



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 07:19 pm BST

PDB ID : 3K8T  
Title : Structure of eukaryotic rnr large subunit R1 complexed with designed adp analog compound  
Authors : Sun, D.; Xu, H.; Dealwis, C.; Lee, R.E.  
Deposited on : 2009-10-14  
Resolution : 2.10 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](mailto: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.

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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

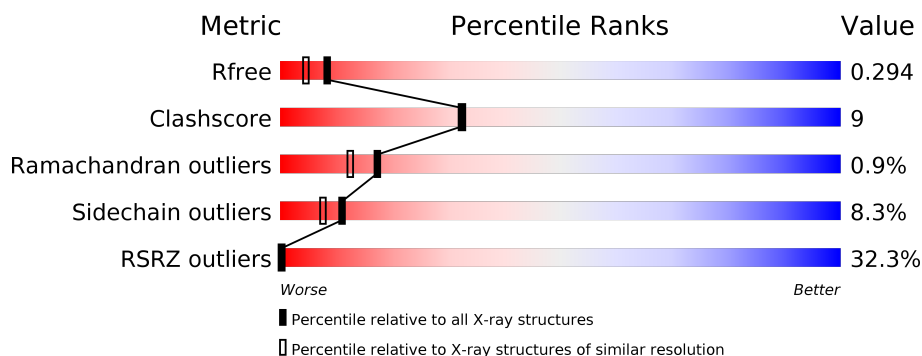
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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  $\geq 3$ , 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	888	<div> <div>23%</div> <div>55%</div> <div>14%</div> <div>•</div> <div>28%</div> </div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5322 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.

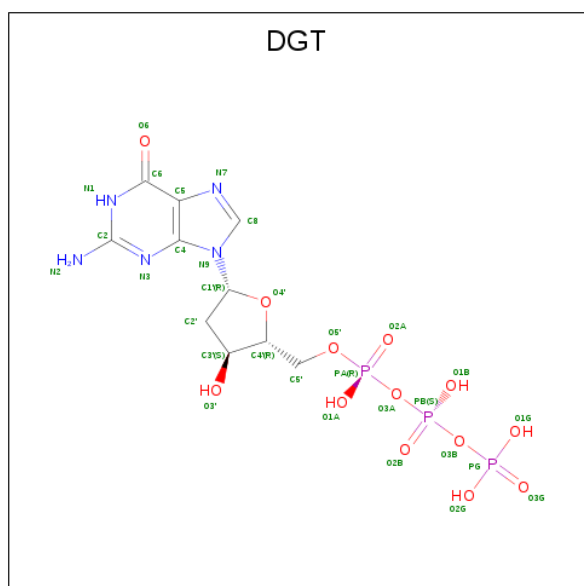
- Molecule 1 is a protein called Ribonucleoside-diphosphate reductase large chain 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	640	Total	C	N	O	S	0	0	0
			5120	3266	866	957	31			

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

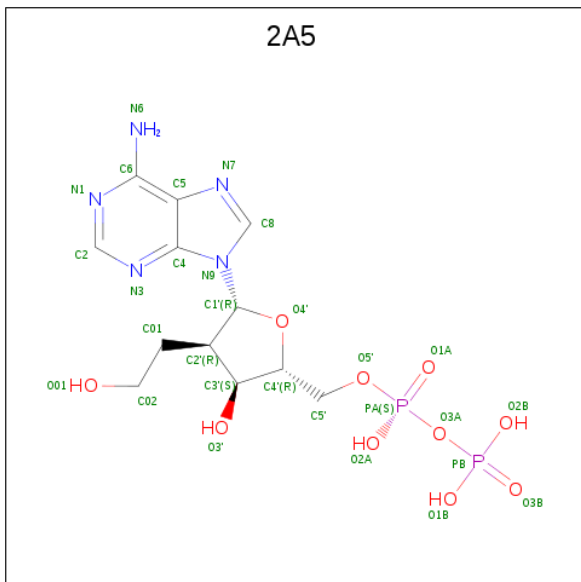
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DGT) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



