



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 02:27 am BST

PDB ID : 5AO0
Title : Crystal structure of human SAMHD1 (amino acid residues 41-583) bound to ddGTP
Authors : Schwefel, D.; Taylor, I.A.
Deposited on : 2015-09-09
Resolution : 3.73 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

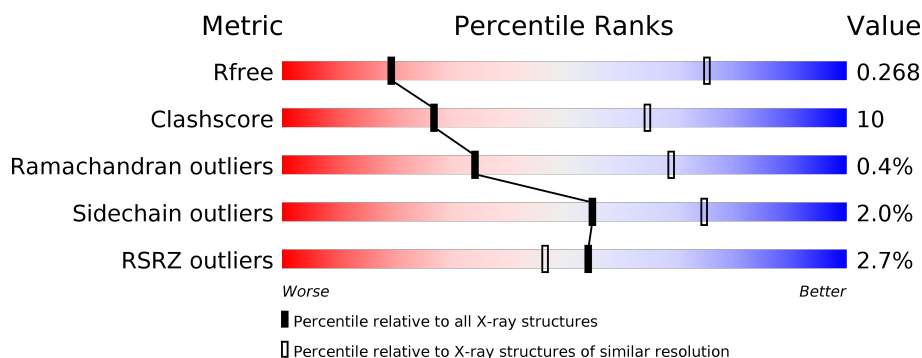
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.73 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	1001 (3.90-3.58)
Clashscore	141614	1063 (3.90-3.58)
Ramachandran outliers	138981	1027 (3.90-3.58)
Sidechain outliers	138945	1023 (3.90-3.58)
RSRZ outliers	127900	1006 (3.92-3.56)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	565	<div> <div>3%</div> <div>66%</div> <div>11%</div> <div>22%</div> </div>
1	B	565	<div> <div>%</div> <div>58%</div> <div>18%</div> <div>23%</div> </div>

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
4	MG	A	3001	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6912 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 DEOXYNUCLEOSIDE TRIPHOSPHATE TRIPHOSPHO-HYDROLASE SAMHD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	0	2	0
			3372	2169	577	606	20			
1	B	435	Total	C	N	O	S	0	0	0
			3413	2181	584	629	19			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	MET	-	expression tag	UNP Q9Y3Z3
A	20	ALA	-	expression tag	UNP Q9Y3Z3
A	21	SER	-	expression tag	UNP Q9Y3Z3
A	22	TRP	-	expression tag	UNP Q9Y3Z3
A	23	SER	-	expression tag	UNP Q9Y3Z3
A	24	HIS	-	expression tag	UNP Q9Y3Z3
A	25	PRO	-	expression tag	UNP Q9Y3Z3
A	26	GLN	-	expression tag	UNP Q9Y3Z3
A	27	PHE	-	expression tag	UNP Q9Y3Z3
A	28	GLU	-	expression tag	UNP Q9Y3Z3
A	29	LYS	-	expression tag	UNP Q9Y3Z3
A	30	GLY	-	expression tag	UNP Q9Y3Z3
A	31	ALA	-	expression tag	UNP Q9Y3Z3
A	32	LEU	-	expression tag	UNP Q9Y3Z3
A	33	GLU	-	expression tag	UNP Q9Y3Z3
A	34	VAL	-	expression tag	UNP Q9Y3Z3
A	35	LEU	-	expression tag	UNP Q9Y3Z3
A	36	PHE	-	expression tag	UNP Q9Y3Z3
A	37	GLN	-	expression tag	UNP Q9Y3Z3
A	38	GLY	-	expression tag	UNP Q9Y3Z3
A	39	PRO	-	expression tag	UNP Q9Y3Z3
A	40	GLY	-	expression tag	UNP Q9Y3Z3
B	19	MET	-	expression tag	UNP Q9Y3Z3
B	20	ALA	-	expression tag	UNP Q9Y3Z3

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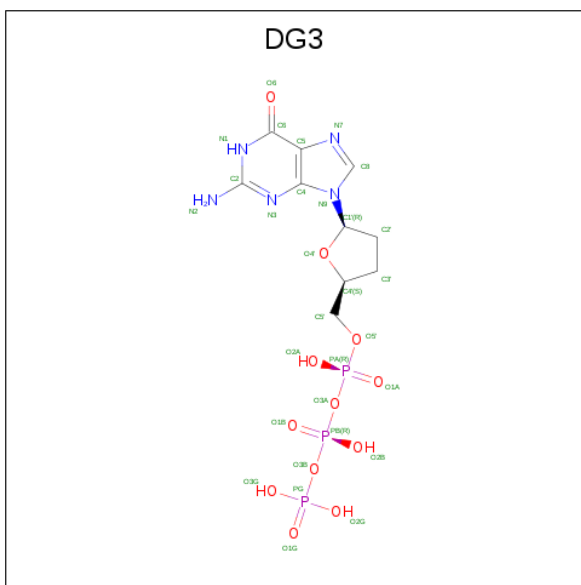
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Chain	Residue	Modelled	Actual	Comment	Reference
B	21	SER	-	expression tag	UNP Q9Y3Z3
B	22	TRP	-	expression tag	UNP Q9Y3Z3
B	23	SER	-	expression tag	UNP Q9Y3Z3
B	24	HIS	-	expression tag	UNP Q9Y3Z3
B	25	PRO	-	expression tag	UNP Q9Y3Z3
B	26	GLN	-	expression tag	UNP Q9Y3Z3
B	27	PHE	-	expression tag	UNP Q9Y3Z3
B	28	GLU	-	expression tag	UNP Q9Y3Z3
B	29	LYS	-	expression tag	UNP Q9Y3Z3
B	30	GLY	-	expression tag	UNP Q9Y3Z3
B	31	ALA	-	expression tag	UNP Q9Y3Z3
B	32	LEU	-	expression tag	UNP Q9Y3Z3
B	33	GLU	-	expression tag	UNP Q9Y3Z3
B	34	VAL	-	expression tag	UNP Q9Y3Z3
B	35	LEU	-	expression tag	UNP Q9Y3Z3
B	36	PHE	-	expression tag	UNP Q9Y3Z3
B	37	GLN	-	expression tag	UNP Q9Y3Z3
B	38	GLY	-	expression tag	UNP Q9Y3Z3
B	39	PRO	-	expression tag	UNP Q9Y3Z3
B	40	GLY	-	expression tag	UNP Q9Y3Z3

