	1:B:551:ILE:CD1	2.07	0.85
1:B:343:VAL:HG21	1:B:369:LEU:HD21	1.62	0.82
1:A:58:LEU:HB3	1:A:59:PRO:HD3	1.61	0.80
1:B:133:LEU:HD13	1:B:136:PHE:HB3	1.64	0.78
1:A:125:LEU:CD1	1:A:130:LEU:HD12	2.15	0.76
1:B:130:LEU:C	1:B:133:LEU:HD11	2.06	0.74
1:B:133:LEU:HD12	1:B:133:LEU:N	2.02	0.74
1:A:343:VAL:HG21	1:A:369:LEU:HD21	1.70	0.72
2:E:23:DT:H3'	2:E:24:DC:C5'	2.20	0.72
1:B:343:VAL:CG2	1:B:369:LEU:HD21	2.20	0.71
1:B:549:ALA:CB	1:B:551:ILE:CD1	2.70	0.69
1:A:1:MET:N	1:A:481:GLU:OE2	2.29	0.65
1:B:154:ALA:HB1	6:B:637:HOH:O	1.96	0.65
1:B:94:GLU:HG3	1:B:118:LEU:HD12	1.78	0.64
1:B:92:VAL:HG22	1:B:96:MET:CE	2.27	0.64
1:A:42:THR:HG22	1:A:513:LEU:HD23	1.79	0.63
1:B:92:VAL:HG22	1:B:96:MET:HE2	1.79	0.63
1:B:132:ARG:C	1:B:133:LEU:HD12	2.19	0.63
1:A:89:PRO:O	1:A:92:VAL:HG12	1.99	0.62
1:B:133:LEU:HD13	1:B:136:PHE:CB	2.28	0.62
1:A:64:ASP:HB3	2:D:1:DG:H3'	1.81	0.61
1:A:58:LEU:HB3	1:A:59:PRO:CD	2.31	0.61
1:A:45:GLU:HA	1:A:48:ALA:HB3	1.83	0.61
2:E:19:DG:C8	2:E:21:DT:H72	2.35	0.61
1:B:6:LEU:HD13	1:B:72:PHE:CG	2.37	0.60
1:B:19:PHE:CE1	1:B:92:VAL:HG21	2.36	0.60
1:B:40:LEU:HD11	1:B:42:THR:HG22	1.84	0.60
1:B:45:GLU:HG2	1:B:73:LEU:HD22	1.84	0.59
1:A:42:THR:HG23	1:A:512:ASP:OD1	2.02	0.59
1:A:202:LEU:HD23	1:A:256:LEU:HD23	1.84	0.59
1:A:352:ASN:ND2	1:A:532:GLN:HA	2.18	0.58
1:B:6:LEU:HD13	1:B:72:PHE:CD2	2.39	0.57
1:B:558:ASN:H	1:B:558:ASN:HD22	1.51	0.57
1:A:133:LEU:HD23	1:A:134:LYS:N	2.18	0.57
2:D:20:DT:C2	2:D:21:DT:H72	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:PRO:HD2	1:B:313:LEU:HD12	1.86	0.56
1:B:113:LEU:HD21	1:B:133:LEU:HD23	1.87	0.56
1:A:352:ASN:HD21	1:A:532:GLN:HA	1.71	0.56
1:B:526:LEU:H	1:B:558:ASN:HD21	1.54	0.56
1:A:63:PRO:O	1:A:66:ALA:HB3	2.07	0.54
1:B:450:GLN:HE22	1:B:453:ARG:HH11	1.55	0.54
2:E:23:DT:H3'	2:E:24:DC:H5'	1.89	0.54
1:B:130:LEU:HD23	1:B:133:LEU:HD21	1.90	0.54
1:B:40:LEU:HD11	1:B:42:THR:CG2	2.38	0.53
1:B:113:LEU:CD2	1:B:133:LEU:HD23	2.38	0.53
1:B:112:GLY:C	1:B:113:LEU:HD22	2.29	0.53