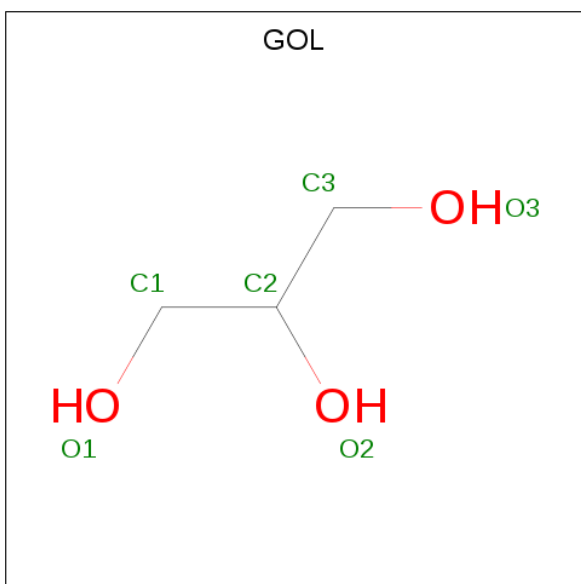
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is 2'-deoxy-2'-(2-hydroxyethyl)adenosine 5'-(trihydrogen diphosphate) (three-letter code: 2A5) (formula:  $C_{12}H_{19}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			29	12	5	10	2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	135	Total 135	O 135	0	0



TYR  
ASN  
SER  
LYS  
VAL  
ILE  
ALA  
CYS  
ALA  
ILE  
ASP  
ASN  
PRO  
GLU  
ALA  
CYS  
GLU  
MET  
CYS  
SER  
GLY

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.53Å 116.92Å 64.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.84 – 2.10 38.84 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.3 (38.84-2.10) 99.3 (38.84-2.10)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.42 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0007	Depositor
R, $R_{free}$	0.252 , 0.290 0.254 , 0.294	Depositor DCC
$R_{free}$ test set	2409 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.8	Xtriage
Anisotropy	0.421	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 64.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5322	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.89% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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: GOL, MG, 2A5, 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	0.77	1/5238 (0.0%)	0.97	25/7089 (0.4%)

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	A	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	707	ASP	CB-CG	-8.16	1.34	1.51

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	707	ASP	CB-CG-OD1	-15.32	104.51	118.30
1	A	707	ASP	CB-CG-OD2	11.93	129.04	118.30
1	A	226	ASP	CB-CG-OD2	8.49	125.94	118.30
1	A	365	ASP	CB-CG-OD2	8.16	125.64	118.30
1	A	182	ASP	CB-CG-OD2	7.72	125.24	118.30
1	A	233	ASP	CB-CG-OD2	7.13	124.72	118.30
1	A	324	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	A	379	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	A	586	ASP	CB-CG-OD2	6.40	124.06	118.30
1	A	100	ASP	CB-CG-OD2	6.30	123.97	118.30
1	A	707	ASP	N-CA-C	6.13	127.55	111.00
1	A	361	ASP	CB-CG-OD2	6.12	123.81	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	379	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	A	573	ASP	CB-CG-OD2	6.00	123.70	118.30
1	A	520	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	A	170	LEU	CA-CB-CG	5.89	128.85	115.30
1	A	287	ASP	CB-CG-OD2	5.85	123.56	118.30
1	A	118	ASP	CB-CG-OD2	5.75	123.47	118.30
1	A	576	ASP	CB-CG-OD2	5.63	123.37	118.30
1	A	140	ASP	CB-CG-OD2	5.54	123.29	118.30
1	A	524	ASP	CB-CG-OD2	5.42	123.17	118.30
1	A	324	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	A	648	ASP	CB-CG-OD2	5.34	123.10	118.30
1	A	138	ASP	CB-CG-OD2	5.21	122.98	118.30
1	A	220	LEU	CA-CB-CG	5.06	126.93	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	318	HIS	Peptide
1	A	319	GLY	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	5120	0	5055	90	0
2	A	1	0	0	0	0
3	A	31	0	12	0	0
4	A	29	0	16	8	0
5	A	6	0	8	0	0
6	A	135	0	0	7	0
All	All	5322	0	5091	90	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 9.