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Fe 1 1	0	0
2	A	1	Total Fe 1 1	0	0

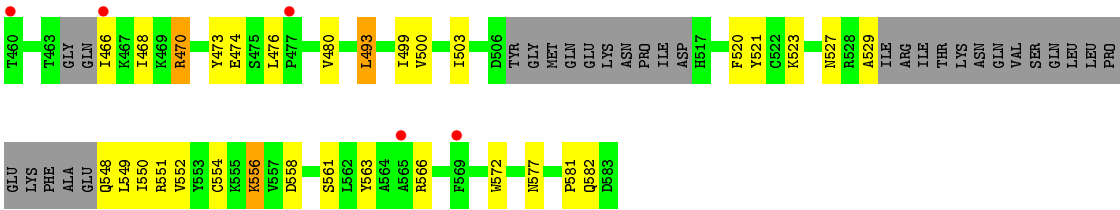
- Molecule 3 is 2'-3'-DIDEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DG3) (formula: C₁₀H₁₆N₅O₁₂P₃).



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 ($\text{RSRZ} > 2$). 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.

- [illegible]

- Chain B:
-
- 58% 18% 23%
- MET ALA SER TRP SER HIS PRO GLN PHE GLU LYS GLY ALA LEU GLU VAL LEU PHE GLN GLY PRO GLY ASP TYR LYS THR TRP GLY PRO GLU GLN VAL HIS CYS PHE LEU ARG ARG GLY GLY PHE GLU GLU PRO VAL LEU LEU LYS ASN ILE ARG GLU ASN GLU ILE THR GLY ALA LEU LEU PRO CYS LEU ASP GLU VAL SER SER LEU GLY GLU ARG LYS LYS LEU TYR ILE GLN ARG LEU VAL GLN ILE HIS VAL D113 K116 V117 I118 N119 D120 I126 R143 G172 Y173 L174 A175 V179 H180 E184 E188 L189 Q190 R194 L197 C198 Y199 Q200 I201 L204 H215 D218 G219 R220 P227 T232 H233 E234 Q235 V236 L244 N248 G249 I250 M254 L259 D264 K269 V273 E277 SER PRO VAL GLU ASP SER L284 W285 T286 P291 E292 I293 K294 I300 P306



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	163.17Å 163.17Å 260.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.42 – 3.73 49.42 – 3.73	Depositor EDS
% Data completeness (in resolution range)	98.7 (49.42-3.73) 98.8 (49.42-3.73)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.33 (at 3.77Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.219 , 0.268 0.222 , 0.268	Depositor DCC
R_{free} test set	703 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	96.4	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 77.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	6912	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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: DG3, MG, FE

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	0.29	0/3461	0.49	1/4709 (0.0%)
1	B	0.38	1/3495 (0.0%)	0.61	2/4749 (0.0%)
All	All	0.34	1/6956 (0.0%)	0.55	3/9458 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	341	CYS	CB-SG	-5.44	1.73	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	493	LEU	CB-CG-CD2	-5.30	101.98	111.00
1	A	431	LEU	CB-CG-CD1	-5.10	102.33	111.00
1	B	312	LYS	CD-CE-NZ	5.03	123.26	111.70

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	3372	0	3136	49	0
1	B	3413	0	3194	86	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	60	0	24	2	0
3	B	60	0	24	6	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	2	0	0	0	0
5	B	1	0	0	0	0
All	All	6912	0	6378	135	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 10.