1:A:526:LEU:H	1:A:558:ASN:HD21	1.54	0.53
1:A:518:TYR:CE1	1:A:551:ILE:HG23	2.43	0.53
1:B:438:SER:HB3	1:B:467:ALA:HB3	1.91	0.53
1:A:72:PHE:O	1:A:76:GLY:N	2.42	0.52
1:B:150:LEU:O	1:B:154:ALA:HB3	2.10	0.52
1:A:133:LEU:HD23	1:A:134:LYS:H	1.74	0.51
2:E:20:DT:H1'	2:E:21:DT:H73	1.92	0.51
1:B:154:ALA:HB2	1:B:235:PHE:CE1	2.46	0.51
1:A:450:GLN:HE22	1:A:453:ARG:HH11	1.59	0.51
1:B:373:ASP:OD2	1:B:392:ARG:NH1	2.43	0.51
1:A:343:VAL:CG2	1:A:369:LEU:HD21	2.38	0.51
1:B:301:TYR:CE2	1:B:309:ILE:HD12	2.47	0.50
1:A:204:ALA:HB2	1:A:252:TYR:CD1	2.46	0.50
1:A:58:LEU:CB	1:A:59:PRO:CD	2.90	0.49
1:B:130:LEU:CA	1:B:133:LEU:HD11	2.42	0.49
1:B:369:LEU:C	1:B:369:LEU:HD23	2.32	0.49
2:D:20:DT:N1	2:D:21:DT:H72	2.27	0.49
2:E:21:DT:H2'	2:E:21:DT:O2	2.13	0.48
1:B:6:LEU:HD21	1:B:69:ILE:HG12	1.94	0.48
1:B:12:GLU:HG2	1:B:93:LEU:HD23	1.95	0.48
2:E:20:DT:H1'	2:E:21:DT:C7	2.44	0.48
1:B:392:ARG:NH2	1:B:411:GLY:O	2.47	0.48
1:A:55:LEU:HD22	1:A:66:ALA:CB	2.45	0.47
1:A:296:THR:O	1:A:300:VAL:HG23	2.13	0.47
1:A:19:PHE:CE1	1:A:92:VAL:HG21	2.49	0.47
1:A:57:GLU:O	1:A:58:LEU:O	2.32	0.47
1:B:130:LEU:HA	1:B:133:LEU:HD21	1.96	0.47
1:B:132:ARG:N	1:B:133:LEU:HD12	2.30	0.47
1:B:190:ARG:NH1	1:B:260:THR:OG1	2.45	0.47
1:A:105:THR:HG23	1:A:136:PHE:HE2	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:375:SER:HB2	1:B:376:PRO:HD2	1.97	0.46
2:E:23:DT:H3'	2:E:24:DC:H5''	1.97	0.46
1:A:131:THR:HG22	1:A:138:PRO:HA	1.98	0.46
1:B:130:LEU:HA	1:B:133:LEU:HD11	1.96	0.46
1:A:150:LEU:HD23	1:A:235:PHE:CE2	2.51	0.46
1:B:372:THR:HG22	1:B:411:GLY:HA3	1.98	0.46
1:B:133:LEU:CD1	1:B:133:LEU:N	2.75	0.46
1:B:464:HIS:ND1	1:B:569:LEU:HD22	2.30	0.46
1:B:467:ALA:O	1:B:468:HIS:C	2.53	0.46
2:E:19:DG:H2'	2:E:21:DT:H72	1.98	0.46
1:A:199:LEU:HG	1:A:240:LEU:HD11	1.98	0.45
2:E:20:DT:C1'	2:E:21:DT:H73	2.46	0.45
1:A:231:ARG:NH1	6:A:625:HOH:O	2.48	0.45
1:A:473:LEU:HD13	1:A:476:ARG:HD2	1.98	0.45
1:A:558:ASN:HD22	1:A:558:ASN:N	2.15	0.45
1:A:562:TYR:CE2	1:A:566:LEU:HD11	2.51	0.45
1:A:310:PRO:HD2	1:A:313:LEU:HD12	1.99	0.45
