



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:03 PM UTC

PDB ID : 3K8T / pdb_00003k8t
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

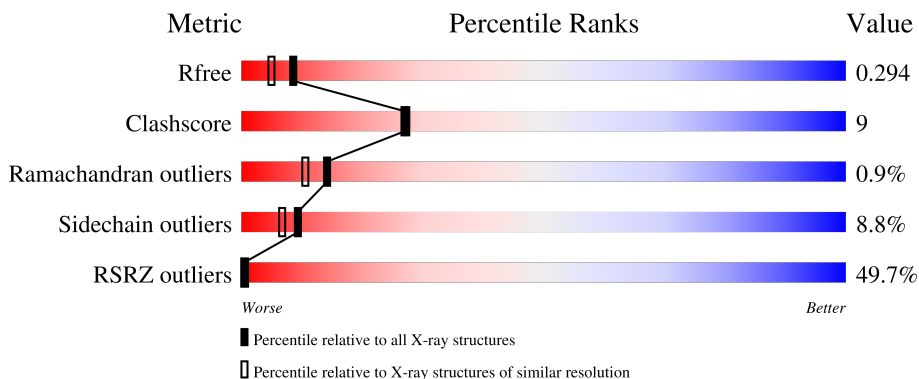
1 Overall quality at a glance

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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	888	36% 54% 15% • 28%

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.

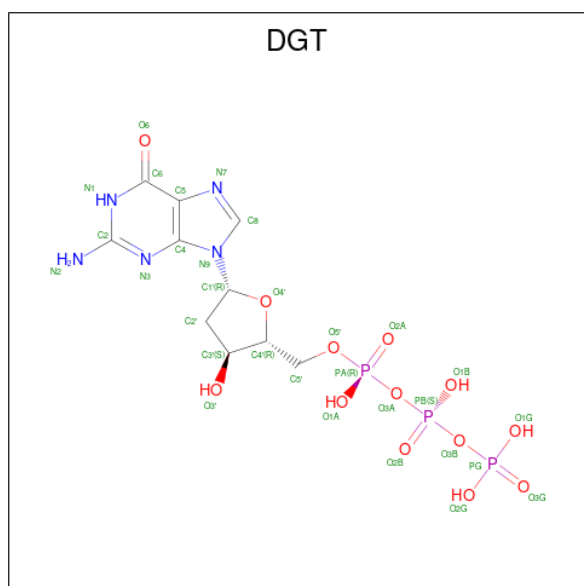
- Molecule 1 is a protein called Ribonucleoside-diphosphate reductase large chain 1.

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

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

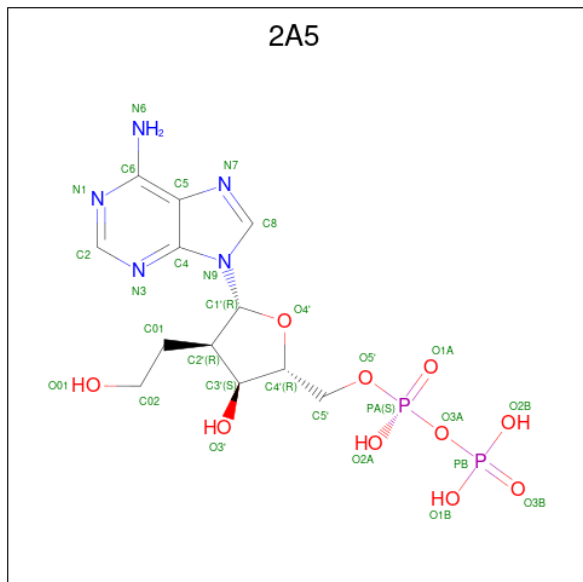
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (CCD ID: DGT) (formula: C₁₀H₁₆N₅O₁₃P₃).