All (135) 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:B:398:GLU:HB3	1:B:406:LYS:HE2	1.50	0.93
1:B:232:THR:OG1	1:B:235:GLN:NE2	2.02	0.92
1:B:308:ILE:HA	1:B:312:LYS:HZ3	1.35	0.92
1:B:172:GLY:HA3	1:B:204:LEU:HD12	1.52	0.91
1:B:307:GLY:O	1:B:312:LYS:NZ	2.04	0.89
1:B:500:VAL:HG12	1:B:552:VAL:HG22	1.55	0.89
1:B:218:ASP:O	1:B:470:ARG:NH2	2.09	0.85
1:B:328:ASN:HB2	1:B:365:THR:OG1	1.77	0.84
1:B:468:ILE:H	1:B:548:GLN:HE22	1.24	0.81
1:B:548:GLN:HE21	1:B:550:ILE:HD11	1.44	0.81
1:B:339:ARG:HD3	1:B:521:TYR:CE2	2.17	0.79
1:B:308:ILE:HA	1:B:312:LYS:NZ	2.00	0.75
1:A:185:LYS:NZ	1:A:336:LYS:O	2.20	0.73
1:B:493:LEU:HD11	1:B:556:LYS:HZ3	1.53	0.73
1:B:116:LYS:HE2	3:B:2002:DG3:H5'2	1.71	0.71
1:B:459:GLU:OE2	1:B:549:LEU:HB3	1.92	0.69
1:A:120:ASP:OD1	1:A:318:ARG:NH2	2.27	0.68
1:B:118:ILE:HG12	3:B:2002:DG3:H2'2	1.76	0.67
1:B:554:CYS:SG	1:B:556:LYS:HE2	2.34	0.67
1:B:352:ARG:NH1	1:B:523:LYS:HA	2.10	0.66
1:B:316:PHE:CZ	1:B:366:ARG:HG3	2.31	0.65
1:A:326:GLN:NE2	1:A:328:ASN:OD1	2.30	0.64
1:A:446:LYS:HA	1:A:446:LYS:HE3	1.81	0.63
1:B:493:LEU:HD11	1:B:556:LYS:NZ	2.14	0.63
1:A:233:HIS:NE2	3:A:2001:DG3:O2G	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:493:LEU:CD1	1:B:556:LYS:HZ3	2.13	0.62
1:B:312:LYS:HA	1:B:315:TYR:CE2	2.35	0.61
1:B:558:ASP:OD1	1:B:561:SER:HB2	2.01	0.60
1:B:233:HIS:NE2	3:B:2001:DG3:O1G	2.35	0.60
1:A:179:VAL:HG12	1:A:300:ILE:HD13	1.84	0.59
1:A:178:LEU:HD23	1:A:300:ILE:HG23	1.84	0.59
1:B:293:ASN:C	1:B:294:LYS:HD3	2.23	0.58
1:A:496:GLU:O	1:A:555:LYS:HE2	2.03	0.58
1:A:431:LEU:HD13	1:A:446:LYS:NZ	2.19	0.58
1:A:446:LYS:HD2	1:A:446:LYS:N	2.19	0.58
1:A:446:LYS:HZ2	1:A:449:GLU:HG3	1.68	0.58
1:B:232:THR:HG1	1:B:235:GLN:NE2	2.02	0.58
1:B:312:LYS:HA	1:B:315:TYR:CD2	2.40	0.56
1:A:500:VAL:HG23	1:A:552:VAL:HG22	1.87	0.55
1:B:493:LEU:HD21	1:B:556:LYS:NZ	2.22	0.55
1:A:320:CYS:HB3	1:A:325:ILE:O	2.06	0.55
1:A:376:HIS:O	1:A:380:ASN:ND2	2.39	0.55
1:A:497:ASP:HA	1:A:555:LYS:HG3	1.89	0.55
1:B:238:VAL:HG13	1:B:269:LYS:HD3	1.87	0.55
1:A:470:ARG:HA	1:A:473:TYR:CE1	2.42	0.54
1:B:220:ARG:NH2	1:B:500:VAL:O	2.40	0.54
1:A:431:LEU:HD13	1:A:446:LYS:HZ3	1.72	0.54
1:B:175:ALA:HB1	1:B:199:VAL:HG12	1.89	0.54
1:A:446:LYS:HA	1:A:446:LYS:CE	2.38	0.53
1:A:446:LYS:NZ	1:A:449:GLU:HG3	2.24	0.53
1:B:120:ASP:OD1	1:B:318:ARG:NH2	2.42	0.52
1:B:380:ASN:O	1:B:384:THR:HG23	2.10	0.52
1:B:503:ILE:HB	1:B:549:LEU:HB2	1.91	0.52
1:A:175:ALA:HB1	1:A:199:VAL:HG12	1.92	0.52
1:B:180:HIS:O	1:B:184:GLU:HG2	2.10	0.52
1:B:190:GLN:HB2	1:B:294:LYS:NZ	2.26	0.51
1:B:309:ASP:H	1:B:312:LYS:HZ3	1.59	0.51
1:B:352:ARG:NH1	1:B:521:TYR:CE2	2.78	0.51
1:B:563:TYR:O	1:B:566:ARG:HB3	2.11	0.51
1:B:215:HIS:NE2	3:B:2001:DG3:O2B	2.39	0.51
1:B:468:ILE:HG21	1:B:476:LEU:HD11	1.94	0.50
1:B:179:VAL:HG22	1:B:300:ILE:HD13	1.92	0.50
1:B:493:LEU:HD21	1:B:556:LYS:HZ3	1.75	0.50
1:A:468:ILE:HG21	1:A:476:LEU:HD11	1.92	0.50
1:B:227:PRO:HG2	1:B:474:GLU:OE1	2.11	0.50
1:B:480:VAL:HG22	1:B:572:TRP:CD2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:ILE:HG13	1:A:204:LEU:HD21	1.95	0.49
1:A:431:LEU:HD12	1:A:431:LEU:O	2.13	0.49
1:A:530:ILE:HG22	1:A:531:ARG:H	1.78	0.49
1:B:316:PHE:HZ	1:B:366:ARG:CZ	2.25	0.49
1:A:118:ILE:HG12	3:A:2002:DG3:H2'1	1.95	0.49
1:A:238:VAL:HG13	1:A:269:LYS:HD3	1.94	0.49
1:B:556:LYS:CE	1:B:561:SER:HB3	2.43	0.48
1:B:476:LEU:HB2	1:B:500:VAL:HG21	1.96	0.48
1:B:291:PRO:HB2	1:B:293:ASN:OD1	2.14	0.48
1:B:433:SER:O	1:B:442:ARG:NH1	2.47	0.48
1:B:312:LYS:CE	1:B:366:ARG:HH22	2.28	0.47
1:B:397:ILE:HD11	1:B:430:ILE:HG12	1.96	0.47
1:A:557:VAL:HA	1:A:562:LEU:HG	1.97	0.47
1:B:433:SER:OG	1:B:442:ARG:NH1	2.48	0.47
1:B:443:GLU:O	1:B:447:GLN:HG2	2.15	0.47
1:A:179:VAL:HG21	1:A:196:VAL:HA	1.97	0.46
1:A:312:LYS:HA	1:A:315:TYR:CE2	2.50	0.46
1:B:293:ASN:O	1:B:294:LYS:HD3	2.16	0.46
1:A:380:ASN:O	1:A:384:THR:HG23	2.16	0.46
1:B:293:ASN:ND2	1:B:294:LYS:HE2	2.31	0.46
1:B:197:LEU:O	1:B:201:ILE:HG13	2.16	0.45
1:B:581:PRO:CB	1:B:582:GLN:HA	2.45	0.45
1:B:308:ILE:CA	1:B:312:LYS:HZ3	2.17	0.45
1:B:320:CYS:HB3	1:B:325:ILE:O	2.17	0.45
1:B:305:ARG:O	1:B:306:ASN:HB3	2.17	0.45
1:B:116:LYS:NZ	3:B:2002:DG3:HN22	2.14	0.44
1:A:294:LYS:HA	1:A:296:PHE:CE1	2.52	0.44
1:B:470:ARG:HA	1:B:473:TYR:CD1	2.53	0.44
1:B:244:LEU:O	1:B:248:ASN:ND2	2.46	0.44
1:A:470:ARG:HA	1:A:473:TYR:CD1	2.53	0.44
1:B:520:PHE:O	1:B:529:ALA:HA	2.18	0.44
1:A:167:HIS:CE1	1:A:315:TYR:HB3	2.53	0.44
1:A:447:GLN:HB3	1:A:452:ASN:O	2.18	0.44
1:B:377:LYS:HA	1:B:551:ARG:NH1	2.32	0.44
1:B:476:LEU:CB	1:B:500:VAL:HG21	2.48	0.43
1:B:126:ILE:HG23	1:B:173:TYR:CD1	2.54	0.43
1:B:194:ARG:HH21	1:B:264:ASP:CG	2.22	0.43
1:B:334:PHE:HD1	1:B:355:GLU:HG2	1.83	0.43
1:B:143:ARG:HD2	1:B:420:THR:HA	2.01	0.43
1:B:548:GLN:NE2	1:B:550:ILE:HD11	2.23	0.43
1:A:359:LEU:HD23	1:A:359:LEU:HA	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:ASN:CB	1:A:361:ASP:HB3	2.49	0.43
1:A:431:LEU:C	1:A:431:LEU:HD12	2.39	0.43
1:B:116:LYS:HE3	3:B:2002:DG3:O1G	2.18	0.43
1:B:250:ILE:HG22	1:B:254:MET:HG3	2.01	0.43
1:A:395:ASP:HA	1:A:408:ARG:HE	1.84	0.42
1:B:493:LEU:CD2	1:B:556:LYS:HZ3	2.32	0.42
1:A:129:HIS:H	1:A:132:LEU:HD12	1.84	0.42
1:B:326:GLN:OE1	1:B:326:GLN:C	2.58	0.42
1:A:179:VAL:CG2	1:A:196:VAL:HG22	2.50	0.42
1:A:285:TRP:HA	1:A:286:PRO:HD3	1.86	0.42
1:B:466:ILE:HD13	1:B:466:ILE:HG21	1.75	0.42
1:B:470:ARG:HA	1:B:473:TYR:CE1	2.55	0.42
1:A:427:PHE:CE2	1:A:445:LEU:HD22	2.54	0.42
1:A:557:VAL:HG13	1:A:562:LEU:HD11	2.01	0.42
1:B:269:LYS:O	1:B:273:VAL:HG12	2.20	0.41
1:B:294:LYS:HD3	1:B:294:LYS:N	2.34	0.41
1:A:530:ILE:HG22	1:A:531:ARG:N	2.34	0.41
1:B:273:VAL:O	1:B:273:VAL:HG22	2.20	0.41
1:B:334:PHE:CD1	1:B:355:GLU:HG2	2.55	0.41
1:A:197:LEU:O	1:A:201:ILE:HG13	2.20	0.41
1:B:470:ARG:HG2	1:B:470:ARG:H	1.52	0.41
1:B:468:ILE:H	1:B:548:GLN:NE2	2.05	0.41
1:A:446:LYS:CD	1:A:446:LYS:N	2.83	0.41
1:B:285:TRP:HA	1:B:286:PRO:HD3	1.90	0.41
1:B:454:PHE:CE2	1:B:499:ILE:HG13	2.56	0.40
1:A:485:PRO:HG3	1:A:568:TYR:HE1	1.86	0.40
1:A:455:LYS:HB2	1:A:557:VAL:HG22	2.02	0.40
1:A:446:LYS:CA	1:A:446:LYS:CE	2.99	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	433/565 (77%)	427 (99%)	6 (1%)	0	100	100
1	B	425/565 (75%)	417 (98%)	5 (1%)	3 (1%)	22	59
All	All	858/1130 (76%)	844 (98%)	11 (1%)	3 (0%)	34	74

