Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2023 – 12:34 AM EDT

PDB ID	:	1XJJ
Title	:	Structural mechanism of allosteric substrate specificity in a ribonucleotide reductase: dGTP complex
Authors	:	Larsson, K.-M.; Jordan, A.; Eliasson, R.; Reichard, P.; Logan, D.T.; Nordlund, P.
Deposited on	:	2004-09-23
Resolution	:	1.86 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

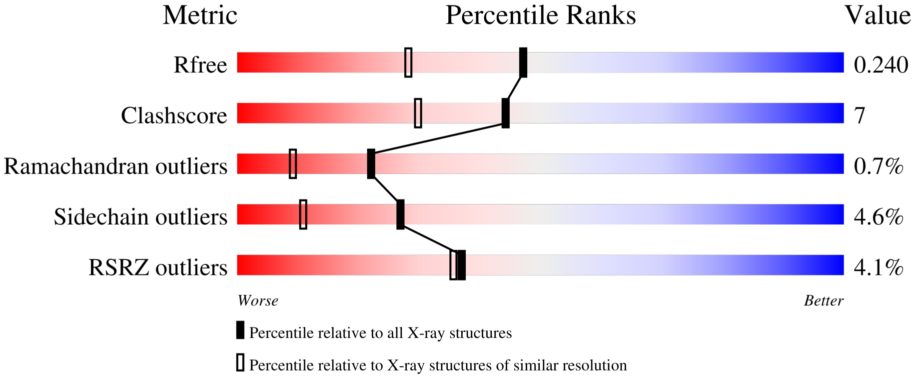
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

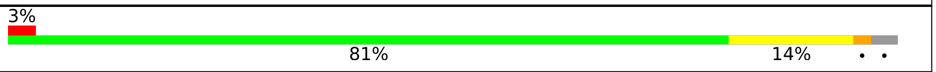
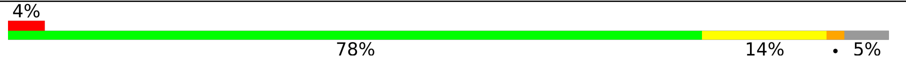
The reported resolution of this entry is 1.86 Å.

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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	644	
1	B	644	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10591 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 ribonucleotide reductase, B12-dependent.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	623	Total 5005	C 3208	N 848	O 929	S 20	0	0	0
1	B	611	Total 4910	C 3149	N 833	O 908	S 20	0	0	0

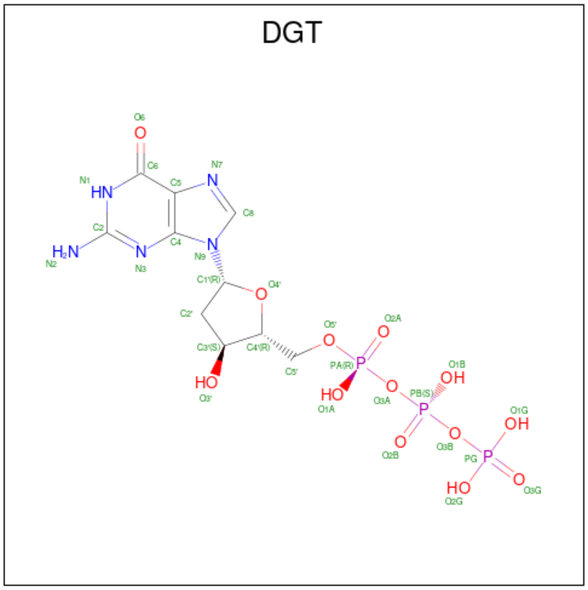
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	205	SER	TYR	SEE REMARK 999	UNP O33839
B	205	SER	TYR	SEE REMARK 999	UNP O33839

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DGT) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 31 10 5 13 3	0	0
3	A	1	Total C N O P 31 10 5 13 3	0	0
3	B	1	Total C N O P 31 10 5 13 3	0	0
3	B	1	Total C N O P 31 10 5 13 3	0	0

- Molecule 4 is water.

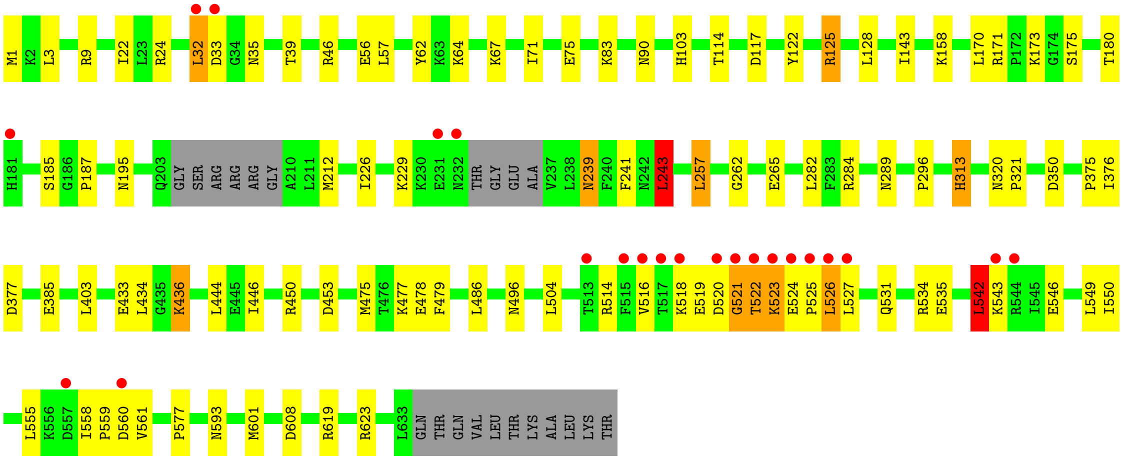
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	292	Total O 292 292	0	0
4	B	258	Total O 258 258	0	0

3 Residue-property plots ⓘ

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.

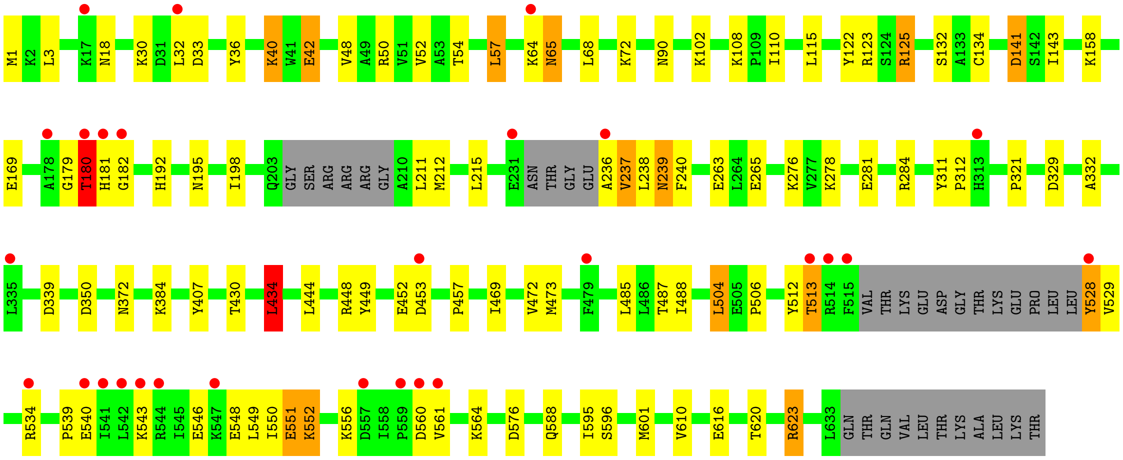
- Molecule 1: ribonucleotide reductase, B12-dependent