1:A:113:LEU:CD2	1:A:133:LEU:HD12	2.47	0.44
1:A:237:LYS:O	1:A:238:ASN:HB3	2.17	0.44
1:A:332:LEU:HD21	1:A:526:LEU:HD21	1.99	0.44
1:B:468:HIS:O	1:B:468:HIS:ND1	2.46	0.44
1:A:113:LEU:HD23	1:A:133:LEU:HD12	2.00	0.44
1:B:280:LEU:HD12	1:B:281:SER:N	2.32	0.44
1:A:18:GLU:HG2	1:A:103:PRO:HB3	1.99	0.44
1:A:133:LEU:HB3	1:A:136:PHE:HB3	2.00	0.44
1:A:375:SER:O	1:A:378:VAL:HG12	2.18	0.44
1:A:6:LEU:HA	1:A:9:ILE:HD12	1.99	0.44
1:B:321:GLU:N	1:B:321:GLU:OE1	2.47	0.44
1:A:467:ALA:O	1:A:468:HIS:C	2.56	0.44
1:B:150:LEU:HD21	1:B:223:GLU:HG3	1.99	0.44
1:B:42:THR:HB	1:B:516:MET:HE3	2.00	0.44
1:B:352:ASN:OD1	1:B:532:GLN:HA	2.18	0.44
1:B:558:ASN:ND2	1:B:558:ASN:N	2.66	0.43
1:B:40:LEU:CD1	1:B:42:THR:HG22	2.48	0.43
1:A:155:GLY:N	6:A:588:HOH:O	2.52	0.43
1:A:409:LEU:HD12	1:A:409:LEU:N	2.34	0.43
1:A:341:LEU:HA	1:A:370:ALA:HB3	2.01	0.43
1:B:175:ARG:HG3	1:B:183:ALA:HB3	2.01	0.42
2:D:8:DT:H4'	2:D:9:DC:C2	2.54	0.42
1:A:558:ASN:H	1:A:558:ASN:HD22	1.66	0.42
3:A:576:DG3:C8	2:D:29:DDG:H2''	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:SER:HB3	1:A:283:TYR:HA	2.01	0.42
1:B:125:LEU:HD13	1:B:125:LEU:O	2.19	0.41
1:A:122:LYS:HG2	1:A:148:LEU:HD21	2.03	0.41
1:B:248:PRO:HB2	1:B:250:GLU:HG3	2.03	0.41
1:A:121:LEU:O	1:A:125:LEU:HD22	2.20	0.41
1:B:131:THR:HG22	1:B:131:THR:O	2.21	0.41
2:D:23:DT:H2"	2:D:24:DC:OP2	2.21	0.41
1:B:385:SER:HB2	1:B:386:PRO:HD2	2.02	0.41
1:A:110:TYR:O	1:A:114:GLY:HA2	2.21	0.41
1:A:3:ASN:CG	1:A:44:ILE:HG23	2.42	0.40
1:B:508:ASP:OD2	1:B:509:LEU:HA	2.21	0.40
1:B:89:PRO:O	1:B:92:VAL:HG12	2.20	0.40
1:B:301:TYR:HE2	1:B:309:ILE:HD12	1.86	0.40
1:A:361:ALA:HB2	1:A:369:LEU:HD13	2.03	0.40
1:A:372:THR:HG22	1:A:411:GLY:HA3	2.03	0.40
1:A:498:VAL:CG2	1:A:524:ILE:HD13	2.52	0.40
1:B:451:THR:HG22	1:B:455:LEU:HD12	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	570/575 (99%)	534 (94%)	27 (5%)	9 (2%)	9	24
1	B	570/575 (99%)	542 (95%)	26 (5%)	2 (0%)	34	60
All	All	1140/1150 (99%)	1076 (94%)	53 (5%)	11 (1%)	15	37