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	306	ASN
1	B	577	ASN
1	B	305	ARG

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	334/501 (67%)	327 (98%)	7 (2%)	53	74
1	B	351/501 (70%)	343 (98%)	8 (2%)	50	71
All	All	685/1002 (68%)	670 (98%)	15 (2%)	55	72

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	190	GLN
1	A	228	GLU
1	A	341[A]	CYS
1	A	341[B]	CYS
1	A	366	ARG
1	A	446	LYS
1	A	491	VAL
1	B	188	GLU
1	B	312	LYS
1	B	342	GLU
1	B	348	ARG
1	B	406	LYS
1	B	470	ARG

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Mol	Chain	Res	Type
1	B	527	ASN
1	B	556	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	326	GLN
1	A	328	ASN
1	B	548	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	A	2002	4	25,32,32	2.18	5 (20%)	28,50,50	2.09	9 (32%)
3	DG3	B	2001	2	25,32,32	2.22	5 (20%)	28,50,50	2.10	10 (35%)
3	DG3	A	2001	2	25,32,32	2.21	5 (20%)	28,50,50	2.08	10 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	DG3	B	2002	4	25,32,32	2.16	5 (20%)	28,50,50	2.09	11 (39%)

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	A	2002	4	-	0/18/31/31	0/3/3/3
3	DG3	B	2001	2	-	1/18/31/31	0/3/3/3
3	DG3	A	2001	2	-	1/18/31/31	0/3/3/3
3	DG3	B	2002	4	-	9/18/31/31	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2001	DG3	C4-N3	6.85	1.46	1.35
3	A	2001	DG3	C4-N3	6.80	1.46	1.35
3	A	2002	DG3	C4-N3	6.72	1.46	1.35
3	B	2002	DG3	C4-N3	6.68	1.46	1.35
3	B	2001	DG3	C2-N1	5.21	1.44	1.35
3	A	2001	DG3	C2-N1	5.17	1.44	1.35
3	A	2002	DG3	C2-N1	5.11	1.44	1.35
3	B	2002	DG3	C2-N1	5.05	1.44	1.35
3	A	2001	DG3	C2-N2	3.80	1.41	1.33
3	B	2001	DG3	C2-N2	3.79	1.41	1.33
3	A	2002	DG3	C2-N2	3.74	1.41	1.33
3	B	2002	DG3	C2-N2	3.72	1.41	1.33
3	A	2001	DG3	C6-C5	3.57	1.47	1.41
3	B	2002	DG3	C6-C5	3.55	1.47	1.41
3	B	2001	DG3	C6-C5	3.55	1.47	1.41
3	A	2002	DG3	C6-C5	3.43	1.47	1.41
3	B	2001	DG3	C6-N1	3.32	1.38	1.33
3	A	2002	DG3	C6-N1	3.28	1.38	1.33
3	A	2001	DG3	C6-N1	3.25	1.38	1.33
3	B	2002	DG3	C6-N1	3.13	1.38	1.33