All (90) 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:426:ASN:HD22	4:A:891:2A5:H02	1.15	1.11
1:A:686:THR:HG21	6:A:985:HOH:O	1.74	0.86
1:A:426:ASN:HD22	4:A:891:2A5:C02	1.88	0.85
1:A:482:ASN:OD1	1:A:503:ARG:NH1	2.11	0.84
1:A:364:GLY:O	1:A:368:GLU:HG3	1.87	0.75
1:A:191:ASN:HB3	6:A:973:HOH:O	1.87	0.75
1:A:534:GLN:O	1:A:538:THR:HG22	1.88	0.74
1:A:251:HIS:HD2	6:A:896:HOH:O	1.73	0.71
1:A:502:HIS:ND1	1:A:559:THR:HG21	2.07	0.69
1:A:538:THR:HB	1:A:583:TRP:NE1	2.08	0.69
1:A:426:ASN:ND2	4:A:891:2A5:H02	1.99	0.69
1:A:126:GLU:OE2	1:A:181:ARG:NH1	2.18	0.68
1:A:505:ILE:HG22	1:A:602:THR:HA	1.76	0.67
1:A:606:MET:HE1	6:A:895:HOH:O	1.96	0.64
1:A:220:LEU:HD21	1:A:426:ASN:HB3	1.78	0.64
1:A:662:TYR:CE1	1:A:666:GLN:HG3	2.34	0.63
1:A:245:ALA:HA	1:A:288:GLN:HE21	1.64	0.62
1:A:560:PHE:CZ	1:A:596:GLY:HA2	2.34	0.62
1:A:106:ASN:OD1	1:A:109:THR:HG22	2.00	0.61
1:A:538:THR:HB	1:A:583:TRP:HE1	1.65	0.61
1:A:485:ILE:HD11	1:A:505:ILE:HD12	1.83	0.61
1:A:467:PHE:CZ	1:A:534:GLN:HG3	2.38	0.59
1:A:145:TYR:OH	1:A:640:VAL:HG11	2.02	0.59
1:A:716:LEU:HD21	1:A:723:LYS:HG2	1.85	0.58
1:A:109:THR:HG23	1:A:111:LYS:H	1.69	0.57
1:A:428:CYS:SG	4:A:891:2A5:H3'	2.44	0.57
1:A:510:GLN:OE1	1:A:612:SER:HA	2.05	0.57
1:A:426:ASN:ND2	4:A:891:2A5:C02	2.62	0.56
1:A:564:PRO:HG2	1:A:574:MET:HE1	1.88	0.56
1:A:447:SER:HB3	1:A:606:MET:HE3	1.87	0.55
1:A:401:THR:HB	1:A:402:PRO:HA	1.89	0.55
1:A:524:ASP:OD2	1:A:685:LYS:NZ	2.30	0.55
1:A:220:LEU:CD2	1:A:426:ASN:HB3	2.37	0.54
1:A:316:LYS:HD3	1:A:318:HIS:CE1	2.44	0.52
1:A:557:TYR:HE1	1:A:559:THR:HG23	1.75	0.52
1:A:486:ASP:OD1	1:A:503:ARG:NH2	2.43	0.51
1:A:454:ILE:HD13	1:A:518:LEU:HB3	1.91	0.51
1:A:481:LEU:CB	1:A:505:ILE:HG12	2.41	0.51
1:A:251:HIS:HE1	1:A:435:SER:OG	1.95	0.50
1:A:661:GLN:C	1:A:663:LEU:H	2.15	0.50
1:A:713:ASN:HD22	1:A:742:TYR:H	1.60	0.50
1:A:714:LEU:HD22	1:A:740:MET:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:686:THR:CG2	6:A:985:HOH:O	2.45	0.49
1:A:606:MET:HE2	1:A:608:THR:CG2	2.43	0.49
1:A:509:VAL:O	1:A:620:CYS:HA	2.13	0.48
1:A:663:LEU:HD11	1:A:670:ILE:HG22	1.94	0.48
1:A:649:LEU:HD13	1:A:655:TRP:CE3	2.49	0.47
1:A:168:GLN:NE2	1:A:190:TYR:OH	2.44	0.47
1:A:520:ARG:HH22	1:A:648:ASP:CG	2.17	0.47
1:A:273:ILE:HD12	1:A:314:ILE:HD11	1.96	0.47
1:A:439:GLU:OE2	1:A:497:LYS:NZ	2.47	0.47
1:A:481:LEU:HB2	1:A:505:ILE:HG12	1.95	0.47
1:A:170:LEU:HD22	1:A:173:ARG:NH2	2.31	0.46
1:A:702:ARG:HH11	1:A:710:HIS:CE1	2.33	0.46
1:A:606:MET:HE2	1:A:608:THR:HG23	1.98	0.46
1:A:450:LEU:N	1:A:451:PRO:CD	2.80	0.45
1:A:444:ASN:N	1:A:444:ASN:ND2	2.64	0.45
1:A:312:ILE:HD13	1:A:392:ILE:HD13	1.98	0.45
1:A:427:LEU:HB3	4:A:891:2A5:H02A	1.99	0.45
1:A:557:TYR:CE1	1:A:559:THR:HG23	2.52	0.44
1:A:642:ASN:HB3	1:A:645:LEU:HB3	1.99	0.44
1:A:276:ILE:HD13	1:A:276:ILE:N	2.33	0.44
1:A:140:ASP:OD2	1:A:168:GLN:HG2	2.19	0.43
1:A:662:TYR:CD1	1:A:666:GLN:HG3	2.54	0.43
1:A:686:THR:HG22	1:A:688:TRP:H	1.84	0.43
1:A:713:ASN:ND2	1:A:742:TYR:H	2.17	0.43
1:A:445:LEU:CD2	1:A:506:ALA:HB3	2.49	0.43
1:A:135:ILE:HG23	1:A:168:GLN:HB3	2.01	0.43
1:A:273:ILE:CD1	1:A:314:ILE:HD11	2.49	0.42
1:A:319:GLY:O	1:A:320:LYS:HB2	2.20	0.42
1:A:356:ALA:HB1	1:A:374:TYR:CD1	2.55	0.42
1:A:745:THR:OG1	1:A:746:GLN:N	2.52	0.42
1:A:475:LYS:O	1:A:479:ARG:HG3	2.20	0.42
1:A:468:LYS:NZ	6:A:1007:HOH:O	2.53	0.42
1:A:534:GLN:O	1:A:538:THR:CG2	2.64	0.41
1:A:247:GLY:N	4:A:891:2A5:N3	2.68	0.41
1:A:594:LYS:HA	1:A:594:LYS:HE3	2.02	0.41
1:A:253:HIS:ND1	1:A:301:LEU:HA	2.35	0.41
1:A:377:GLU:OE1	1:A:379:ARG:HD2	2.21	0.41
1:A:135:ILE:HG21	1:A:137:TYR:CE2	2.55	0.41
1:A:244:THR:O	1:A:245:ALA:O	2.39	0.41
1:A:481:LEU:HB3	1:A:505:ILE:CG1	2.49	0.41
1:A:191:ASN:CB	6:A:973:HOH:O	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:661:GLN:O	1:A:664:ILE:HG12	2.21	0.41
1:A:693:LYS:HD2	1:A:730:TYR:CD2	2.56	0.41
1:A:299:LEU:HD11	1:A:328:LEU:HD13	2.03	0.40
1:A:467:PHE:CE2	1:A:534:GLN:HG3	2.56	0.40
1:A:481:LEU:HB3	1:A:505:ILE:HG12	2.03	0.40
1:A:475:LYS:NZ	1:A:549:GLU:OE1	2.55	0.40
1:A:218:CYS:SG	4:A:891:2A5:H02	2.62	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	632/888 (71%)	609 (96%)	17 (3%)	6 (1%)	17 12