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	LEU

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Mol	Chain	Res	Type
1	A	59	PRO
1	A	238	ASN
1	A	384	PRO
1	A	51	GLY
1	A	380	VAL
1	B	380	VAL
1	A	155	GLY
1	A	383	GLY
1	B	468	HIS
1	A	101	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	464/466 (100%)	438 (94%)	26 (6%)	21	45
1	B	464/466 (100%)	442 (95%)	22 (5%)	26	54
All	All	928/932 (100%)	880 (95%)	48 (5%)	23	49

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	ARG
1	A	3	ASN
1	A	32	GLN
1	A	38	TYR
1	A	45	GLU
1	A	79	ARG
1	A	82	GLU
1	A	104	LYS
1	A	132	ARG
1	A	166	LEU
1	A	170	LEU
1	A	181	GLU

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Mol	Chain	Res	Type
1	A	210	ARG
1	A	213	GLU
1	A	237	LYS
1	A	245	ARG
1	A	272	LEU
1	A	295	GLU
1	A	298	GLU
1	A	343	VAL
1	A	367	ARG
1	A	415	ASP
1	A	558	ASN
1	A	570	LYS
1	A	572	ARG
1	B	23	ASN
1	B	80	LYS
1	B	90	ARG
1	B	104	LYS
1	B	127	ARG
1	B	132	ARG
1	B	133	LEU
1	B	134	LYS
1	B	156	LYS
1	B	158	ARG
1	B	182	ARG
1	B	223	GLU
1	B	229	LYS
1	B	231	ARG
1	B	240	LEU
1	B	245	ARG
1	B	282	GLU
1	B	317	GLN
1	B	380	VAL
1	B	512	ASP
1	B	558	ASN
1	B	570	LYS

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

Mol	Chain	Res	Type
1	A	317	GLN
1	A	351	GLN
1	A	352	ASN

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Mol	Chain	Res	Type
1	A	440	HIS
1	A	450	GLN
1	A	558	ASN
1	B	23	ASN
1	B	317	GLN
1	B	450	GLN
1	B	558	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are 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	DDG	D	29	2	17,23,24	1.26	2 (11%)	15,33,36	2.66	7 (46%)
2	DDG	E	29	2	17,23,24	1.30	2 (11%)	15,33,36	2.58	6 (40%)

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	DDG	D	29	2	-	0/3/18/19	0/3/3/3
2	DDG	E	29	2	-	0/3/18/19	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	29	DDG	C6-C5	4.17	1.48	1.41
2	D	29	DDG	C6-C5	4.12	1.48	1.41
2	E	29	DDG	C5-C4	2.50	1.47	1.40
2	D	29	DDG	C5-C4	2.43	1.47	1.40

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	29	DDG	C2-N3-C4	4.70	120.72	115.36
2	E	29	DDG	C2-N3-C4	4.48	120.48	115.36
2	D	29	DDG	C5-C6-N1	-4.13	117.78	123.43
2	D	29	DDG	C6-N1-C2	4.13	122.48	115.93
2	E	29	DDG	C5-C6-N1	-4.09	117.84	123.43
2	D	29	DDG	C6-C5-C4	-4.07	116.91	120.80
2	E	29	DDG	C6-N1-C2	4.05	122.36	115.93
2	E	29	DDG	C6-C5-C4	-3.98	117.00	120.80
2	D	29	DDG	N3-C2-N1	-3.24	122.90	127.22
2	E	29	DDG	N3-C2-N1	-3.06	123.14	127.22
2	D	29	DDG	C4-C5-N7	-2.98	106.29	109.40
2	E	29	DDG	C4-C5-N7	-2.85	106.43	109.40
2	D	29	DDG	C3'-C2'-C1'	2.53	105.70	102.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	29	DDG	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 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
3	DG3	B	576	4	25,32,32	1.10	2 (8%)	28,50,50	2.24	10 (35%)
3	DG3	A	576	4	25,32,32	1.13	2 (8%)	28,50,50	2.19	8 (28%)

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
3	DG3	B	576	4	-	3/18/31/31	0/3/3/3
3	DG3	A	576	4	-	5/18/31/31	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	576	DG3	C6-C5	4.19	1.48	1.41
3	B	576	DG3	C6-C5	4.06	1.48	1.41
3	A	576	DG3	C5-C4	2.25	1.46	1.40
3	B	576	DG3	C5-C4	2.23	1.46	1.40

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	576	DG3	C2-N3-C4	5.26	121.36	115.36
3	A	576	DG3	C2-N3-C4	5.17	121.26	115.36
3	B	576	DG3	C6-C5-C4	-4.54	116.46	120.80
3	A	576	DG3	C6-C5-C4	-4.37	116.62	120.80
3	B	576	DG3	C6-N1-C2	3.84	122.03	115.93
3	A	576	DG3	C6-N1-C2	3.77	121.92	115.93
3	B	576	DG3	N3-C2-N1	-3.68	122.32	127.22
3	A	576	DG3	C5-C6-N1	-3.61	118.49	123.43
3	B	576	DG3	C5-C6-N1	-3.50	118.65	123.43
3	A	576	DG3	N3-C2-N1	-3.34	122.77	127.22
3	A	576	DG3	PB-O3B-PG	-2.87	122.99	132.83
3	A	576	DG3	C4-C5-N7	-2.74	106.55	109.40
3	B	576	DG3	PB-O3B-PG	-2.68	123.64	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	576	DG3	C4-C5-N7	-2.56	106.73	109.40
3	A	576	DG3	C3'-C2'-C1'	2.35	105.49	102.78
3	B	576	DG3	PA-O3A-PB	-2.20	125.28	132.83
3	B	576	DG3	O4'-C1'-C2'	2.08	108.92	106.67
3	B	576	DG3	C3'-C2'-C1'	2.04	105.13	102.78