Chain A:



- Molecule 1: ribonucleotide reductase, B12-dependent

Chain B:



4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	118.07Å 123.88Å 106.30Å 90.00° 103.70° 90.00°	Depositor
Resolution (Å)	42.26 – 1.86 42.08 – 1.86	Depositor EDS
% Data completeness (in resolution range)	99.9 (42.26-1.86) 99.9 (42.08-1.86)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.196 , 0.241 0.195 , 0.240	Depositor DCC
R_{free} test set	6217 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	25.4	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 45.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10591	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.72% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, DGT

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	0.87	0/5104	0.87	7/6891 (0.1%)
1	B	0.83	0/5007	0.89	7/6758 (0.1%)
All	All	0.85	0/10111	0.88	14/13649 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	623	ARG	NE-CZ-NH1	14.35	127.48	120.30
1	B	623	ARG	NE-CZ-NH2	-12.18	114.21	120.30
1	A	623	ARG	NE-CZ-NH1	-7.38	116.61	120.30
1	A	377	ASP	CB-CG-OD1	6.68	124.31	118.30
1	B	125	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	243	LEU	CB-CG-CD1	5.46	120.27	111.00
1	A	125	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	B	576	ASP	CB-CG-OD1	5.29	123.06	118.30
1	B	329	ASP	CB-CG-OD1	-5.25	113.57	118.30
1	B	141	ASP	CB-CG-OD1	5.20	122.98	118.30
1	A	125	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	403	LEU	CB-CG-CD2	-5.11	102.32	111.00
1	B	434	LEU	CB-CG-CD1	5.07	119.61	111.00
1	A	542	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	237	VAL	Peptide
1	B	560	ASP	Peptide

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	5005	0	5057	64	0
1	B	4910	0	4958	75	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	62	0	24	0	0
3	B	62	0	24	0	0
4	A	292	0	0	6	0
4	B	258	0	0	3	0
All	All	10591	0	10063	133	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 (133) 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:522:THR:HB	1:A:523:LYS:HA	1.41	1.02
1:A:128:LEU:HD13	1:B:179:GLY:HA2	1.47	0.95
1:B:180:THR:HG22	1:B:181:HIS:H	1.30	0.94
1:B:487:THR:O	1:B:488:ILE:HD13	1.64	0.94
1:A:128:LEU:CD1	1:B:179:GLY:HA2	2.00	0.92
1:B:449:TYR:HE1	1:B:473:MET:CE	1.83	0.91
1:B:195:ASN:HD21	1:B:240:PHE:H	1.14	0.87
1:B:449:TYR:HE1	1:B:473:MET:HE1	1.40	0.85
1:B:551:GLU:O	1:B:552:LYS:HB2	1.78	0.81
1:B:512:TYR:O	1:B:513:THR:HG23	1.81	0.80
1:A:542:LEU:O	1:A:546:GLU:HG3	1.87	0.75

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:A:385:GLU:OE1	4:A:1262:HOH:O	2.05	0.75
1:B:64:LYS:O	1:B:65:ASN:HB2	1.88	0.72
1:A:522:THR:CB	1:A:523:LYS:HA	2.18	0.72
1:B:1:MET:HB3	1:B:350:ASP:OD2	1.89	0.72
1:B:239:ASN:H	1:B:239:ASN:HD22	1.37	0.71
1:B:180:THR:HG22	1:B:181:HIS:N	2.04	0.70
1:A:524:GLU:HG2	1:A:525:PRO:HD2	1.74	0.70
1:A:619:ARG:NH1	4:A:1204:HOH:O	2.26	0.69
1:A:241:PHE:HB3	1:A:243:LEU:HD13	1.75	0.69
1:B:457:PRO:HD3	1:B:473:MET:CE	2.24	0.68
1:A:1:MET:HB3	1:A:350:ASP:OD2	1.96	0.66
1:B:180:THR:CG2	1:B:181:HIS:H	2.09	0.65
1:B:623:ARG:HD2	4:B:1017:HOH:O	1.97	0.64
1:B:263:GLU:HG2	1:B:278:LYS:HD3	1.80	0.64
1:A:475:MET:O	1:A:478:GLU:HG2	1.98	0.64
1:B:449:TYR:CE1	1:B:473:MET:CE	2.74	0.63
1:B:122:TYR:O	1:B:125:ARG:HD3	1.99	0.63
1:B:212:MET:HB2	1:B:321:PRO:HA	1.81	0.62
1:B:449:TYR:CE1	1:B:473:MET:HE1	2.30	0.62
1:B:192:HIS:HE1	1:B:236:ALA:O	1.82	0.62
1:A:24:ARG:HH22	1:A:39:THR:HB	1.64	0.62
1:B:449:TYR:HE1	1:B:473:MET:HE3	1.65	0.60
1:A:284:ARG:NH2	1:A:608:ASP:OD1	2.27	0.59
1:B:18:ASN:ND2	1:B:528:TYR:OH	2.35	0.59
1:A:549:LEU:HD13	1:A:555:LEU:HD23	1.84	0.59
1:B:457:PRO:HD3	1:B:473:MET:HE1	1.83	0.59
1:A:226:ILE:HG22	1:A:289:ASN:HD22	1.67	0.58
1:B:539:PRO:O	1:B:540:GLU:HB2	2.03	0.58
1:A:257:LEU:HD22	1:A:262:GLY:HA3	1.85	0.58
1:B:601:MET:HE1	1:B:610:VAL:HG22	1.85	0.58
1:B:64:LYS:HE3	1:B:115:LEU:HD21	1.86	0.58
1:B:449:TYR:CE1	1:B:473:MET:HE3	2.39	0.57
1:A:577:PRO:HG3	1:A:601:MET:HG2	1.86	0.57
1:A:128:LEU:HD11	1:B:179:GLY:HA2	1.84	0.57
1:A:518:LYS:H	1:A:522:THR:CG2	2.18	0.57
1:B:40:LYS:HB3	1:B:40:LYS:NZ	2.20	0.57
1:B:265:GLU:OE1	1:B:276:LYS:HG2	2.05	0.56
1:A:195:ASN:HD21	1:A:239:ASN:ND2	2.04	0.55
1:B:180:THR:CG2	1:B:181:HIS:N	2.67	0.55
1:B:548:GLU:O	1:B:551:GLU:O	2.23	0.55
1:B:40:LYS:NZ	1:B:40:LYS:CB	2.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:GLY:HA3	1:A:522:THR:O	2.06	0.54
1:A:212:MET:HB2	1:A:321:PRO:HA	1.89	0.54
1:B:50:ARG:NH1	1:B:108:LYS:O	2.37	0.54
1:A:229:LYS:HG3	1:A:243:LEU:HD22	1.90	0.54
1:A:313:HIS:HD2	1:A:446:ILE:HD12	1.73	0.53
1:B:64:LYS:O	1:B:65:ASN:CB	2.57	0.53
1:B:601:MET:CE	1:B:610:VAL:HG22	2.39	0.52
1:A:523:LYS:HB3	1:A:524:GLU:HA	1.90	0.52
1:A:239:ASN:HD22	1:A:239:ASN:H	1.57	0.52
1:B:195:ASN:ND2	1:B:240:PHE:H	1.96	0.52
1:B:457:PRO:HD3	1:B:473:MET:HE2	1.93	0.51
1:A:516:VAL:HG23	1:A:526:LEU:HD22	1.94	0.50
1:A:103:HIS:HE1	4:A:1191:HOH:O	1.94	0.50
1:B:134:CYS:O	1:B:332:ALA:HA	2.12	0.50
1:B:488:ILE:HG21	1:B:504:LEU:HG	1.93	0.50
1:A:453:ASP:HA	4:A:1233:HOH:O	2.13	0.49
1:A:433:GLU:CA	1:A:436:LYS:HE3	2.43	0.49
1:B:453:ASP:HA	4:B:1211:HOH:O	2.12	0.49
1:A:128:LEU:HD13	1:B:179:GLY:CA	2.32	0.49
1:B:469:ILE:O	1:B:473:MET:HG2	2.14	0.48
1:B:239:ASN:HD22	1:B:239:ASN:N	2.09	0.48
1:B:430:THR:HG22	1:B:434:LEU:HD22	1.95	0.48
1:A:143:ILE:HG13	1:B:158:LYS:HD2	1.95	0.48
1:B:50:ARG:NH2	1:B:108:LYS:O	2.46	0.48
1:A:433:GLU:HA	1:A:436:LYS:HE3	1.95	0.47
1:A:46:ARG:HH21	1:A:75:GLU:HG2	1.78	0.47
1:A:56:GLU:HB2	1:A:71:ILE:HG12	1.95	0.47
1:B:30:LYS:HE2	1:B:36:TYR:CE1	2.49	0.47
1:B:529:VAL:HB	1:B:534:ARG:NH2	2.30	0.47
1:B:448:ARG:O	1:B:452:GLU:HB2	2.15	0.46
1:A:313:HIS:CD2	1:A:446:ILE:HD12	2.51	0.46
1:A:122:TYR:O	1:A:125:ARG:HD3	2.15	0.46
1:B:311:TYR:CD1	1:B:312:PRO:HA	2.51	0.46
1:A:531:GLN:HE21	1:A:534:ARG:HH21	1.62	0.46
1:A:62:TYR:HB2	1:A:67:LYS:HE3	1.97	0.46
1:B:54:THR:O	1:B:57:LEU:HB2	2.15	0.45
1:A:22:ILE:CD1	1:A:496:ASN:HB3	2.47	0.45
1:B:68:LEU:O	1:B:72:LYS:HG3	2.17	0.45
1:A:320:ASN:HB2	1:A:321:PRO:HD2	1.99	0.44
1:A:375:PRO:C	1:A:376:ILE:HG13	2.38	0.44
1:B:265:GLU:OE2	1:B:276:LYS:HE3	2.17	0.44