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	245	ALA
1	A	320	LYS
1	A	707	ASP
1	A	662	TYR
1	A	321	GLU
1	A	642	ASN

### 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	555/761 (73%)	509 (92%)	46 (8%)	11 7

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	131	LEU
1	A	138	ASP
1	A	153	ARG
1	A	170	LEU
1	A	176	LEU
1	A	187	LEU
1	A	214	GLN
1	A	276	ILE
1	A	277	ARG
1	A	297	PHE
1	A	301	LEU
1	A	314	ILE
1	A	320	LYS
1	A	321	GLU
1	A	324	ARG
1	A	337	LEU
1	A	359	LEU
1	A	388	LEU
1	A	443	CYS
1	A	462	THR
1	A	468	LYS
1	A	505	ILE
1	A	512	LEU
1	A	518	LEU
1	A	520	ARG
1	A	530	LEU
1	A	538	THR
1	A	594	LYS
1	A	606	MET
1	A	610	SER
1	A	611	THR
1	A	639	GLN
1	A	656	ASP
1	A	659	MET
1	A	663	LEU
1	A	673	LEU

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Mol	Chain	Res	Type
1	A	679	GLU
1	A	686	THR
1	A	696	ILE
1	A	712	LEU
1	A	714	LEU
1	A	716	LEU
1	A	717	ARG
1	A	721	MET
1	A	724	LEU
1	A	743	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	GLN
1	A	214	GLN
1	A	251	HIS
1	A	266	ASN
1	A	270	ASN
1	A	288	GLN
1	A	317	ASN
1	A	561	GLN
1	A	567	GLN
1	A	692	GLN
1	A	710	HIS
1	A	713	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	DGT	A	890	2	26,33,33	0.95	1 (3%)	32,52,52	1.55	8 (25%)
5	GOL	A	892	-	5,5,5	0.44	0	5,5,5	0.53	0
4	2A5	A	891	-	26,31,31	1.06	3 (11%)	28,47,47	1.38	3 (10%)

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	A	890	2	-	3/18/34/34	0/3/3/3
5	GOL	A	892	-	-	3/4/4/4	-
4	2A5	A	891	-	-	4/15/35/35	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	891	2A5	O4'-C1'	2.72	1.44	1.41
4	A	891	2A5	C5-C4	2.54	1.47	1.40
4	A	891	2A5	C2-N3	2.32	1.35	1.32
3	A	890	DGT	O4'-C4'	-2.12	1.40	1.45

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	890	DGT	N3-C2-N1	-4.00	121.89	127.22
4	A	891	2A5	N3-C2-N1	-3.93	122.53	128.68
3	A	890	DGT	O1G-PG-O3B	3.36	115.92	104.64
3	A	890	DGT	C5-C6-N1	-2.85	119.54	123.43
3	A	890	DGT	C6-N1-C2	2.67	120.17	115.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	891	2A5	C01-C2'-C1'	-2.57	108.17	115.31
3	A	890	DGT	PB-O3B-PG	-2.54	124.11	132.83
3	A	890	DGT	C2-N3-C4	2.33	118.02	115.36
3	A	890	DGT	PA-O3A-PB	-2.12	125.57	132.83
4	A	891	2A5	C4-C5-N7	-2.06	107.25	109.40
3	A	890	DGT	N2-C2-N3	2.05	121.13	117.79

There are no chirality outliers.