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2001	DG3	N3-C2-N1	-5.23	120.25	127.22
3	A	2002	DG3	N3-C2-N1	-5.21	120.28	127.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2001	DG3	N3-C2-N1	-5.16	120.34	127.22
3	B	2002	DG3	N3-C2-N1	-5.12	120.39	127.22
3	A	2002	DG3	C2-N3-C4	4.61	120.63	115.36
3	B	2002	DG3	C2-N3-C4	4.43	120.41	115.36
3	A	2001	DG3	C2-N3-C4	4.38	120.36	115.36
3	B	2001	DG3	C2-N3-C4	4.38	120.36	115.36
3	B	2002	DG3	C4'-O4'-C1'	-3.90	106.13	109.81
3	A	2001	DG3	C4'-O4'-C1'	-3.63	106.38	109.81
3	A	2002	DG3	C4'-O4'-C1'	-3.32	106.67	109.81
3	B	2001	DG3	O4'-C4'-C3'	3.22	110.14	104.80
3	B	2001	DG3	PB-O3B-PG	-2.94	122.73	132.83
3	A	2002	DG3	O4'-C4'-C3'	2.92	109.64	104.80
3	B	2001	DG3	C4'-O4'-C1'	-2.90	107.07	109.81
3	B	2001	DG3	C6-N1-C2	2.79	120.37	115.93
3	A	2001	DG3	C6-N1-C2	2.78	120.35	115.93
3	B	2002	DG3	C6-N1-C2	2.76	120.32	115.93
3	A	2002	DG3	PB-O3B-PG	-2.73	123.45	132.83
3	A	2002	DG3	C6-N1-C2	2.73	120.26	115.93
3	A	2001	DG3	O4'-C4'-C3'	2.71	109.31	104.80
3	B	2001	DG3	PA-O3A-PB	-2.63	123.78	132.83
3	A	2001	DG3	PB-O3B-PG	-2.63	123.81	132.83
3	A	2001	DG3	C5-C6-N1	-2.56	119.94	123.43
3	A	2002	DG3	C5-C6-N1	-2.53	119.97	123.43
3	A	2002	DG3	PA-O3A-PB	-2.51	124.21	132.83
3	B	2002	DG3	C5-C6-N1	-2.50	120.01	123.43
3	B	2001	DG3	C5-C6-N1	-2.49	120.02	123.43
3	B	2002	DG3	O4'-C4'-C3'	2.49	108.94	104.80
3	B	2002	DG3	PA-O3A-PB	-2.45	124.41	132.83
3	A	2001	DG3	PA-O3A-PB	-2.34	124.78	132.83
3	B	2002	DG3	PB-O3B-PG	-2.31	124.89	132.83
3	B	2001	DG3	O4'-C1'-C2'	2.28	109.14	106.67
3	B	2001	DG3	C6-C5-C4	-2.22	118.68	120.80
3	B	2002	DG3	O4'-C1'-C2'	2.17	109.03	106.67
3	B	2002	DG3	C6-C5-C4	-2.16	118.74	120.80
3	A	2002	DG3	O4'-C1'-C2'	2.15	109.00	106.67
3	A	2001	DG3	O4'-C1'-C2'	2.09	108.93	106.67
3	A	2001	DG3	C6-C5-C4	-2.05	118.84	120.80
3	B	2002	DG3	C3'-C2'-C1'	2.04	105.13	102.78

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2002	DG3	PB-O3B-PG-O2G
3	B	2002	DG3	PB-O3B-PG-O3G
3	B	2002	DG3	C5'-O5'-PA-O3A
3	B	2002	DG3	C3'-C4'-C5'-O5'
3	B	2002	DG3	O4'-C4'-C5'-O5'
3	B	2001	DG3	C3'-C4'-C5'-O5'
3	A	2001	DG3	PB-O3A-PA-O5'
3	B	2002	DG3	C5'-O5'-PA-O1A
3	B	2002	DG3	C5'-O5'-PA-O2A
3	B	2002	DG3	PB-O3A-PA-O1A
3	B	2002	DG3	PB-O3B-PG-O1G