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:A:170:LEU:HD12	1:A:187:PRO:HA	1.99	0.44
1:A:450:ARG:HA	1:A:477:LYS:HG3	1.99	0.44
1:B:588:GLN:HB2	1:B:595:ILE:HD12	1.99	0.44
1:A:33:ASP:HB2	1:A:35:ASN:HD22	1.83	0.43
1:B:72:LYS:O	1:B:110:ILE:HD11	2.18	0.43
1:B:237:VAL:HA	1:B:238:LEU:HB2	1.99	0.43
1:A:478:GLU:HG3	1:A:479:PHE:CD2	2.54	0.43
1:A:527:LEU:CD1	1:A:550:ILE:HD11	2.47	0.43
1:A:114:THR:O	1:A:117:ASP:HB2	2.18	0.43
1:A:527:LEU:HD12	1:A:550:ILE:HD11	1.99	0.43
1:B:616:GLU:O	1:B:620:THR:HG23	2.19	0.43
1:A:226:ILE:HG22	1:A:289:ASN:ND2	2.32	0.43
1:B:181:HIS:HB3	1:B:182:GLY:HA2	2.00	0.42
1:A:9:ARG:NH2	4:A:1095:HOH:O	2.52	0.42
1:A:83:LYS:NZ	4:A:1202:HOH:O	2.53	0.42
1:B:384:LYS:HG3	4:B:1123:HOH:O	2.19	0.42
1:A:486:LEU:O	1:A:593:ASN:HB2	2.20	0.42
1:A:523:LYS:H	1:A:524:GLU:CB	2.32	0.42
1:A:313:HIS:N	1:A:313:HIS:ND1	2.68	0.41
1:B:215:LEU:HA	1:B:215:LEU:HD12	1.90	0.41
1:B:546:GLU:O	1:B:550:ILE:HG13	2.19	0.41
1:A:32:LEU:H	1:A:32:LEU:HG	1.69	0.41
1:B:469:ILE:O	1:B:472:VAL:HG12	2.20	0.41
1:B:239:ASN:H	1:B:239:ASN:ND2	2.09	0.41
1:A:173:LYS:HG3	1:A:185:SER:O	2.20	0.41
1:B:339:ASP:OD1	1:B:339:ASP:C	2.59	0.41
1:A:518:LYS:H	1:A:522:THR:HG22	1.85	0.41
1:B:40:LYS:HG3	1:B:42:GLU:HG2	2.02	0.41
1:B:198:ILE:HG13	1:B:211:LEU:HD11	2.03	0.41
1:A:158:LYS:HD2	1:B:143:ILE:HG13	2.03	0.41
1:A:171:ARG:HG3	1:A:175:SER:HB2	2.02	0.41
1:A:518:LYS:O	1:A:522:THR:HG23	2.21	0.41
1:A:22:ILE:HD13	1:A:496:ASN:HB3	2.03	0.41
1:B:588:GLN:CD	1:B:623:ARG:HD3	2.41	0.41
1:A:558:ILE:HA	1:A:559:PRO:HD2	1.96	0.40
1:B:48:VAL:O	1:B:52:VAL:HG23	2.21	0.40
1:B:141:ASP:HB2	1:B:169:GLU:O	2.20	0.40
1:B:132:SER:OG	1:B:372:ASN:ND2	2.53	0.40
1:B:407:TYR:CZ	1:B:506:PRO:HD3	2.56	0.40
1:A:433:GLU:O	1:A:436:LYS:HE3	2.22	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	617/644 (96%)	595 (96%)	20 (3%)	2 (0%)	41	26
1	B	603/644 (94%)	574 (95%)	23 (4%)	6 (1%)	15	5
All	All	1220/1288 (95%)	1169 (96%)	43 (4%)	8 (1%)	22	9

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	65	ASN
1	B	180	THR
1	B	32	LEU
1	B	513	THR
1	B	552	LYS
1	A	522	THR
1	B	556	LYS
1	A	521	GLY

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	550/566 (97%)	523 (95%)	27 (5%)	25	9
1	B	538/566 (95%)	515 (96%)	23 (4%)	29	12
All	All	1088/1132 (96%)	1038 (95%)	50 (5%)	27	11