All (10) torsion outliers are listed below:

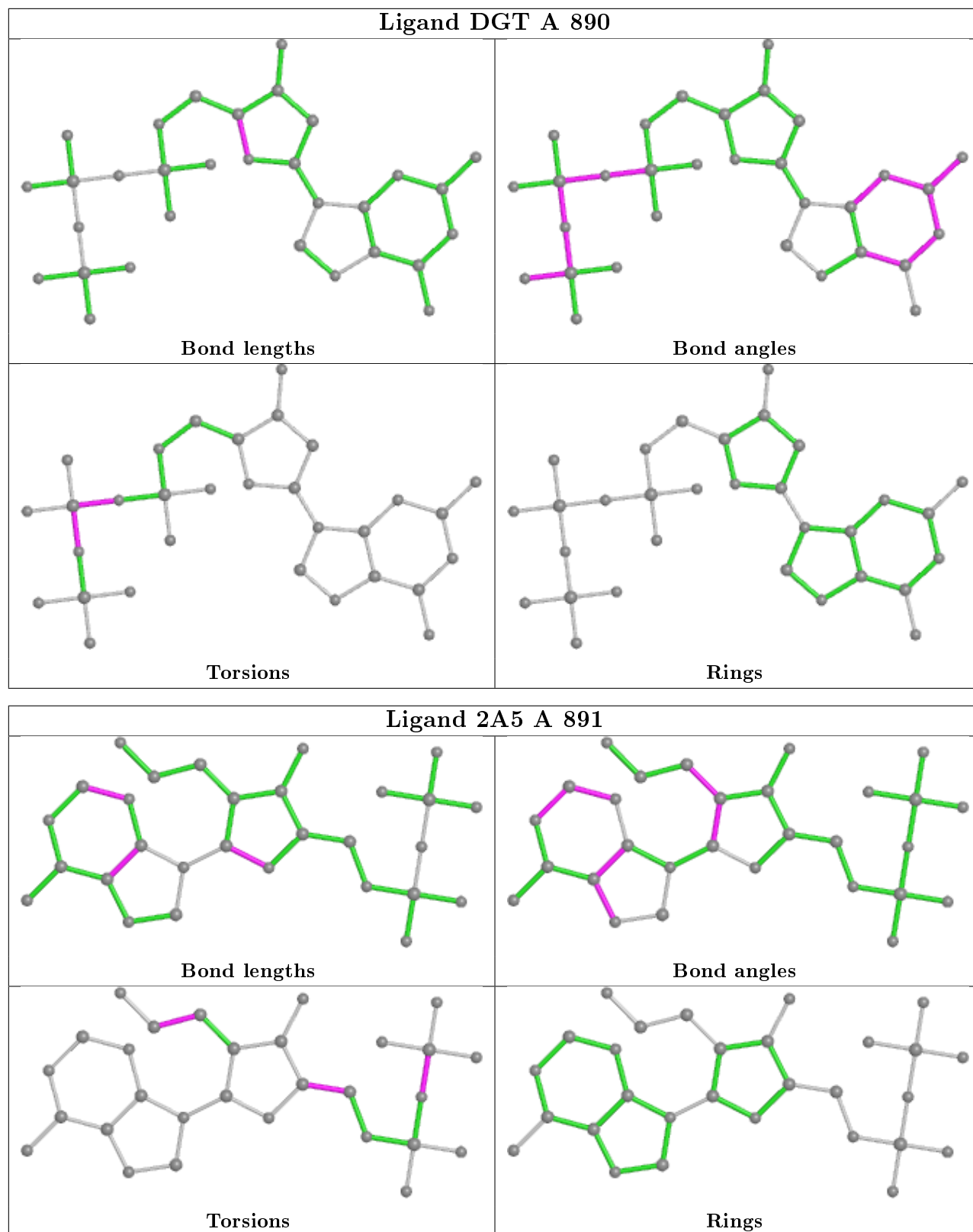
Mol	Chain	Res	Type	Atoms
5	A	892	GOL	O1-C1-C2-C3
5	A	892	GOL	C1-C2-C3-O3
5	A	892	GOL	O1-C1-C2-O2
4	A	891	2A5	C2'-C01-C02-O01
3	A	890	DGT	PG-O3B-PB-O2B
3	A	890	DGT	PA-O3A-PB-O1B
4	A	891	2A5	PA-O3A-PB-O2B
4	A	891	2A5	PA-O3A-PB-O1B
4	A	891	2A5	O4'-C4'-C5'-O5'
3	A	890	DGT	PA-O3A-PB-O2B