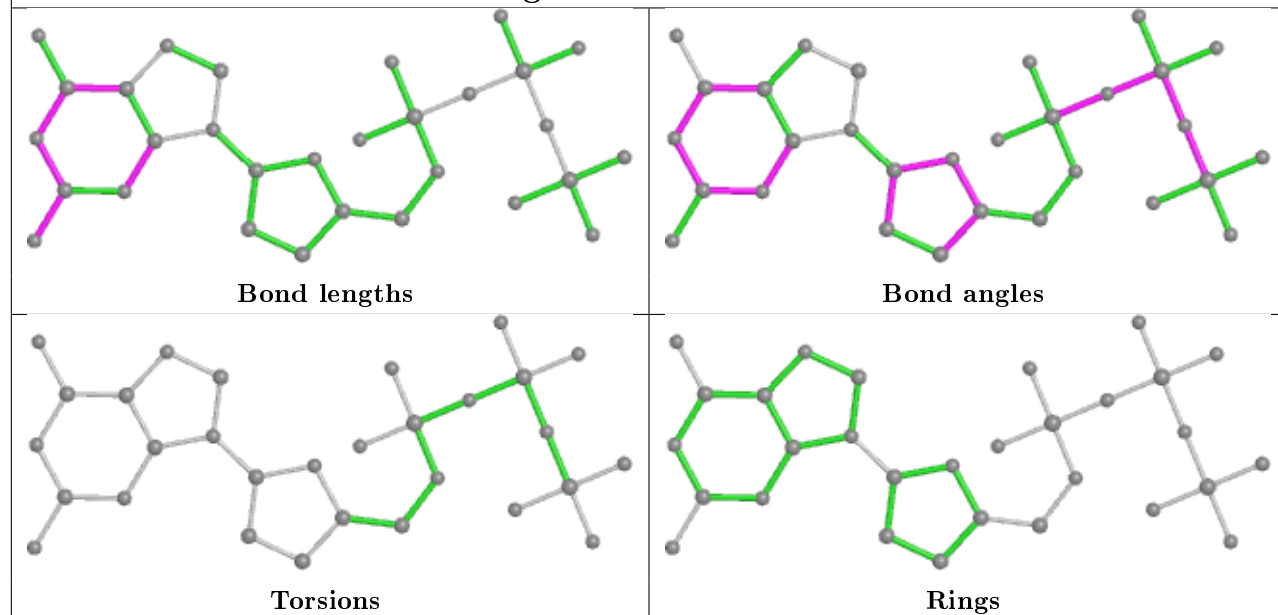
There are no ring outliers.

4 monomers are involved in 8 short contacts:

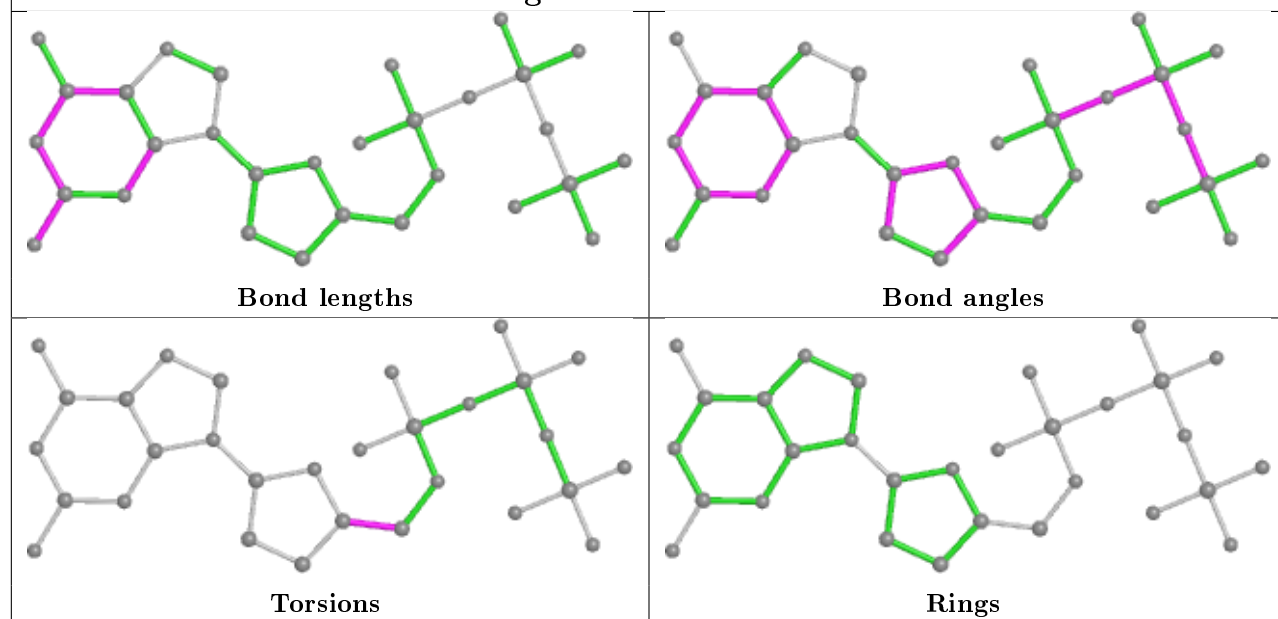
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2002	DG3	1	0
3	B	2001	DG3	2	0
3	A	2001	DG3	1	0
3	B	2002	DG3	4	0