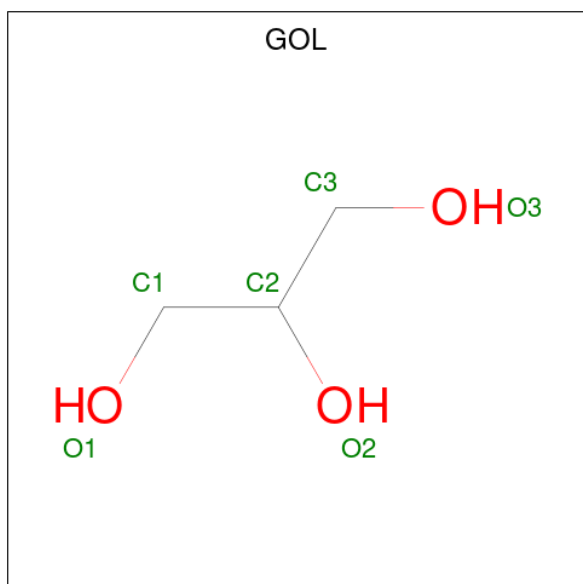
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is 2'-deoxy-2'-(2-hydroxyethyl)adenosine 5'-(trihydrogen diphosphate) (CCD ID: 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 (CCD ID: 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

GLY																																																												
	GLY	MET	ALA	GLU	LEU	ASN	VAL	GLN	GLU	SER	LYS	VAL	GLU	VAL	PRO	GLU	VAL	PRO	ALA	PRO	THR	THR	LYS	ASN	GLU	LYS	ALA	PRO	ILE	VAL	VAL	ALA	VAL	ALA	ALA	ALA	ASP	TYR	ASN	SER	GLU	LYS	VAL	ILE	VAL	CYS	ILE	ASP	ASN	PRO	PRO	GLU	ALA	ALA	CYS	GLU	MET	CYS	THR	LYS
VAL	I706	D707	Q708	S709	H710	S711	L712	N713	L714	F715	L716	R717	A718	F719	T720	M721	G722	K723	L724	T725	S726	N727	H728	F729	Y730	G731	H732	K733	L736	G739	N740	Y741	Y742	L743	R744	T745	Q746	ALA	ALA	SER	SER	ALA	ALA	ALA	ILE	GLN	PHE	THR	ILE	ASP	GLN	LYS	ILE	ALA	ASP	GLN	ALA	THR	GLU	ASN

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	43.8	Xtriage
Anisotropy	0.421	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5322	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DGT, GOL, MG, 2A5

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	0.99	7/5238 (0.1%)	1.09	8/7089 (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	A	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	676	VAL	CA-CB	7.91	1.60	1.54
1	A	707	ASP	CB-CG	-6.97	1.34	1.52
1	A	276	ILE	CA-CB	5.82	1.61	1.54
1	A	538	THR	CA-CB	5.81	1.62	1.53
1	A	298	ALA	C-O	5.80	1.30	1.23
1	A	664	ILE	CA-CB	5.59	1.60	1.54
1	A	604	ALA	CA-CB	-5.48	1.46	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	676	VAL	CA-C-O	10.76	126.18	119.51
1	A	334	ILE	N-CA-C	8.26	116.10	107.76
1	A	707	ASP	N-CA-C	7.87	127.55	110.80
1	A	319	GLY	N-CA-C	7.63	122.88	110.97
1	A	707	ASP	CB-CG-OD1	-6.04	104.51	118.40
1	A	229	GLU	N-CA-C	5.29	116.74	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	352	SER	N-CA-C	-5.20	103.52	110.07
1	A	357	PRO	N-CA-C	5.08	119.07	111.14

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 [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	5120	0	5055	95	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	6	0
All	All	5322	0	5091	95	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 (95) 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:606:MET:HE3	1:A:608:THR:HG22	1.65	0.78
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:606:MET:HE3	1:A:608:THR:CG2	2.17	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:220:LEU:HD21	1:A:426:ASN:HB3	1.78	0.64
1:A:659:MET:O	1:A:659:MET:HE2	1.98	0.64
1:A:659:MET:HE3	1:A:673:LEU:HD11	1.80	0.63
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:606:MET:HE2	6:A:895:HOH:O	2.02	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:659:MET:HE3	1:A:673:LEU:CD1	2.35	0.56
1:A:426:ASN:ND2	4:A:891:2A5:C02	2.62	0.56
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:661:GLN:C	1:A:663:LEU:H	2.15	0.54
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:520:ARG:HH22	1:A:648:ASP:CG	2.17	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:713:ASN:HD22	1:A:742:TYR:H	1.60	0.50
1:A:648:ASP:OD2	1:A:684:TYR:OH	2.27	0.49
1:A:124:VAL:HG12	1:A:125:MET:HE2	1.93	0.49
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: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: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:564:PRO:HG2	1:A:574:MET:HE1	1.98	0.46
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: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:N	1:A:276:ILE:HD13	2.33	0.44
1:A:486:ASP:OD2	1:A:500:MET:HE1	2.18	0.43
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: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:HE3	1:A:594:LYS:HA	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:641:VAL:O	1:A:642:ASN:C	2.63	0.40
1:A:218:CYS:SG	4:A:891:2A5:H02	2.62	0.40
1:A:475:LYS:NZ	1:A:549:GLU:OE1	2.55	0.40
1:A:481:LEU:HB3	1:A:505:ILE:HG12	2.03	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%)	14 10

