



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:49 PM UTC

PDB ID : 4MZ7 / pdb_00004mz7
Title : Structural insight into dGTP-dependent activation of tetrameric SAMHD1 deoxynucleoside triphosphate triphosphohydrolase
Authors : Zhu, C.; Gao, W.; Zhao, K.; Qin, X.; Zhang, Y.; Peng, X.; Zhang, L.; Dong, Y.; Zhang, W.; Li, P.; Wei, W.; Gong, Y.; Yu, X.F.
Deposited on : 2013-09-29
Resolution : 1.80 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

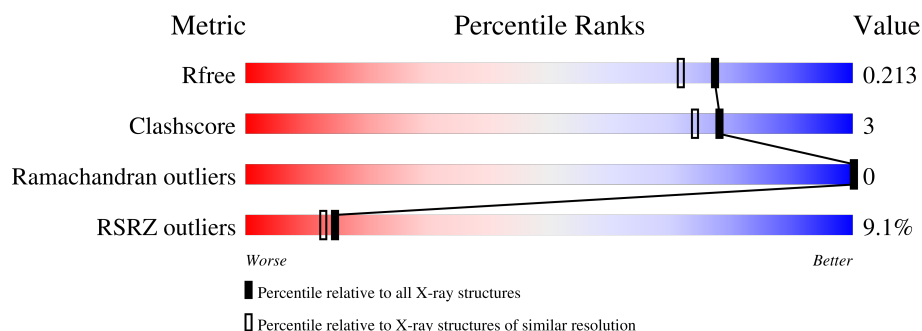
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	539	11% 83% 6% 11%
1	B	539	5% 86% 5% 9%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9013 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 triphosphohydrolase SAMHD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	481	Total	C	N	O	S	0	2	0
			3955	2534	688	714	19			
1	B	493	Total	C	N	O	S	0	2	0
			4050	2596	704	731	19			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	88	MET	-	expression tag	UNP Q9Y3Z3
A	89	GLY	-	expression tag	UNP Q9Y3Z3
A	90	SER	-	expression tag	UNP Q9Y3Z3
A	91	SER	-	expression tag	UNP Q9Y3Z3
A	92	HIS	-	expression tag	UNP Q9Y3Z3
A	93	HIS	-	expression tag	UNP Q9Y3Z3
A	94	HIS	-	expression tag	UNP Q9Y3Z3
A	95	HIS	-	expression tag	UNP Q9Y3Z3
A	96	HIS	-	expression tag	UNP Q9Y3Z3
A	97	HIS	-	expression tag	UNP Q9Y3Z3
A	98	SER	-	expression tag	UNP Q9Y3Z3
A	99	SER	-	expression tag	UNP Q9Y3Z3
A	100	GLY	-	expression tag	UNP Q9Y3Z3
A	101	GLU	-	expression tag	UNP Q9Y3Z3
A	102	ASN	-	expression tag	UNP Q9Y3Z3
A	103	LEU	-	expression tag	UNP Q9Y3Z3
A	104	TYR	-	expression tag	UNP Q9Y3Z3
A	105	PHE	-	expression tag	UNP Q9Y3Z3
A	106	GLN	-	expression tag	UNP Q9Y3Z3
A	107	GLY	-	expression tag	UNP Q9Y3Z3
A	108	SER	-	expression tag	UNP Q9Y3Z3
A	266	TYR	CYS	engineered mutation	UNP Q9Y3Z3
B	88	MET	-	expression tag	UNP Q9Y3Z3
B	89	GLY	-	expression tag	UNP Q9Y3Z3
B	90	SER	-	expression tag	UNP Q9Y3Z3