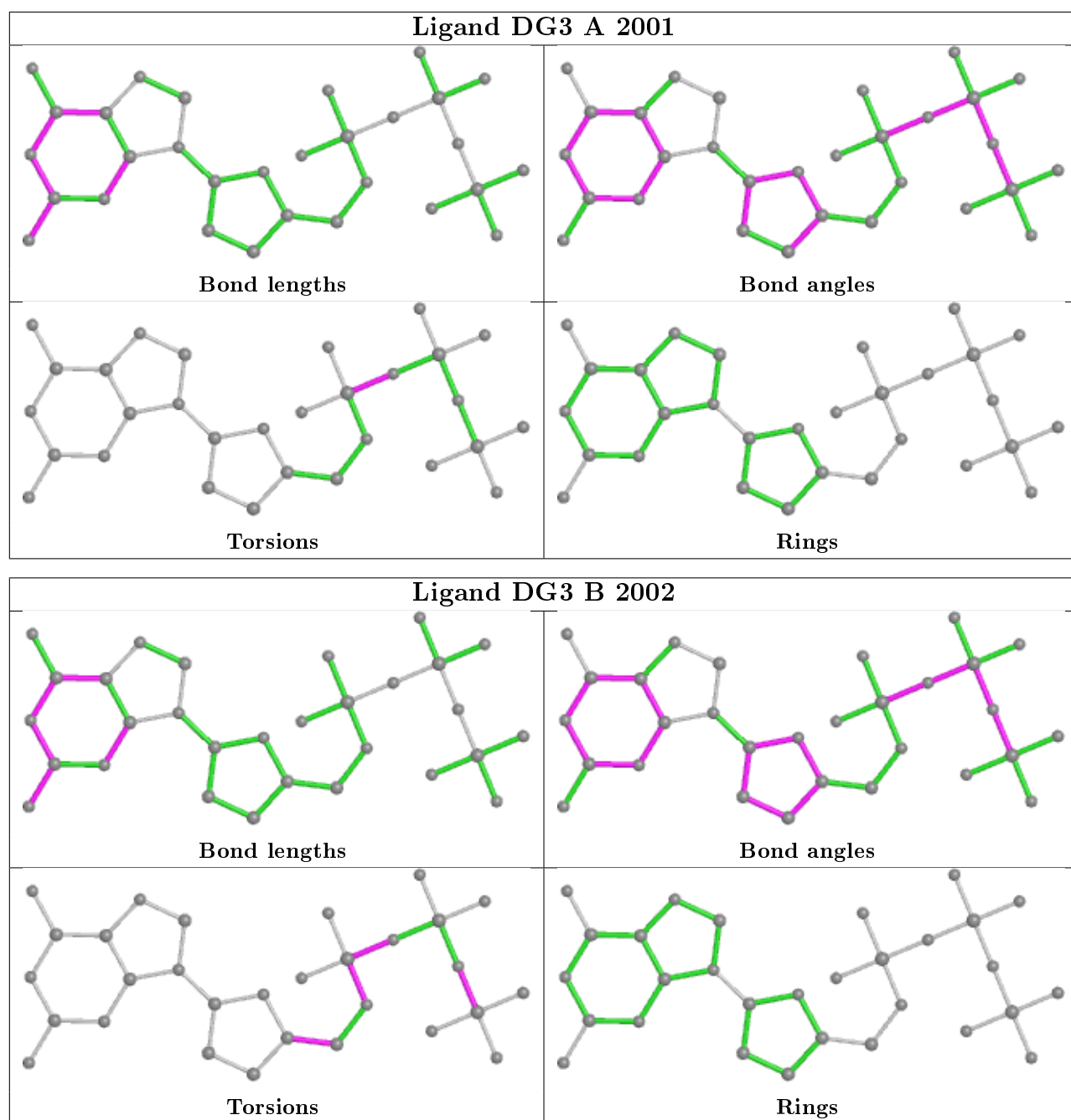
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand DG3 A 2002



Ligand DG3 B 2001





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	439/565 (77%)	-0.05	16 (3%) 42 36	51, 90, 162, 197	0
1	B	435/565 (76%)	-0.05	8 (1%) 68 63	46, 89, 127, 148	0
All	All	874/1130 (77%)	-0.05	24 (2%) 54 46	46, 90, 151, 197	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	463	THR	5.1
1	A	460	THR	4.6
1	A	569	PHE	3.8
1	B	341	CYS	3.6
1	A	462	PRO	3.5
1	A	466	ILE	3.4
1	A	461	GLN	3.4
1	B	477	PRO	3.3
1	A	504	ASN	3.0
1	A	548	GLN	3.0
1	A	575	ASP	3.0
1	A	581	PRO	2.8
1	A	565	ALA	2.8
1	B	565	ALA	2.8
1	A	186	GLN	2.7
1	A	464	GLY	2.7
1	B	259	LEU	2.6
1	B	466	ILE	2.6
1	A	326	GLN	2.4
1	A	328	ASN	2.3
1	B	569	PHE	2.1
1	B	460	THR	2.1
1	B	348	ARG	2.1
1	A	577	ASN	2.0

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 carbohydrates in this entry.

6.4 Ligands [i](#)

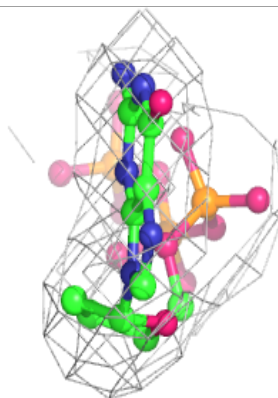
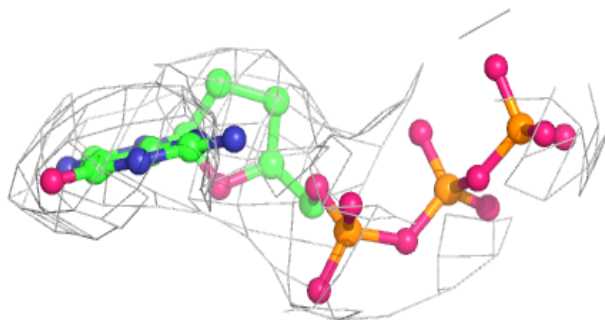
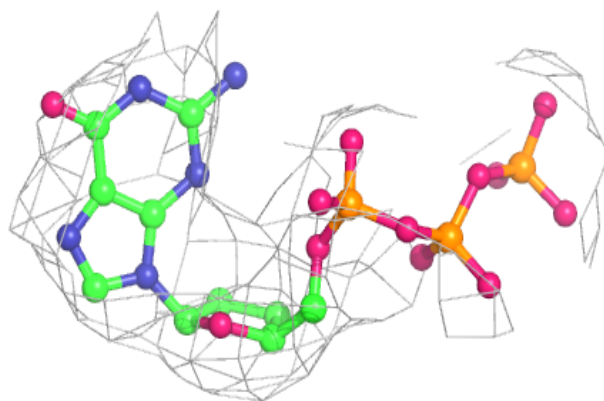
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MG	A	3001	1/1	0.58	0.67	93,93,93,93	0
4	MG	B	3001	1/1	0.82	0.34	65,65,65,65	0
3	DG3	A	2002	30/30	0.94	0.17	47,65,139,141	0
3	DG3	B	2002	30/30	0.94	0.17	65,71,151,163	0
3	DG3	B	2001	30/30	0.94	0.16	55,100,110,165	0
3	DG3	A	2001	30/30	0.95	0.18	69,116,127,188	0
2	FE	A	1001	1/1	0.98	0.12	62,62,62,62	0
2	FE	B	1001	1/1	0.99	0.15	59,59,59,59	0