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%)	506 (91%)	49 (9%)	9 7

All (49) 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	253	HIS
1	A	268	THR
1	A	276	ILE
1	A	277	ARG
1	A	282	THR
1	A	297	PHE
1	A	301	LEU
1	A	314	ILE
1	A	321	GLU
1	A	323	ILE
1	A	324	ARG
1	A	337	LEU
1	A	359	LEU
1	A	388	LEU
1	A	432	VAL
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	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	680	LEU
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	GLN
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	692	GLN
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 oligosaccharides 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	32,33,33	1.66	3 (9%)	48,52,52	1.54	9 (18%)
4	2A5	A	891	-	30,31,31	1.50	5 (16%)	40,47,47	2.03	7 (17%)
5	GOL	A	892	-	5,5,5	0.45	0	5,5,5	0.57	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DGT	A	890	2	-	3/22/34/34	0/3/3/3
4	2A5	A	891	-	-	4/19/35/35	0/3/3/3
5	GOL	A	892	-	-	3/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	890	DGT	PB-O3A	5.50	1.65	1.59
3	A	890	DGT	PA-O3A	5.11	1.65	1.59
4	A	891	2A5	C5-C4	4.80	1.47	1.39
4	A	891	2A5	PA-O3A	3.58	1.63	1.59
4	A	891	2A5	C5-C6	2.65	1.48	1.41
4	A	891	2A5	C8-N7	2.18	1.35	1.31
4	A	891	2A5	C5-N7	-2.17	1.35	1.39
3	A	890	DGT	O4'-C4'	-2.13	1.40	1.45

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	891	2A5	C5-C4-N3	-6.29	118.06	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	891	2A5	N3-C4-N9	5.38	136.31	127.17
3	A	890	DGT	C5-C4-N3	-4.72	120.87	128.39
4	A	891	2A5	C2-N3-C4	4.31	122.35	111.83
4	A	891	2A5	N3-C2-N1	-4.00	122.53	128.58
3	A	890	DGT	N9-C4-N3	3.64	133.24	125.95
3	A	890	DGT	O1G-PG-O3B	3.36	115.92	104.64
3	A	890	DGT	C2-N3-C4	3.32	118.02	112.30
4	A	891	2A5	C4-C5-N7	-2.92	107.25	110.58
4	A	891	2A5	C4-N9-C8	2.82	108.70	105.74
3	A	890	DGT	C2-N1-C6	-2.72	120.17	125.11
3	A	890	DGT	O6-C6-C5	-2.58	119.72	126.53
3	A	890	DGT	N9-C8-N7	-2.54	108.69	113.40
3	A	890	DGT	C5-C6-N1	2.47	119.54	113.25
4	A	891	2A5	C5-N7-C8	2.44	107.29	103.45
3	A	890	DGT	O2G-PG-O1G	-2.01	100.27	107.80