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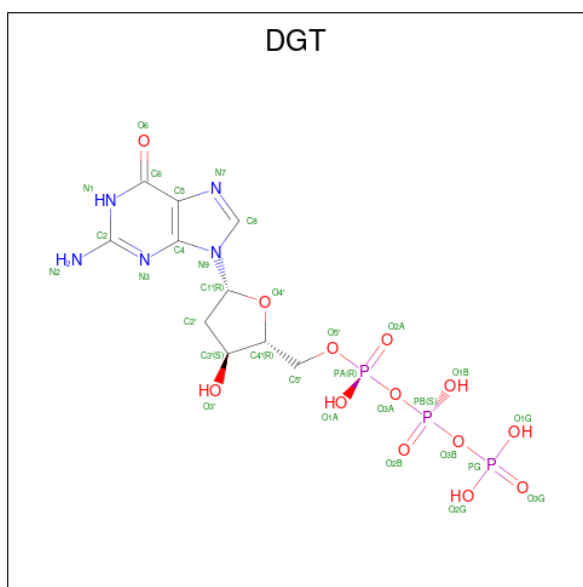
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Chain	Residue	Modelled	Actual	Comment	Reference
B	91	SER	-	expression tag	UNP Q9Y3Z3
B	92	HIS	-	expression tag	UNP Q9Y3Z3
B	93	HIS	-	expression tag	UNP Q9Y3Z3
B	94	HIS	-	expression tag	UNP Q9Y3Z3
B	95	HIS	-	expression tag	UNP Q9Y3Z3
B	96	HIS	-	expression tag	UNP Q9Y3Z3
B	97	HIS	-	expression tag	UNP Q9Y3Z3
B	98	SER	-	expression tag	UNP Q9Y3Z3
B	99	SER	-	expression tag	UNP Q9Y3Z3
B	100	GLY	-	expression tag	UNP Q9Y3Z3
B	101	GLU	-	expression tag	UNP Q9Y3Z3
B	102	ASN	-	expression tag	UNP Q9Y3Z3
B	103	LEU	-	expression tag	UNP Q9Y3Z3
B	104	TYR	-	expression tag	UNP Q9Y3Z3
B	105	PHE	-	expression tag	UNP Q9Y3Z3
B	106	GLN	-	expression tag	UNP Q9Y3Z3
B	107	GLY	-	expression tag	UNP Q9Y3Z3
B	108	SER	-	expression tag	UNP Q9Y3Z3
B	266	TYR	CYS	engineered mutation	UNP Q9Y3Z3

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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

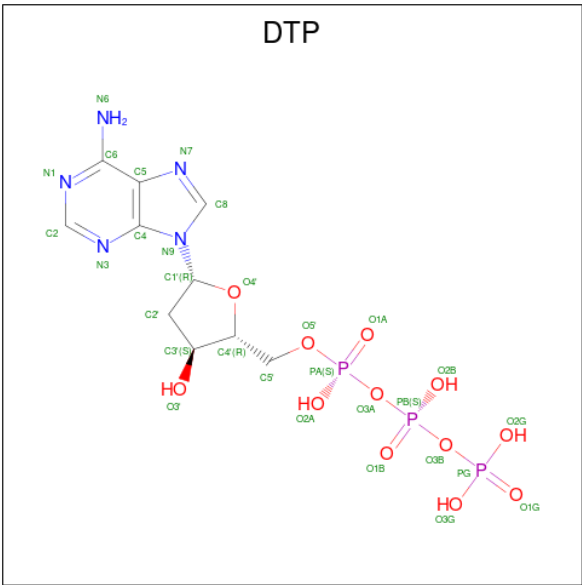


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 5 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (CCD ID: DTP) (formula: C₁₀H₁₆N₅O₁₂P₃).



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

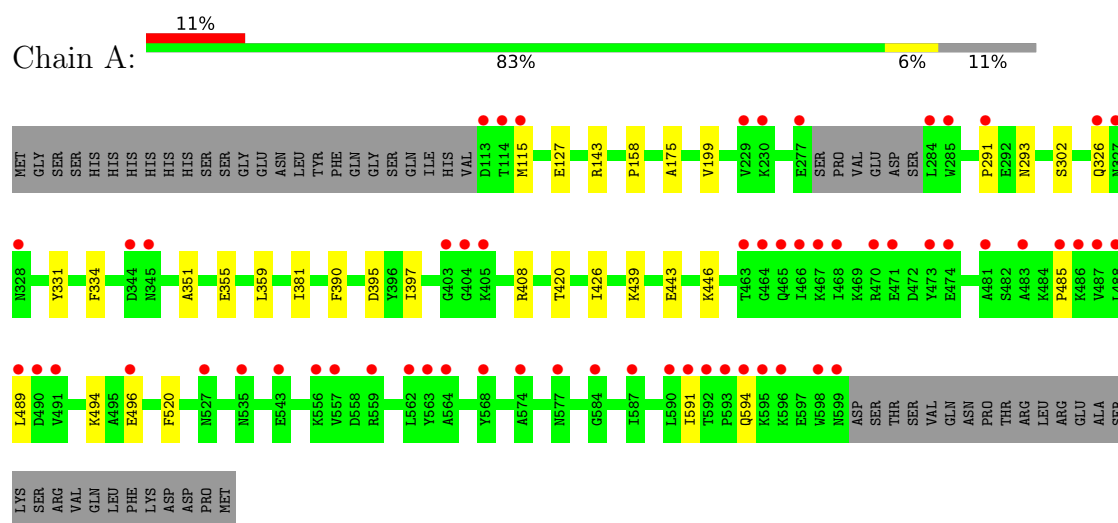
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	347	Total	O	0	0
			347	347		
6	B	472	Total	O	0	0
			472	472		