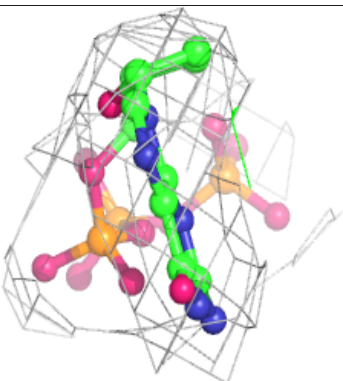
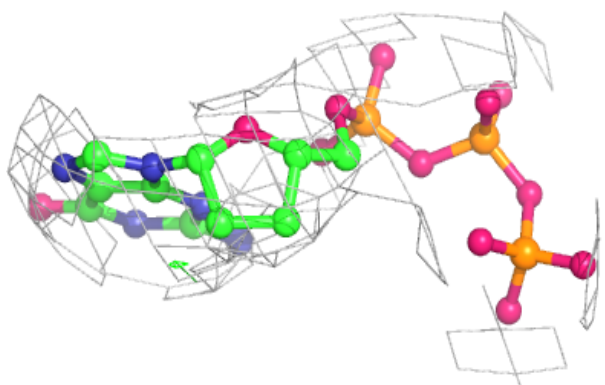
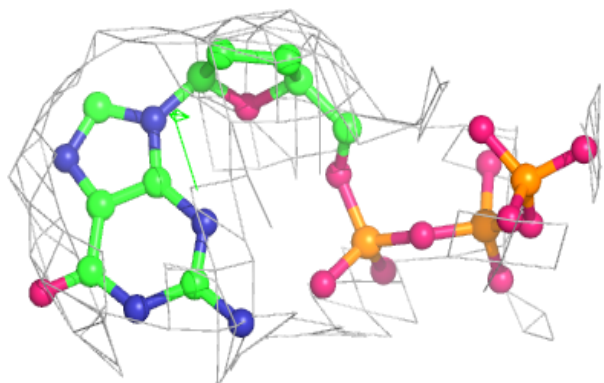
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DG3 A 2002:

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

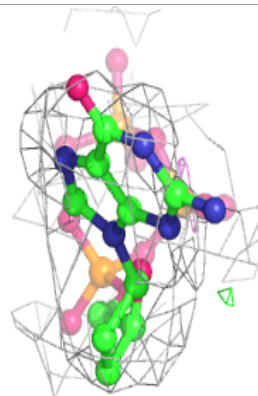
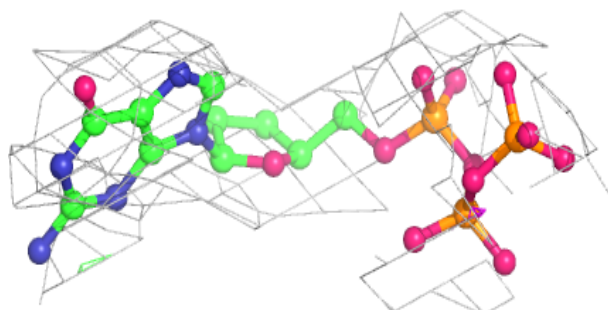
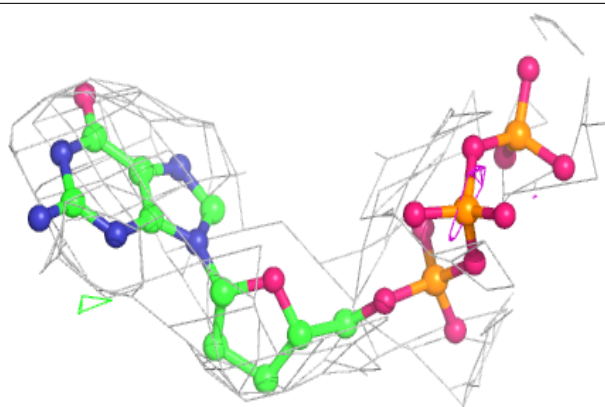
**Electron density around DG3 B 2002:**

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

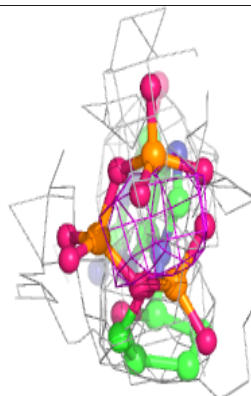
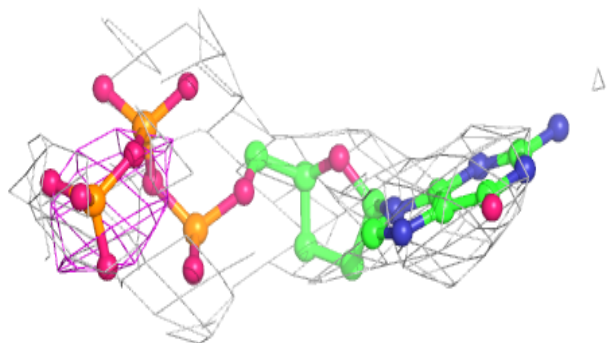
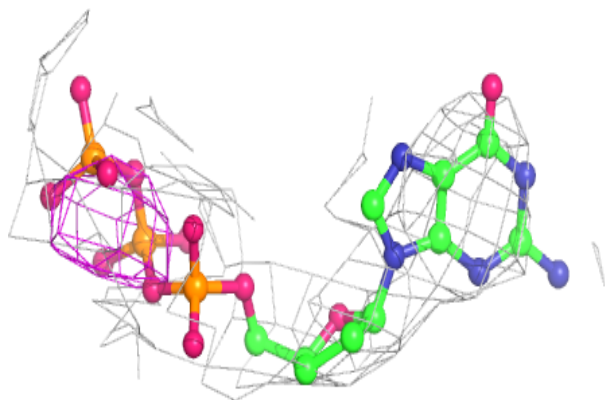


Electron density around DG3 B 2001:

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

**Electron density around DG3 A 2001:**

$2mF_o-DF_c$ (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.