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

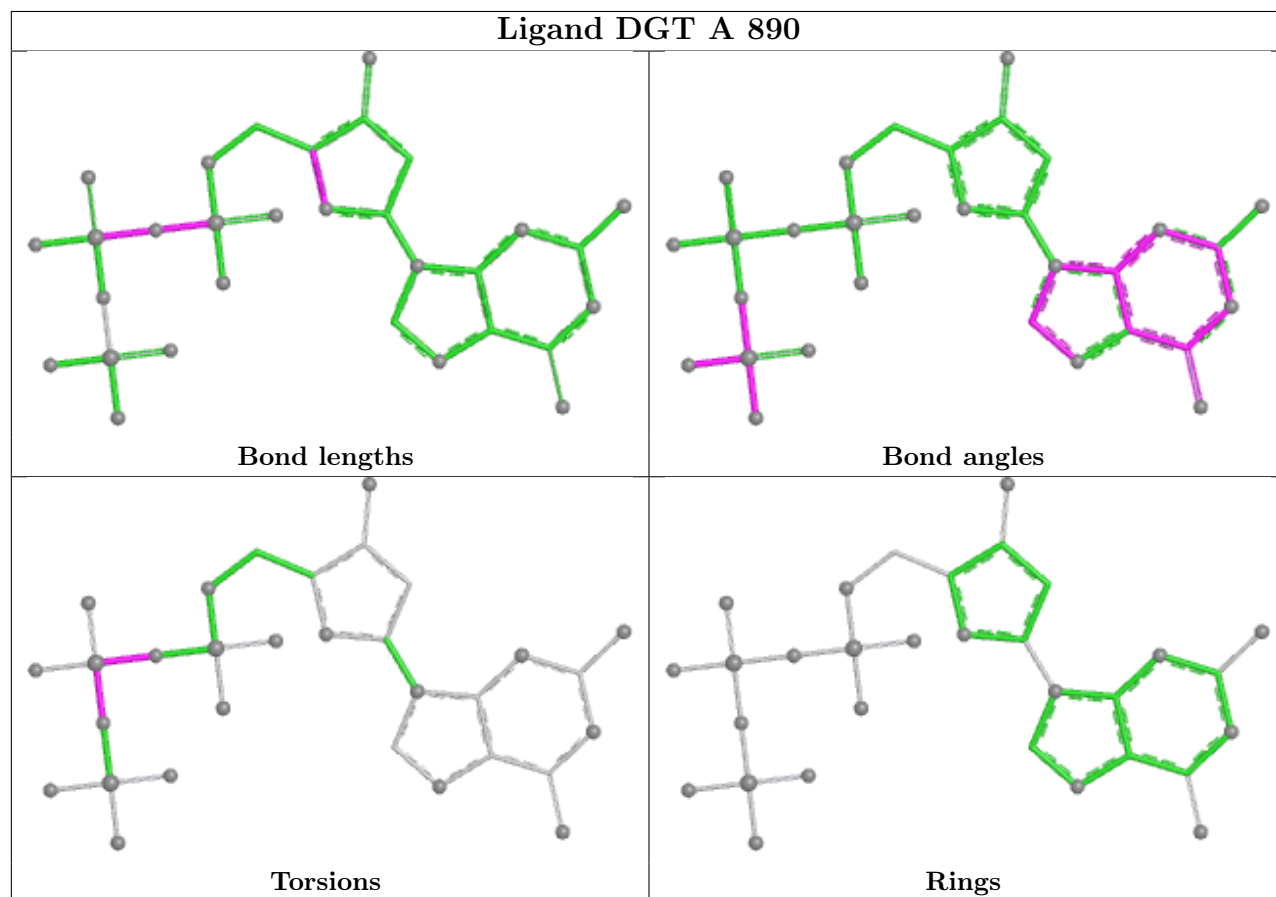
There are no ring outliers.

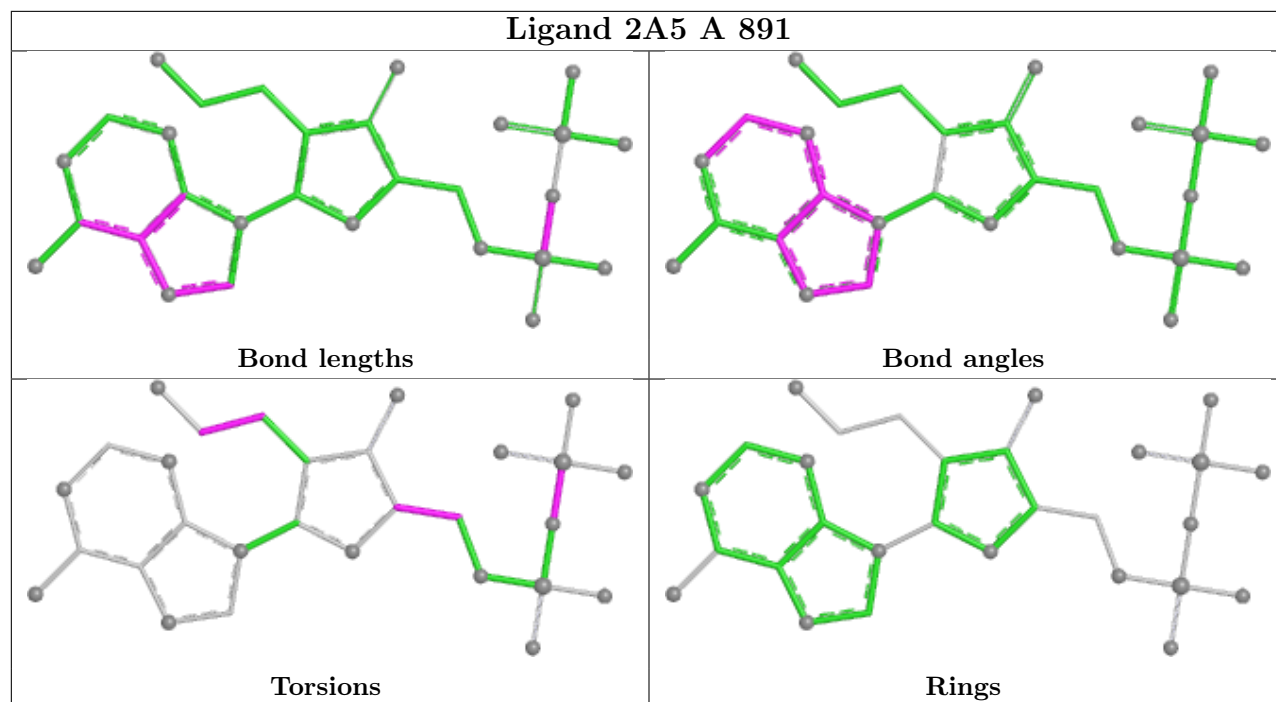
1 monomer is involved in 8 short contacts:

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 [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	640/888 (72%)	2.11	318 (49%) 0 0	41, 52, 70, 79	0

All (318) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	662	TYR	6.8
1	A	145	TYR	5.6
1	A	686	THR	5.5
1	A	518	LEU	5.5
1	A	290	GLY	5.3
1	A	143	TYR	5.2
1	A	718	ALA	5.1
1	A	659	MET	5.1
1	A	148	PHE	5.0
1	A	658	GLY	4.9
1	A	325	ALA	4.7
1	A	675	ASN	4.6
1	A	712	LEU	4.5
1	A	489	TYR	4.4
1	A	655	TRP	4.4
1	A	462	THR	4.4
1	A	137	TYR	4.3
1	A	715	PHE	4.2
1	A	323	ILE	4.2
1	A	646	LEU	4.2
1	A	731	GLY	4.1
1	A	614	ILE	4.1
1	A	652	LEU	4.1
1	A	378	GLY	4.1
1	A	397	THR	4.1
1	A	294	PRO	4.1
1	A	628	MET	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	409	ALA	4.0
1	A	156	LEU	4.0
1	A	146	PHE	4.0
1	A	705	TYR	3.9
1	A	654	ILE	3.9
1	A	163	VAL	3.9
1	A	390	TYR	3.9
1	A	742	TYR	3.8
1	A	383	ILE	3.8
1	A	523	PHE	3.8
1	A	535	ILE	3.8
1	A	644	TYR	3.8
1	A	717	ARG	3.8
1	A	617	TYR	3.7
1	A	665	THR	3.7
1	A	629	TYR	3.7
1	A	268	THR	3.7
1	A	359	LEU	3.7
1	A	276	ILE	3.6
1	A	505	ILE	3.6
1	A	664	ILE	3.6
1	A	700	ALA	3.6
1	A	640	VAL	3.6
1	A	673	LEU	3.6
1	A	190	TYR	3.6
1	A	333	TRP	3.5
1	A	607	PRO	3.5
1	A	674	PRO	3.5
1	A	369	ALA	3.5
1	A	615	LEU	3.5
1	A	641	VAL	3.5
1	A	506	ALA	3.4
1	A	741	TYR	3.4
1	A	720	THR	3.4
1	A	555	GLY	3.4
1	A	218	CYS	3.4
1	A	222	ALA	3.4
1	A	245	ALA	3.4
1	A	454	ILE	3.4
1	A	639	GLN	3.4
1	A	465	TYR	3.3
1	A	569	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	91	THR	3.3
1	A	176	LEU	3.3
1	A	585	TRP	3.3
1	A	371	TYR	3.3
1	A	278	VAL	3.2
1	A	530	LEU	3.2
1	A	432	VAL	3.2
1	A	337	LEU	3.2
1	A	370	LEU	3.2
1	A	351	PHE	3.2
1	A	572	PHE	3.2
1	A	536	PHE	3.2
1	A	582	MET	3.2
1	A	262	ILE	3.1
1	A	388	LEU	3.1
1	A	198	PHE	3.1
1	A	745	THR	3.1
1	A	542	ALA	3.1
1	A	743	LEU	3.1
1	A	559	THR	3.1
1	A	611	THR	3.1
1	A	261	TYR	3.1
1	A	701	ASP	3.1
1	A	509	VAL	3.1
1	A	314	ILE	3.1
1	A	688	TRP	3.0
1	A	374	TYR	3.0
1	A	538	THR	3.0
1	A	504	PRO	3.0
1	A	687	VAL	3.0
1	A	395	ALA	3.0
1	A	613	GLN	3.0
1	A	120	VAL	3.0
1	A	422	ILE	3.0
1	A	670	ILE	3.0
1	A	109	THR	3.0
1	A	464	THR	3.0
1	A	516	PHE	3.0
1	A	570	LEU	3.0
1	A	714	LEU	3.0
1	A	129	ASP	3.0
1	A	320	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	643	PRO	3.0
1	A	560	PHE	3.0
1	A	160	ASN	2.9
1	A	445	LEU	2.9
1	A	663	LEU	2.9
1	A	252	ILE	2.9
1	A	330	PRO	2.9
1	A	357	PRO	2.9
1	A	580	TYR	2.9
1	A	730	TYR	2.9
1	A	240	LEU	2.9
1	A	393	LEU	2.9
1	A	508	GLY	2.9
1	A	739	GLY	2.9
1	A	597	VAL	2.9
1	A	557	TYR	2.9
1	A	355	SER	2.9
1	A	348	TRP	2.9
1	A	431	ILE	2.9
1	A	241	ILE	2.8
1	A	437	PRO	2.8
1	A	447	SER	2.8
1	A	141	PHE	2.8
1	A	297	PHE	2.8
1	A	183	ILE	2.8
1	A	191	ASN	2.8
1	A	281	ASN	2.8
1	A	529	ARG	2.8
1	A	534	GLN	2.8
1	A	151	LEU	2.8
1	A	588	LEU	2.8
1	A	602	THR	2.8
1	A	162	GLN	2.8
1	A	289	GLY	2.8
1	A	144	SER	2.7
1	A	206	PHE	2.7
1	A	296	ALA	2.7
1	A	372	THR	2.7
1	A	608	THR	2.7
1	A	421	VAL	2.7
1	A	228	ILE	2.7
1	A	444	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	304	TRP	2.7