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	32	LEU
1	A	57	LEU
1	A	64	LYS
1	A	90	ASN
1	A	180	THR
1	A	239	ASN
1	A	243	LEU
1	A	257	LEU
1	A	265	GLU
1	A	282	LEU
1	A	296	PRO
1	A	313	HIS
1	A	434	LEU
1	A	436	LYS
1	A	444	LEU
1	A	504	LEU
1	A	514	ARG
1	A	519	GLU
1	A	520	ASP
1	A	523	LYS
1	A	526	LEU
1	A	535	GLU
1	A	542	LEU
1	A	543	LYS
1	A	560	ASP
1	A	561	VAL
1	B	3	LEU
1	B	33	ASP
1	B	40	LYS
1	B	42	GLU
1	B	57	LEU
1	B	90	ASN
1	B	102	LYS
1	B	123	ARG
1	B	180	THR
1	B	239	ASN
1	B	281	GLU
1	B	284	ARG
1	B	434	LEU
1	B	444	LEU
1	B	485	LEU
1	B	504	LEU

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Mol	Chain	Res	Type
1	B	528	TYR
1	B	543	LYS
1	B	549	LEU
1	B	551	GLU
1	B	561	VAL
1	B	564	LYS
1	B	596	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	127	HIS
1	A	181	HIS
1	A	239	ASN
1	A	345	ASN
1	A	355	GLN
1	A	359	GLN
1	A	531	GLN
1	A	584	GLN
1	A	603	GLN
1	B	18	ASN
1	B	127	HIS
1	B	192	HIS
1	B	195	ASN
1	B	239	ASN
1	B	345	ASN
1	B	346	ASN
1	B	359	GLN
1	B	464	ASN
1	B	584	GLN
1	B	603	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 2 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 $\lvert Z\rvert > 2$ 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	$\#\lvert Z\rvert > 2$	Counts	RMSZ	$\#\lvert Z\rvert > 2$
3	DGT	B	1004	-	26,33,33	1.39	3 (11%)	32,52,52	1.50	7 (21%)
3	DGT	B	1002	2	26,33,33	1.62	2 (7%)	32,52,52	2.06	8 (25%)
3	DGT	A	1003	-	26,33,33	1.34	3 (11%)	32,52,52	1.86	11 (34%)
3	DGT	A	1001	2	26,33,33	1.71	4 (15%)	32,52,52	1.63	8 (25%)

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	DGT	B	1004	-	-	3/18/34/34	0/3/3/3
3	DGT	B	1002	2	-	1/18/34/34	0/3/3/3
3	DGT	A	1003	-	-	4/18/34/34	0/3/3/3
3	DGT	A	1001	2	-	2/18/34/34	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	DGT	C5-C6	-5.01	1.37	1.47
3	B	1002	DGT	C5-C6	-4.36	1.38	1.47
3	B	1002	DGT	PG-O3G	3.98	1.63	1.50
3	B	1004	DGT	PG-O3G	3.42	1.61	1.50
3	B	1004	DGT	C5-C6	-3.33	1.40	1.47
3	A	1003	DGT	C5-C6	-3.32	1.40	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1003	DGT	C6-N1	3.08	1.42	1.37
3	B	1004	DGT	C6-N1	2.89	1.42	1.37
3	A	1001	DGT	PG-O3G	2.79	1.59	1.50
3	A	1001	DGT	PG-O1G	-2.45	1.45	1.54
3	A	1003	DGT	PG-O3G	2.29	1.57	1.50
3	A	1001	DGT	C2-N1	2.23	1.43	1.37

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1002	DGT	C2'-C1'-N9	-5.31	102.02	114.27
3	B	1002	DGT	PA-O3A-PB	-4.62	116.98	132.83
3	B	1002	DGT	O6-C6-N1	-4.37	115.49	120.65
3	A	1003	DGT	O4'-C4'-C5'	-3.93	96.43	109.37
3	B	1002	DGT	O2G-PG-O1G	3.32	120.33	107.64
3	A	1001	DGT	O2G-PG-O1G	3.21	119.90	107.64
3	A	1001	DGT	C2-N1-C6	-3.20	119.20	125.10
3	A	1003	DGT	C5-C6-N1	3.18	119.57	113.95
3	A	1003	DGT	C2-N1-C6	-3.17	119.26	125.10
3	B	1004	DGT	C2-N1-C6	-3.11	119.38	125.10
3	A	1003	DGT	O2G-PG-O3B	3.09	115.01	104.64
3	A	1003	DGT	C8-N7-C5	3.06	108.81	102.99
3	B	1004	DGT	C4'-O4'-C1'	-3.04	102.11	109.45
3	A	1003	DGT	PB-O3B-PG	-2.92	122.81	132.83
3	B	1004	DGT	O2G-PG-O1G	2.84	118.47	107.64
3	A	1001	DGT	C2'-C1'-N9	-2.83	107.75	114.27
3	A	1001	DGT	C5-C6-N1	2.80	118.91	113.95
3	B	1004	DGT	C5-C6-N1	2.76	118.82	113.95
3	B	1002	DGT	O4'-C1'-C2'	-2.73	101.10	106.25
3	B	1002	DGT	PB-O3B-PG	-2.71	123.52	132.83
3	A	1003	DGT	O2G-PG-O1G	2.66	117.80	107.64
3	B	1004	DGT	C8-N7-C5	2.59	107.92	102.99
3	B	1002	DGT	C5-C6-N1	2.51	118.38	113.95
3	A	1001	DGT	PA-O3A-PB	-2.43	124.47	132.83
3	A	1001	DGT	O6-C6-C5	-2.43	119.62	124.37
3	B	1002	DGT	C2-N1-C6	-2.39	120.70	125.10
3	A	1003	DGT	O3B-PG-O3G	-2.34	98.20	111.19
3	A	1001	DGT	C8-N7-C5	2.25	107.27	102.99
3	A	1003	DGT	C4'-O4'-C1'	-2.23	104.08	109.45
3	B	1004	DGT	O4'-C1'-C2'	-2.18	102.14	106.25
3	B	1004	DGT	O1A-PA-O2A	2.06	122.43	112.24
3	A	1003	DGT	N1-C2-N3	-2.06	119.47	123.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1001	DGT	O5'-C5'-C4'	2.04	116.00	108.99
3	A	1003	DGT	O1B-PB-O2B	2.01	122.20	112.24

There are no chirality outliers.