There are no chirality outliers.

All (8) torsion outliers are listed below:

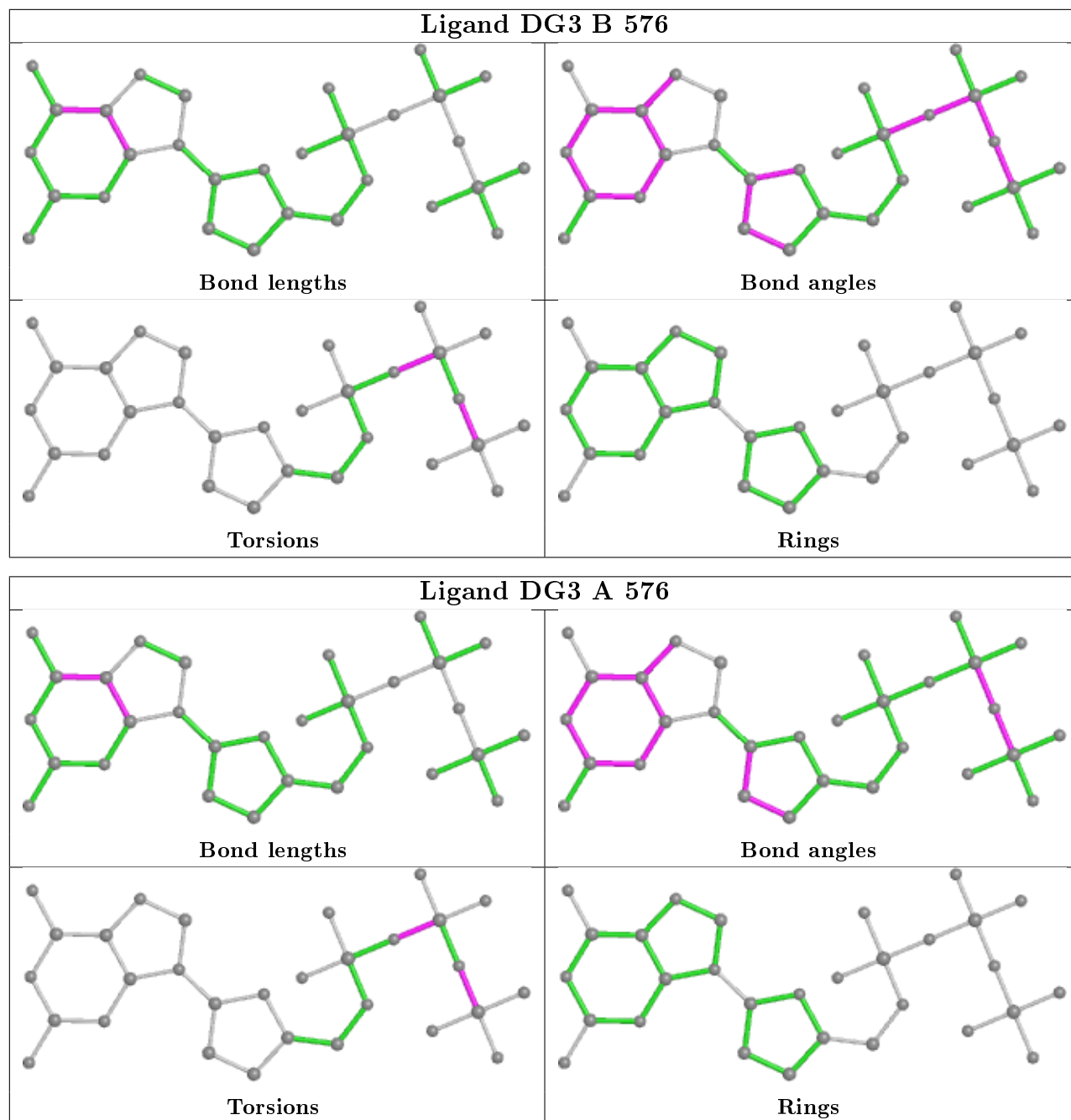
Mol	Chain	Res	Type	Atoms
3	B	576	DG3	PB-O3B-PG-O2G
3	B	576	DG3	PA-O3A-PB-O1B
3	A	576	DG3	PB-O3B-PG-O1G
3	A	576	DG3	PA-O3A-PB-O2B
3	B	576	DG3	PA-O3A-PB-O2B
3	A	576	DG3	PB-O3B-PG-O2G
3	A	576	DG3	PB-O3B-PG-O3G
3	A	576	DG3	PA-O3A-PB-O1B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	576	DG3	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	572/575 (99%)	0.28	35 (6%) 21 20	15, 30, 67, 74	0
1	B	572/575 (99%)	0.17	24 (4%) 36 35	14, 27, 60, 68	0
2	D	28/29 (96%)	0.45	6 (21%) 0 0	17, 41, 82, 88	0
2	E	28/29 (96%)	0.25	3 (10%) 6 4	14, 37, 86, 91	0
All	All	1200/1208 (99%)	0.23	68 (5%) 23 22	14, 29, 66, 91	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	378	VAL	7.7
1	B	383	GLY	7.2
1	B	380	VAL	6.7
1	A	381	ALA	6.5
1	A	384	PRO	6.1
1	A	55	LEU	5.4
1	A	380	VAL	5.3
1	B	384	PRO	5.3
1	B	381	ALA	5.1
2	D	5	DT	4.6
1	A	379	ARG	4.4
1	A	382	GLY	4.4
2	E	23	DT	4.4
1	A	74	ARG	4.3
1	A	75	THR	4.3
1	A	53	GLU	4.3
1	A	56	MET	4.2
1	B	379	ARG	4.1
1	B	136	PHE	4.1