1	A	672	GLY	2.7
1	A	561	GLN	2.7
1	A	405	VAL	2.7
1	A	606	MET	2.7
1	A	624	VAL	2.7
1	A	727	MET	2.7
1	A	231	ILE	2.7
1	A	170	LEU	2.7
1	A	601	LEU	2.7
1	A	334	ILE	2.7
1	A	288	GLN	2.6
1	A	185	ALA	2.6
1	A	619	GLU	2.6
1	A	499	ASN	2.6
1	A	650	VAL	2.6
1	A	147	GLY	2.6
1	A	208	ALA	2.6
1	A	587	THR	2.6
1	A	618	ASN	2.6
1	A	350	LEU	2.6
1	A	367	PHE	2.6
1	A	496	ARG	2.6
1	A	667	ASN	2.6
1	A	412	ARG	2.6
1	A	244	THR	2.6
1	A	579	PRO	2.6
1	A	729	PHE	2.5
1	A	434	TYR	2.5
1	A	721	MET	2.5
1	A	565	ALA	2.5
1	A	719	PRO	2.5
1	A	195	LEU	2.5
1	A	467	PHE	2.5
1	A	364	GLY	2.5
1	A	379	ARG	2.5
1	A	201	ALA	2.5
1	A	455	GLU	2.5
1	A	512	LEU	2.5
1	A	403	PHE	2.5
1	A	583	TRP	2.5
1	A	267	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	468	LYS	2.5
1	A	676	VAL	2.5
1	A	363	TYR	2.5
1	A	398	GLU	2.5
1	A	414	SER	2.5
1	A	435	SER	2.5
1	A	108	ALA	2.5
1	A	263	ALA	2.5
1	A	495	ALA	2.5
1	A	328	LEU	2.5
1	A	594	LYS	2.5
1	A	568	GLY	2.5
1	A	581	GLY	2.5
1	A	696	ILE	2.5
1	A	657	GLU	2.4
1	A	694	THR	2.4
1	A	107	ALA	2.4
1	A	551	ALA	2.4
1	A	593	MET	2.4
1	A	604	ALA	2.4
1	A	683	LEU	2.4
1	A	724	LEU	2.4
1	A	309	PHE	2.4
1	A	415	ASN	2.4
1	A	713	ASN	2.4
1	A	430	GLU	2.4
1	A	473	ILE	2.4
1	A	704	VAL	2.4
1	A	258	THR	2.4
1	A	246	GLY	2.4
1	A	627	ASN	2.4
1	A	342	VAL	2.4
1	A	125	MET	2.4
1	A	461	LYS	2.4
1	A	553	LYS	2.4
1	A	197	TYR	2.4
1	A	595	HIS	2.4
1	A	609	ALA	2.4
1	A	645	LEU	2.4
1	A	319	GLY	2.4
1	A	514	ASP	2.4
1	A	477	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	592	ILE	2.4
1	A	282	THR	2.4
1	A	679	GLU	2.3
1	A	479	ARG	2.3
1	A	442	VAL	2.3
1	A	622	GLU	2.3
1	A	406	TYR	2.3
1	A	697	ASN	2.3
1	A	166	ARG	2.3
1	A	723	LYS	2.3
1	A	242	SER	2.3
1	A	159	ILE	2.3
1	A	392	ILE	2.3
1	A	484	VAL	2.3
1	A	556	PRO	2.3
1	A	623	PRO	2.3
1	A	101	LEU	2.3
1	A	744	ARG	2.3
1	A	626	SER	2.3
1	A	329	PHE	2.3
1	A	513	ALA	2.3
1	A	271	GLY	2.3
1	A	235	LEU	2.3
1	A	229	GLU	2.2
1	A	311	PHE	2.2
1	A	255	ILE	2.2
1	A	180	GLY	2.2
1	A	295	GLY	2.2
1	A	616	GLY	2.2
1	A	577	GLN	2.2
1	A	709	SER	2.2
1	A	352	SER	2.2
1	A	732	TRP	2.2
1	A	115	MET	2.2
1	A	485	ILE	2.2
1	A	286	VAL	2.2
1	A	239	ALA	2.2
1	A	385	ALA	2.2
1	A	205	LEU	2.2
1	A	353	PRO	2.1
1	A	230	GLY	2.1
1	A	259	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	157	LEU	2.1
1	A	481	LEU	2.1
1	A	381	LYS	2.1
1	A	418	ASN	2.1
1	A	591	ASP	2.1
1	A	625	THR	2.1
1	A	725	THR	2.1
1	A	389	TRP	2.1
1	A	116	ILE	2.1
1	A	661	GLN	2.1
1	A	666	GLN	2.1
1	A	492	VAL	2.1
1	A	164	ALA	2.1
1	A	269	SER	2.1
1	A	716	LEU	2.1
1	A	526	GLU	2.1
1	A	265	THR	2.1
1	A	396	GLN	2.1
1	A	171	ILE	2.1
1	A	308	ILE	2.1
1	A	733	LYS	2.1
1	A	260	SER	2.1
1	A	736	LEU	2.1
1	A	620	CYS	2.1
1	A	256	ARG	2.1
1	A	540	TYR	2.1
1	A	105	VAL	2.1
1	A	338	PHE	2.1
1	A	181	ARG	2.0
1	A	277	ARG	2.0
1	A	112	PRO	2.0
1	A	354	THR	2.0
1	A	152	GLU	2.0
1	A	165	GLU	2.0
1	A	448	VAL	2.0
1	A	272	LEU	2.0
1	A	427	LEU	2.0
1	A	450	LEU	2.0
1	A	478	THR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