All (10) torsion outliers are listed below:

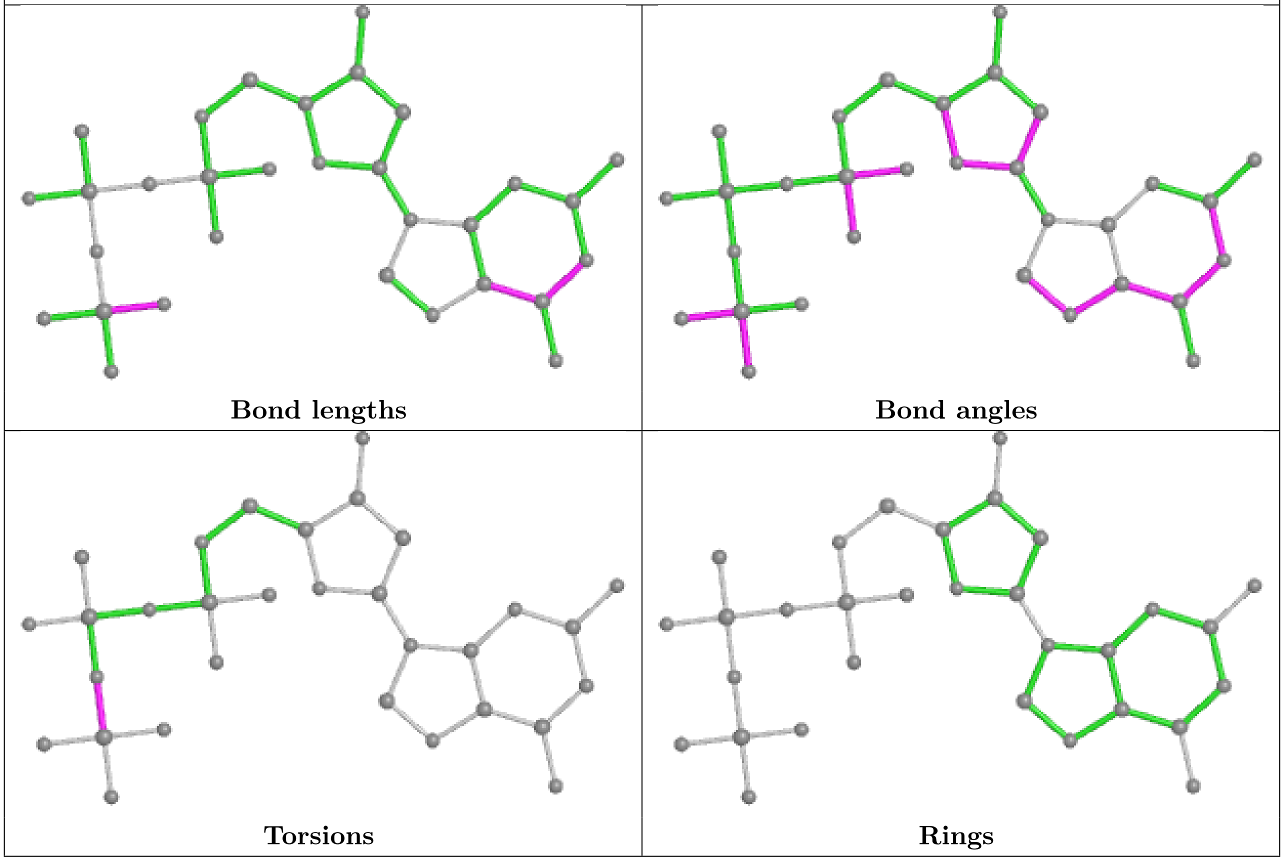
Mol	Chain	Res	Type	Atoms
3	A	1003	DGT	PB-O3B-PG-O2G
3	B	1004	DGT	PB-O3B-PG-O1G
3	B	1004	DGT	PB-O3B-PG-O2G
3	A	1001	DGT	PB-O3B-PG-O2G
3	B	1002	DGT	PB-O3B-PG-O2G
3	A	1001	DGT	PA-O3A-PB-O2B
3	A	1003	DGT	PB-O3A-PA-O2A
3	B	1004	DGT	PB-O3B-PG-O3G
3	A	1003	DGT	PB-O3B-PG-O1G
3	A	1003	DGT	PB-O3B-PG-O3G

There are no ring outliers.

No monomer is involved in short contacts.