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	891	2A5	8	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 ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	640/888 (72%)	1.70	207 (32%) 0 0	41, 52, 70, 79	0

All (207) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	659	MET	12.6
1	A	145	TYR	12.0
1	A	148	PHE	10.0
1	A	662	TYR	9.6
1	A	640	VAL	8.8
1	A	639	GLN	8.6
1	A	319	GLY	8.0
1	A	641	VAL	7.6
1	A	320	LYS	7.5
1	A	718	ALA	7.5
1	A	462	THR	7.4
1	A	629	TYR	7.4
1	A	664	ILE	6.8
1	A	655	TRP	6.8
1	A	91	THR	6.7
1	A	162	GLN	6.4
1	A	146	PHE	6.3
1	A	163	VAL	6.1
1	A	717	ARG	6.1
1	A	686	THR	5.9
1	A	675	ASN	5.9
1	A	628	MET	5.8
1	A	518	LEU	5.7
1	A	137	TYR	5.5
1	A	658	GLY	5.5
1	A	673	LEU	5.4
1	A	431	ILE	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	712	LEU	5.1
1	A	489	TYR	5.1
1	A	429	CYS	5.0
1	A	657	GLU	5.0
1	A	650	VAL	4.9
1	A	506	ALA	4.9
1	A	509	VAL	4.7
1	A	318	HIS	4.7
1	A	317	ASN	4.7
1	A	152	GLU	4.6
1	A	147	GLY	4.6
1	A	604	ALA	4.6
1	A	614	ILE	4.5
1	A	660	LYS	4.5
1	A	445	LEU	4.3
1	A	654	ILE	4.3
1	A	643	PRO	4.3
1	A	183	ILE	4.3
1	A	601	LEU	4.3
1	A	153	ARG	4.2
1	A	432	VAL	4.2
1	A	390	TYR	4.2
1	A	325	ALA	4.2
1	A	646	LEU	4.1
1	A	653	GLY	4.1
1	A	709	SER	4.1
1	A	144	SER	4.0
1	A	333	TRP	4.0
1	A	652	LEU	4.0
1	A	741	TYR	4.0
1	A	505	ILE	3.9
1	A	143	TYR	3.9
1	A	181	ARG	3.9
1	A	160	ASN	3.8
1	A	201	ALA	3.8
1	A	461	LYS	3.7
1	A	323	ILE	3.7
1	A	427	LEU	3.7
1	A	141	PHE	3.7
1	A	723	LYS	3.7
1	A	611	THR	3.6
1	A	582	MET	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	578	LYS	3.5
1	A	156	LEU	3.5
1	A	129	ASP	3.5
1	A	746	GLN	3.5
1	A	447	SER	3.5
1	A	300	TYR	3.5
1	A	481	LEU	3.5
1	A	504	PRO	3.4
1	A	710	HIS	3.4
1	A	477	VAL	3.4
1	A	321	GLU	3.4
1	A	107	ALA	3.3
1	A	607	PRO	3.3
1	A	667	ASN	3.3
1	A	644	TYR	3.3
1	A	149	LYS	3.2
1	A	142	GLN	3.2
1	A	523	PHE	3.2
1	A	133	SER	3.1
1	A	507	LEU	3.1
1	A	621	PHE	3.1
1	A	536	PHE	3.1
1	A	739	GLY	3.1
1	A	605	PRO	3.1
1	A	711	SER	3.1
1	A	656	ASP	3.0
1	A	465	TYR	3.0
1	A	672	GLY	3.0
1	A	742	TYR	3.0
1	A	161	GLY	3.0
1	A	184	GLU	3.0
1	A	508	GLY	3.0
1	A	624	VAL	3.0
1	A	478	THR	3.0
1	A	218	CYS	3.0
1	A	138	ASP	3.0
1	A	688	TRP	2.9
1	A	164	ALA	2.9
1	A	190	TYR	2.9
1	A	331	ALA	2.9
1	A	393	LEU	2.9
1	A	405	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	425	SER	2.9
1	A	397	THR	2.9
1	A	613	GLN	2.9
1	A	647	ARG	2.8
1	A	159	ILE	2.8
1	A	443	CYS	2.8
1	A	663	LEU	2.7
1	A	176	LEU	2.7
1	A	603	MET	2.7
1	A	670	ILE	2.7
1	A	526	GLU	2.7
1	A	166	ARG	2.7
1	A	530	LEU	2.7
1	A	730	TYR	2.7
1	A	572	PHE	2.7
1	A	677	PRO	2.7
1	A	220	LEU	2.7
1	A	90	THR	2.6
1	A	216	SER	2.6
1	A	743	LEU	2.6
1	A	706	ILE	2.6
1	A	403	PHE	2.6
1	A	187	LEU	2.6
1	A	288	GLN	2.6
1	A	720	THR	2.6
1	A	619	GLU	2.6
1	A	406	TYR	2.5
1	A	617	TYR	2.5
1	A	719	PRO	2.5
1	A	383	ILE	2.5
1	A	198	PHE	2.5
1	A	268	THR	2.5
1	A	674	PRO	2.5
1	A	322	GLU	2.5
1	A	455	GLU	2.5
1	A	92	LYS	2.5
1	A	334	ILE	2.5
1	A	473	ILE	2.5
1	A	627	ASN	2.5
1	A	512	LEU	2.4
1	A	496	ARG	2.4
1	A	708	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	414	SER	2.4
1	A	651	ASP	2.4
1	A	738	THR	2.4
1	A	165	GLU	2.4
1	A	737	LYS	2.4
1	A	249	GLY	2.4
1	A	540	TYR	2.4
1	A	705	TYR	2.4
1	A	157	LEU	2.3
1	A	299	LEU	2.3
1	A	206	PHE	2.3
1	A	516	PHE	2.3
1	A	409	ALA	2.3
1	A	534	GLN	2.3
1	A	428	CYS	2.3
1	A	666	GLN	2.3
1	A	485	ILE	2.3
1	A	707	ASP	2.2
1	A	464	THR	2.2
1	A	570	LEU	2.2
1	A	529	ARG	2.2
1	A	727	MET	2.2
1	A	665	THR	2.2
1	A	261	TYR	2.2
1	A	395	ALA	2.2
1	A	626	SER	2.2
1	A	615	LEU	2.2
1	A	158	ARG	2.2
1	A	472	GLU	2.2
1	A	608	THR	2.2
1	A	616	GLY	2.2
1	A	661	GLN	2.1
1	A	120	VAL	2.1
1	A	444	ASN	2.1
1	A	606	MET	2.1
1	A	108	ALA	2.1
1	A	543	SER	2.1
1	A	580	TYR	2.1
1	A	731	GLY	2.1
1	A	474	ALA	2.1
1	A	242	SER	2.1
1	A	535	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	217	SER	2.1
1	A	484	VAL	2.1
1	A	553	LYS	2.1
1	A	704	VAL	2.1
1	A	294	PRO	2.1
1	A	330	PRO	2.1
1	A	555	GLY	2.1
1	A	404	VAL	2.1
1	A	468	LYS	2.1
1	A	191	ASN	2.0
1	A	648	ASP	2.0
1	A	426	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](#)