1	A	51	GLY	4.0
2	D	22	DT	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	57	GLU	3.6
1	B	134	LYS	3.5
1	B	382	GLY	3.4
1	B	154	ALA	3.3
1	A	119	GLU	3.3
2	E	22	DT	3.3
1	B	138	PRO	3.2
1	A	136	PHE	3.2
1	A	38	TYR	3.1
1	A	131	THR	3.0
1	B	155	GLY	3.0
1	A	390	LEU	2.9
1	A	67	GLU	2.8
2	D	23	DT	2.8
1	A	49	GLU	2.8
1	A	70	LEU	2.8
1	A	130	LEU	2.8
2	D	21	DT	2.7
1	A	135	GLY	2.7
2	D	20	DT	2.6
1	B	135	GLY	2.6
1	A	54	ALA	2.5
1	B	132	ARG	2.5
1	B	347	TYR	2.4
1	B	51	GLY	2.4
2	D	6	DT	2.4
1	B	86	ARG	2.4
1	A	154	ALA	2.4
1	A	61	VAL	2.4
1	B	144	ILE	2.3
1	A	383	GLY	2.3
1	A	63	PRO	2.3
1	A	289	GLU	2.3
1	B	79	ARG	2.3
1	A	52	LYS	2.2
2	E	5	DT	2.2
1	A	132	ARG	2.2
1	B	118	LEU	2.1
1	B	153	ALA	2.1
1	B	90	ARG	2.1
1	A	122	LYS	2.1
1	A	125	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	71	GLU	2.1
1	B	57	GLU	2.0
1	B	128	GLY	2.0
1	A	110	TYR	2.0
1	A	121	LEU	2.0

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	DDG	D	29	21/22	0.94	0.16	19,21,22,24	0
2	DDG	E	29	21/22	0.94	0.15	19,21,25,26	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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.