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

Ligand DGT B 1004



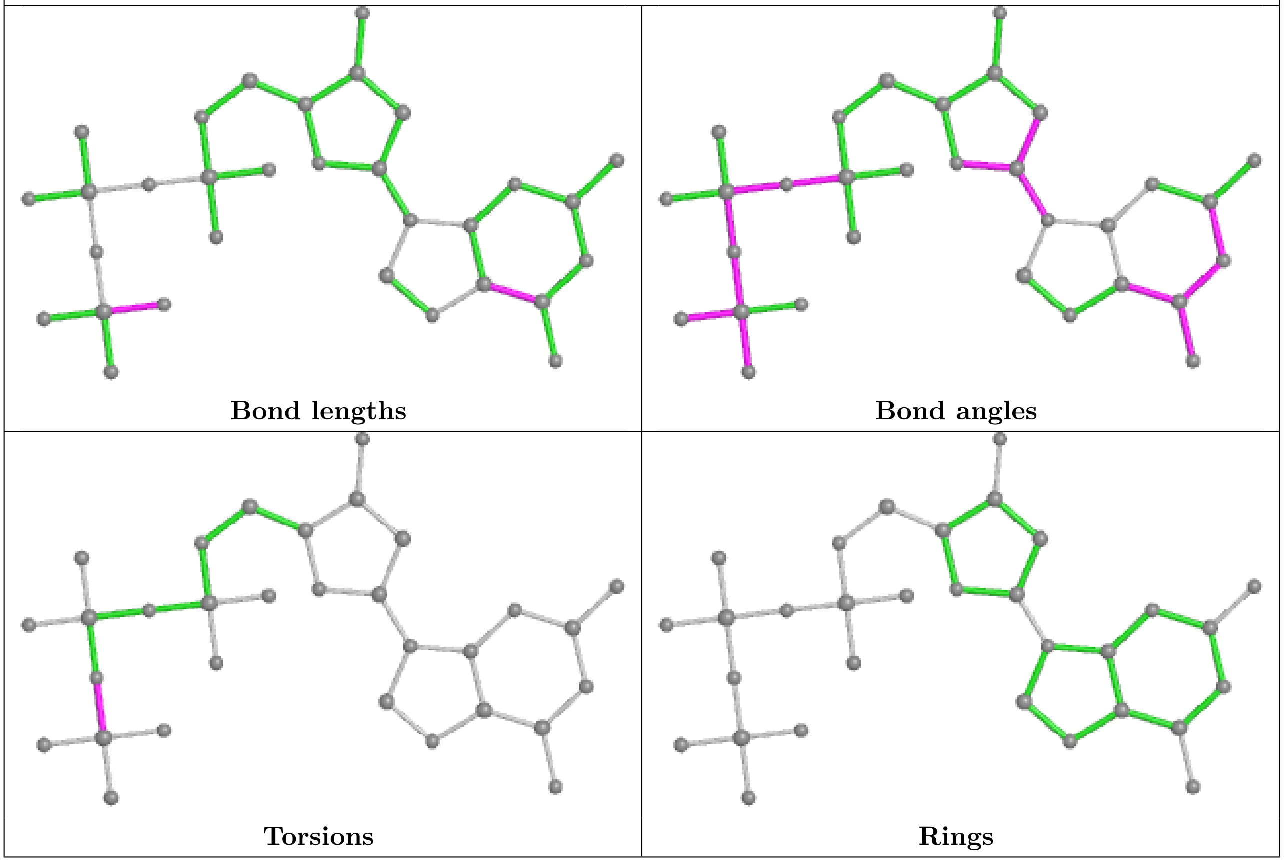
Bond lengths

Bond angles

Torsions

Rings

Ligand DGT B 1002



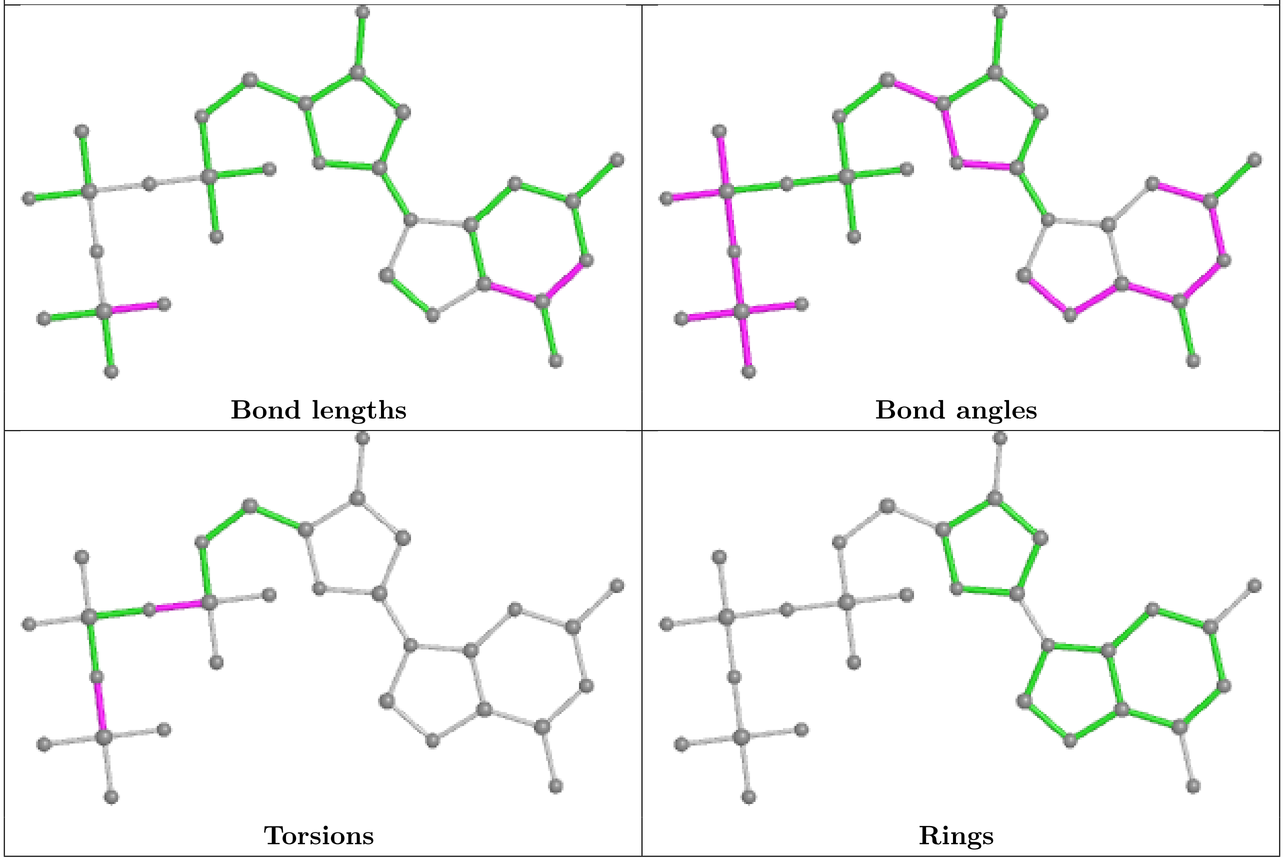
Bond lengths

Bond angles

Torsions

Rings

Ligand DGT A 1003



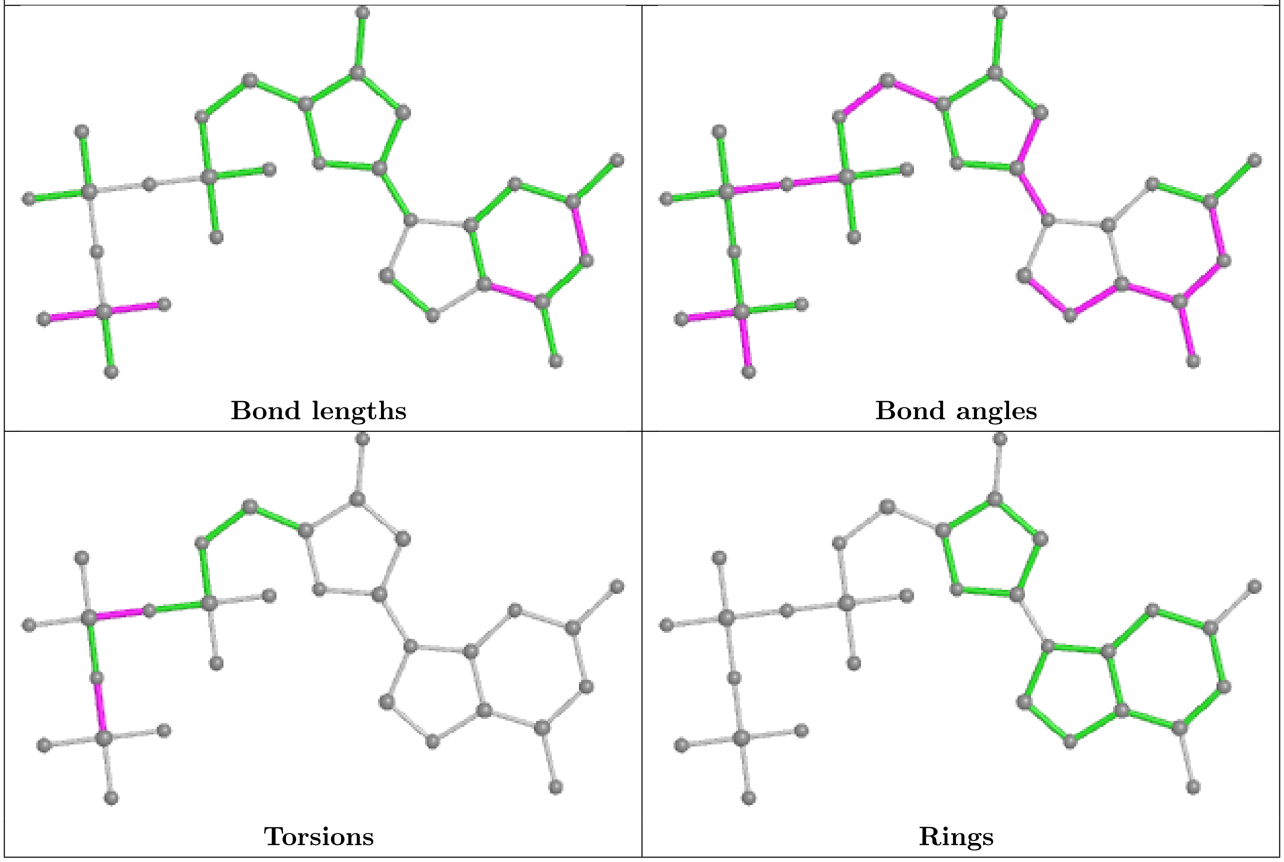
Bond lengths

Bond angles

Torsions

Rings

Ligand DGT A 1001



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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	623/644 (96%)	-0.13	22 (3%)	44	41	15, 27, 56, 88	0
1	B	611/644 (94%)	-0.01	28 (4%)	32	31	17, 29, 59, 75	0
All	All	1234/1288 (95%)	-0.07	50 (4%)	37	35	15, 28, 58, 88	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	521	GLY	6.8
1	A	516	VAL	6.3
1	B	236	ALA	5.7
1	A	523	LYS	5.6
1	A	517	THR	5.2
1	A	522	THR	4.9
1	A	515	PHE	4.8
1	A	520	ASP	4.5
1	B	515	PHE	4.4
1	B	559	PRO	4.3
1	A	526	LEU	4.1
1	A	524	GLU	4.0
1	B	181	HIS	4.0
1	A	560	ASP	3.9
1	B	528	TYR	3.8
1	A	527	LEU	3.6
1	A	525	PRO	3.4
1	B	453	ASP	3.2