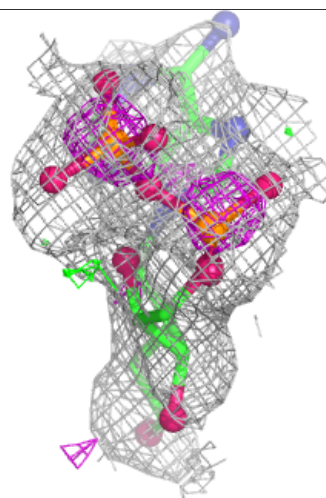
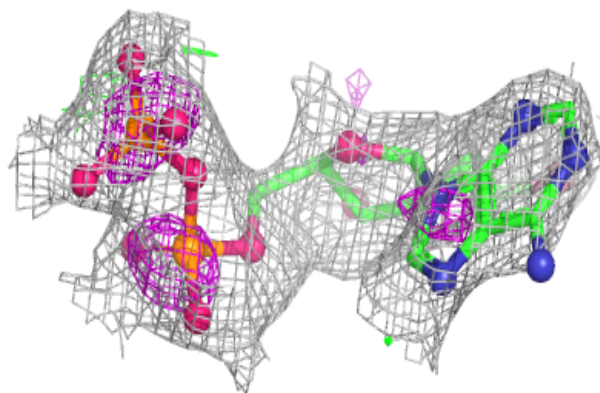
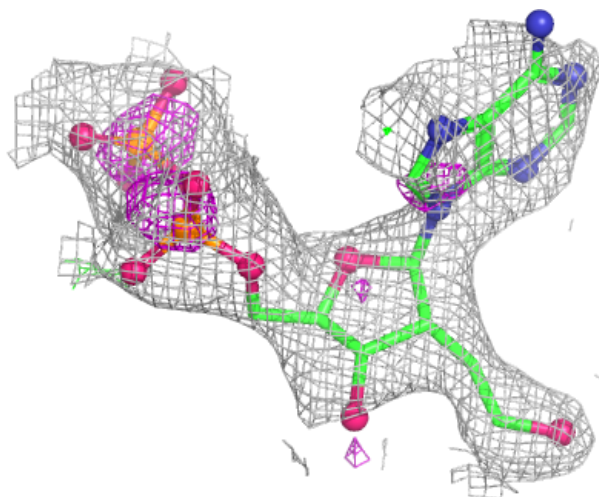
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	2A5	A	891	29/29	0.73	0.17	71,81,83,84	0
5	GOL	A	892	6/6	0.74	0.18	73,76,77,78	0
3	DGT	A	890	31/31	0.93	0.10	36,43,48,49	0
2	MG	A	889	1/1	0.94	0.07	41,41,41,41	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.