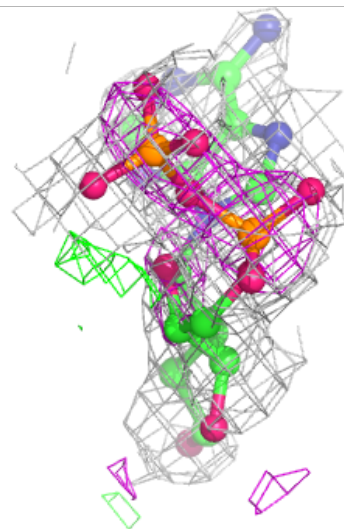
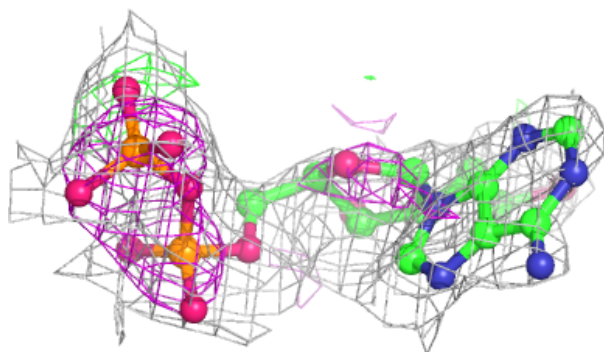
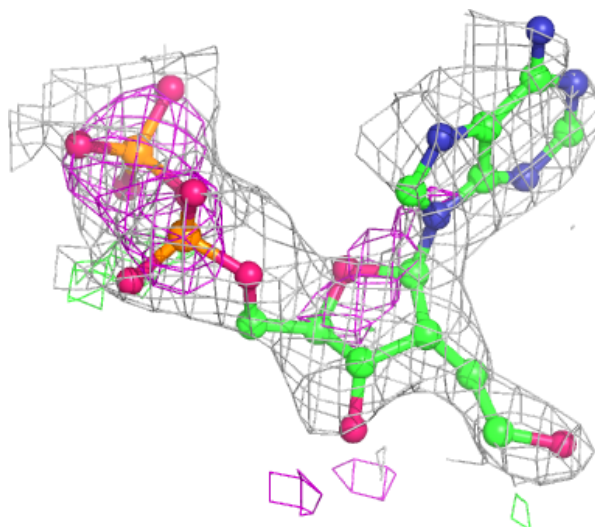
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