1	A	232	ASN	3.1
1	B	231	GLU	3.0
1	B	182	GLY	2.9
1	B	547	LYS	2.9
1	B	514	ARG	2.8
1	A	32	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	231	GLU	2.7
1	B	540	GLU	2.7
1	B	180	THR	2.6
1	B	64	LYS	2.6
1	B	561	VAL	2.6
1	B	557	ASP	2.6
1	B	544	ARG	2.5
1	A	33	ASP	2.5
1	A	518	LYS	2.5
1	B	32	LEU	2.4
1	B	560	ASP	2.4
1	B	543	LYS	2.3
1	A	513	THR	2.3
1	B	513	THR	2.2
1	A	181	HIS	2.2
1	A	557	ASP	2.2
1	B	541	ILE	2.2
1	B	542	LEU	2.1
1	B	534	ARG	2.1
1	A	543	LYS	2.1
1	A	544	ARG	2.1
1	B	313	HIS	2.1
1	B	479	PHE	2.0
1	B	17	LYS	2.0
1	B	178	ALA	2.0
1	B	335	LEU	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)

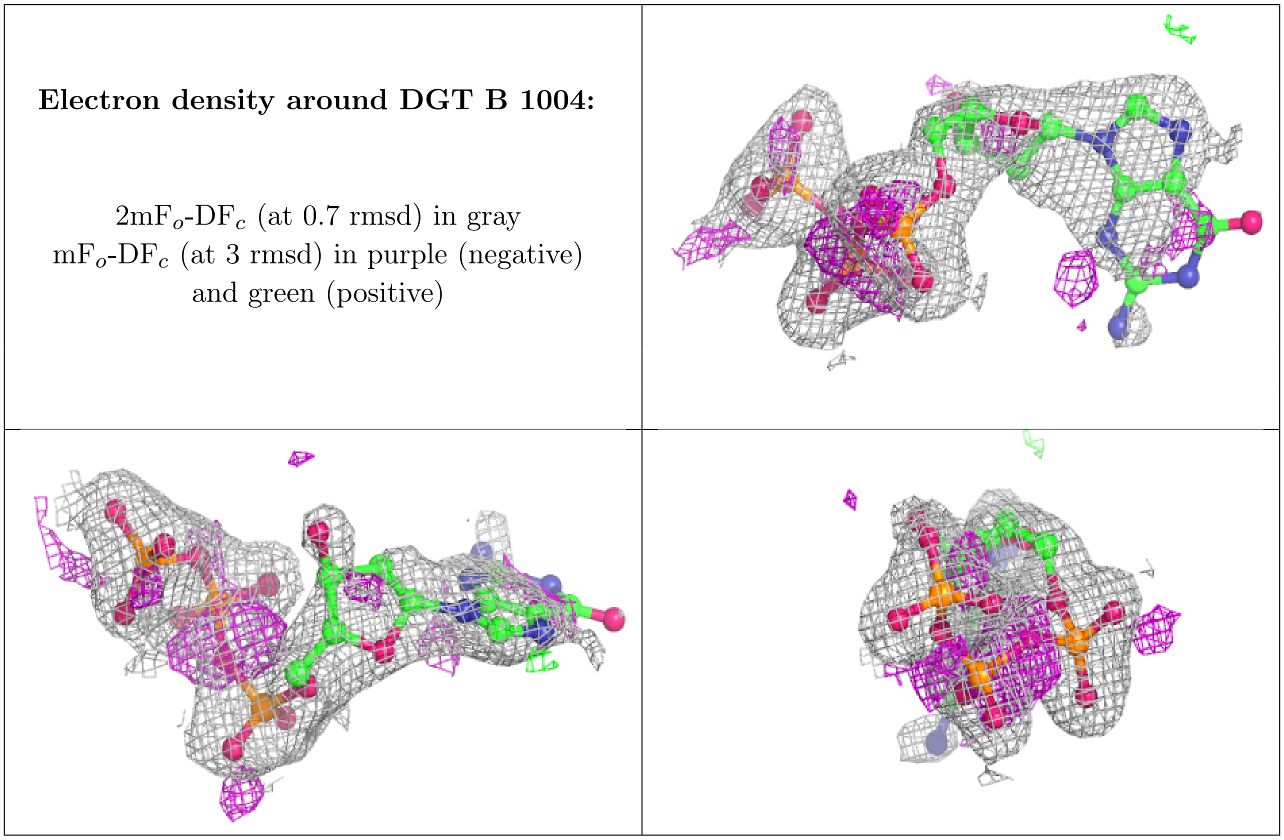
There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	DGT	B	1004	31/31	0.93	0.14	33,62,73,74	0
3	DGT	A	1003	31/31	0.94	0.14	26,63,75,75	0
2	MG	B	1005	1/1	0.95	0.08	36,36,36,36	0
3	DGT	B	1002	31/31	0.96	0.08	14,21,44,44	0
3	DGT	A	1001	31/31	0.98	0.06	17,25,32,34	0
2	MG	A	1006	1/1	0.99	0.02	26,26,26,26	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.