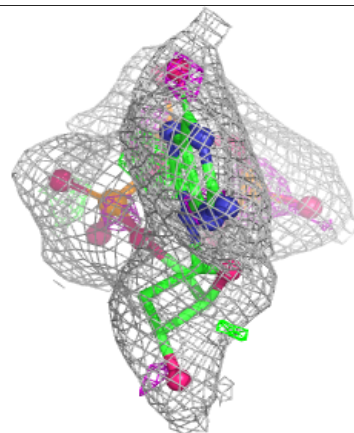
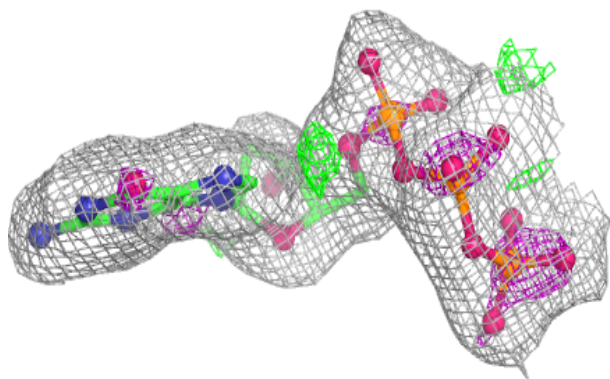
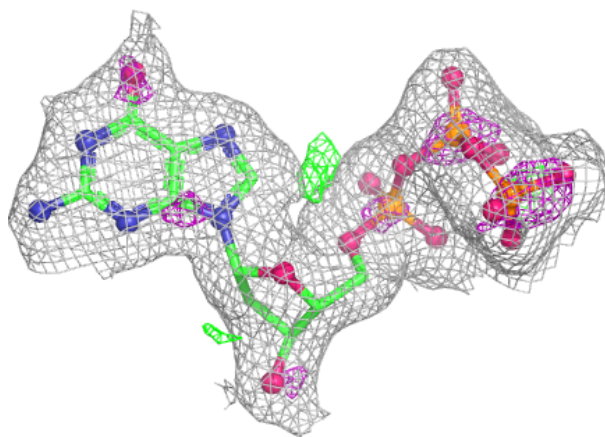
Electron density around 2A5 Å 891:

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



Electron density around DGT A 890:

$2mF_o - DF_c$ (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.