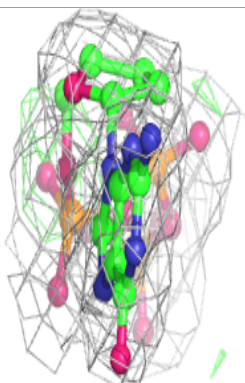
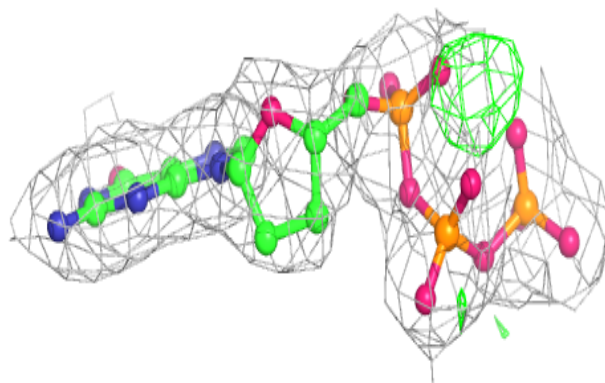
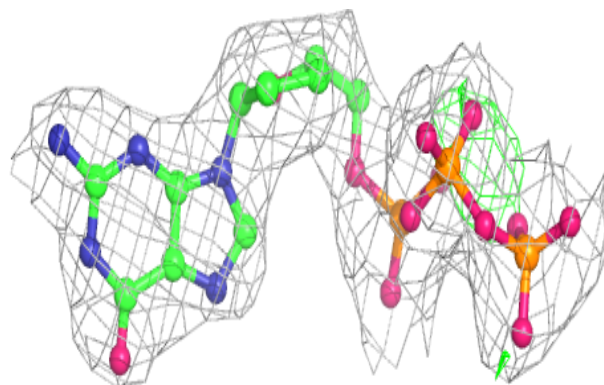
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MG	A	577	1/1	0.84	0.24	13,13,13,13	0
5	ZN	B	579	1/1	0.88	0.07	56,56,56,56	0
4	MG	B	577	1/1	0.91	0.21	17,17,17,17	0
5	ZN	A	579	1/1	0.92	0.11	70,70,70,70	0
4	MG	A	578	1/1	0.93	0.11	31,31,31,31	0
4	MG	B	578	1/1	0.93	0.24	24,24,24,24	0
3	DG3	B	576	30/30	0.96	0.16	9,12,16,16	0
3	DG3	A	576	30/30	0.98	0.14	11,12,13,13	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.

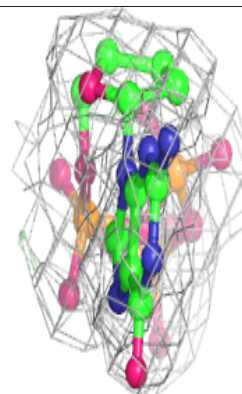
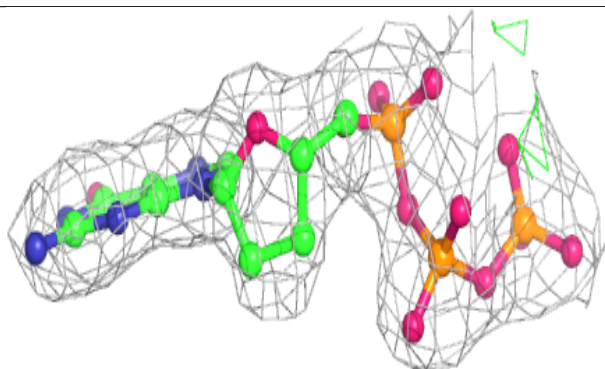
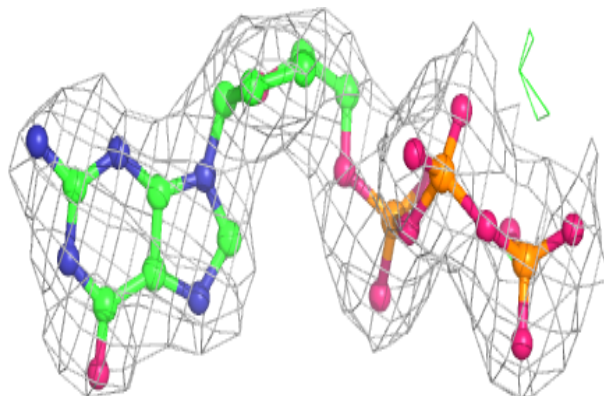
Electron density around DG3 B 576:

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



Electron density around DG3 A 576:

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



6.5 Other polymers

There are no such residues in this entry.