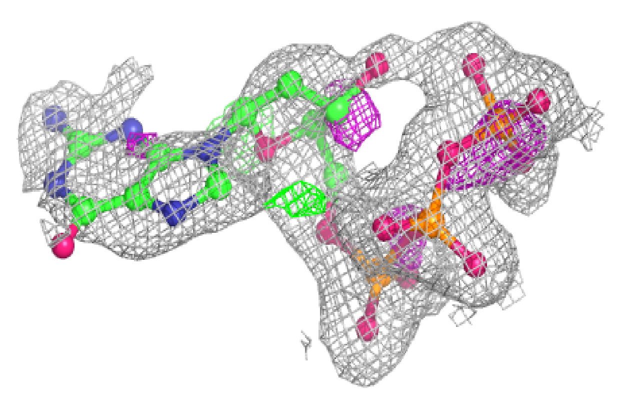


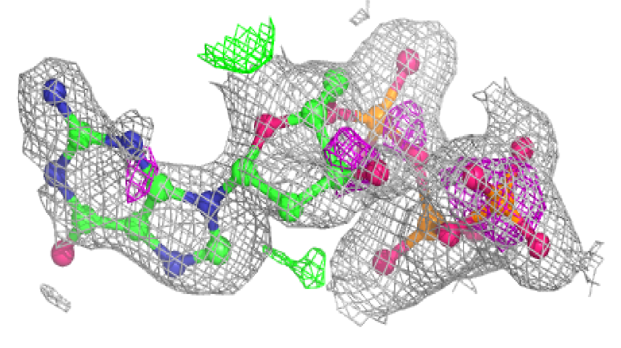
Electron density around DGT B 1004:

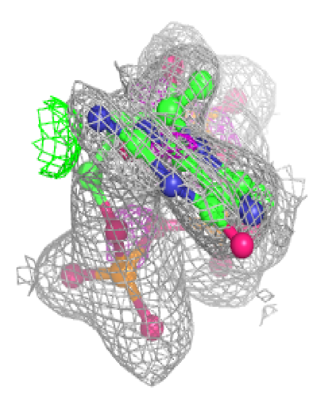
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around DGT A 1003:

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

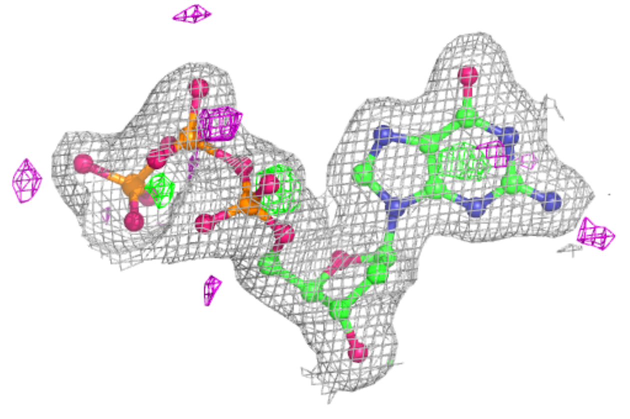


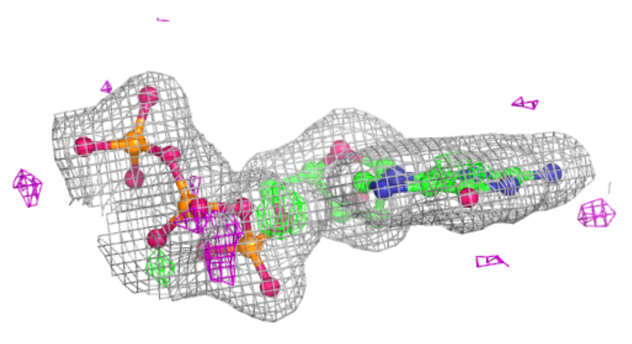


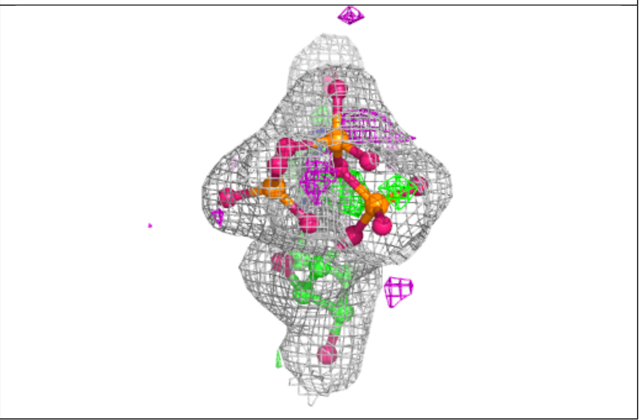


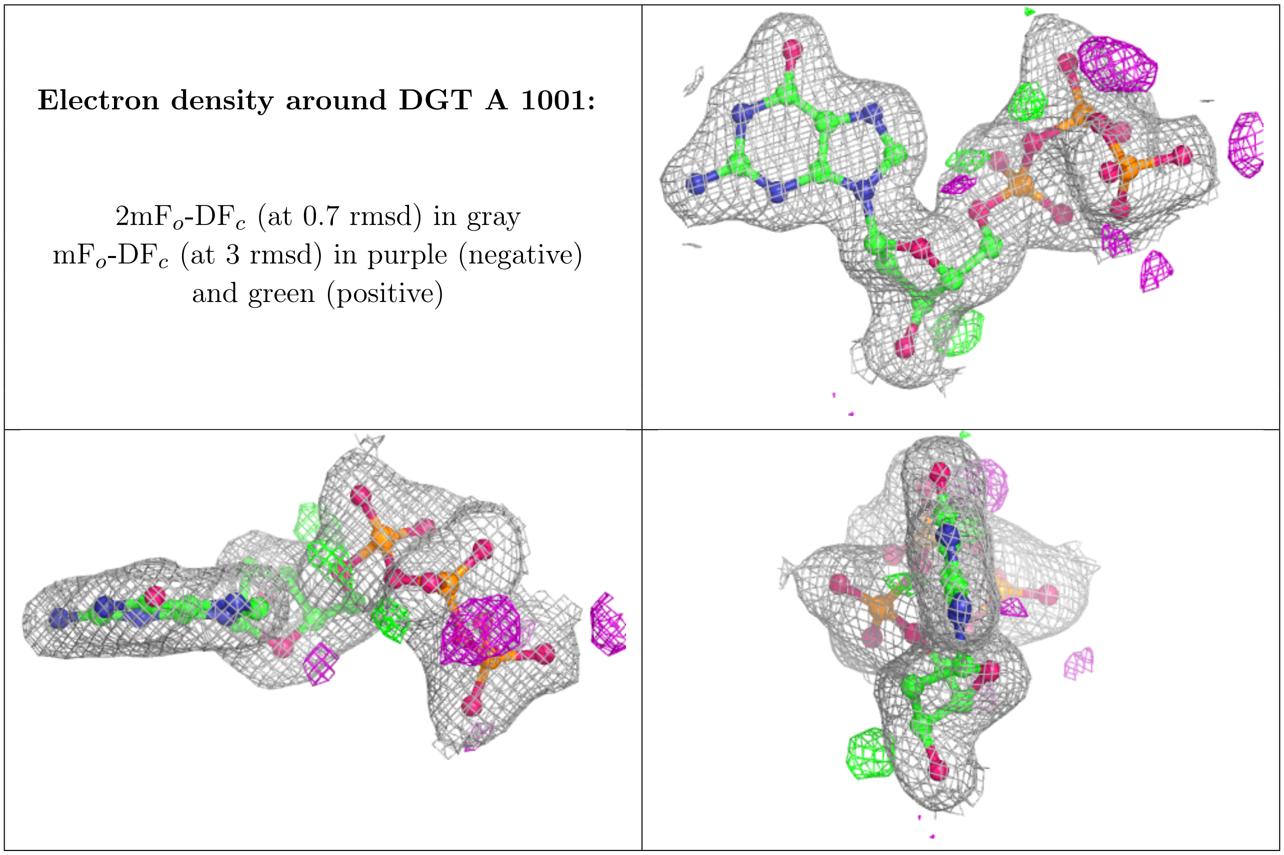
Electron density around DGT B 1002:

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 DGT A 1001:

$2mF_o$-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.