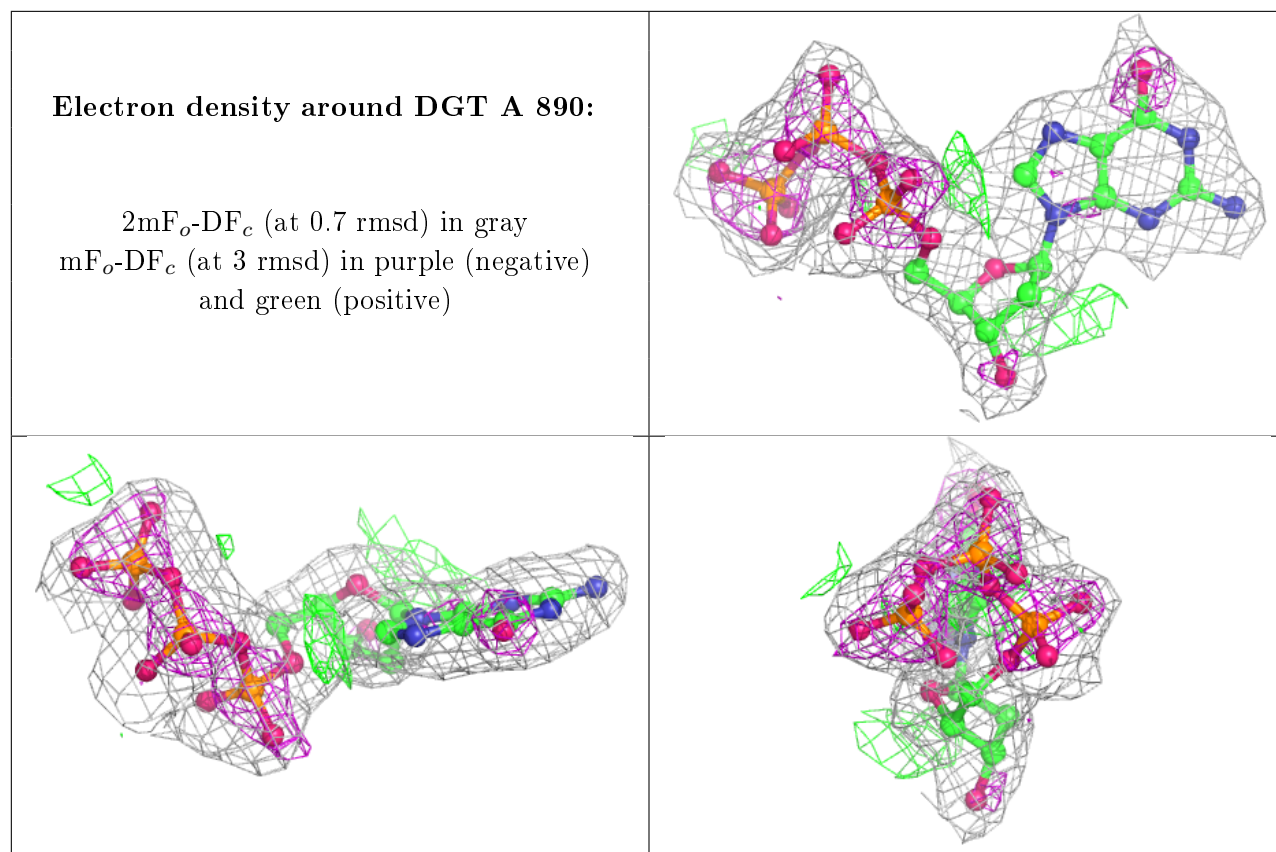
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	GOL	A	892	6/6	0.79	0.19	73,76,77,78	0
4	2A5	A	891	29/29	0.79	0.26	71,81,83,84	0
2	MG	A	889	1/1	0.88	0.08	41,41,41,41	0
3	DGT	A	890	31/31	0.96	0.09	36,43,48,49	0

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 2A5 Å 891:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.