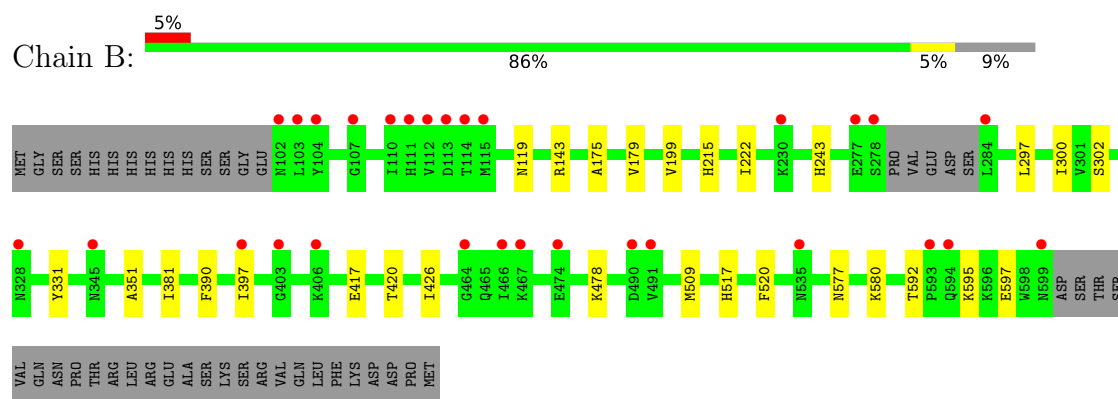
3 Residue-property plots

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: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	147.40Å 103.61Å 92.13Å 90.00° 121.98° 90.00°	Depositor
Resolution (Å)	50.00 – 1.80 50.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.2 (50.00-1.80) 97.2 (50.00-1.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.03 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.194 , 0.226 (Not available) , 0.213	Depositor DCC
R_{free} test set	5284 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	16.5	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9013	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% 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: DTP, MG, ZN, 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	0.71	0/4054	0.78	0/5474
1	B	0.70	0/4155	0.78	1/5611 (0.0%)
All	All	0.70	0/8209	0.78	1/11085 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	222	ILE	N-CA-CB	5.85	114.19	110.50

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	3955	0	3928	20	0
1	B	4050	0	4020	24	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	93	0	36	2	0
3	B	62	0	24	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	30	0	12	0	0
6	A	347	0	0	6	0
6	B	472	0	0	6	0
All	All	9013	0	8020	45	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 3.

All (45) 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:355:GLU:HG3	6:A:1062:HOH:O	1.82	0.80
1:A:591:ILE:O	1:A:594:GLN:HG2	1.83	0.78
1:B:243:HIS:HE1	6:B:1370:HOH:O	1.66	0.77
1:B:179:VAL:HG22	1:B:300:ILE:HD13	1.70	0.72
1:A:158:PRO:HG3	6:A:1059:HOH:O	1.94	0.67
1:B:397:ILE:HG21	1:B:426:ILE:HD11	1.77	0.64
1:A:115:MET:HE1	1:A:127:GLU:CD	2.23	0.64
1:B:509:MET:HE1	1:B:517:HIS:CD2	2.35	0.62
1:A:326:GLN:NE2	6:A:1093:HOH:O	2.32	0.61
1:A:485:PRO:HG2	1:A:489:LEU:HD11	1.83	0.59
1:B:397:ILE:HB	6:B:1054:HOH:O	2.03	0.58
1:B:175:ALA:HB1	1:B:199:VAL:HG12	1.86	0.57
1:A:395:ASP:OD1	1:A:408:ARG:NH2	2.39	0.56
1:B:179:VAL:CG2	1:B:300:ILE:HD13	2.35	0.56
1:A:494:LYS:HG3	1:A:496:GLU:HG2	1.90	0.53
3:A:703:DGT:N2	6:A:859:HOH:O	2.34	0.52
1:A:397:ILE:HG21	1:A:426:ILE:HD11	1.90	0.52
1:A:143:ARG:HD2	1:A:420:THR:HA	1.91	0.51
1:A:446:LYS:HE2	6:A:1147:HOH:O	2.09	0.51
1:A:439:LYS:O	1:A:443:GLU:HG2	2.10	0.51
1:B:297:LEU:HA	1:B:300:ILE:HD12	1.93	0.49
3:A:703:DGT:HN2A	1:B:119:ASN:ND2	2.11	0.49
1:A:175:ALA:HB1	1:A:199:VAL:HG12	1.95	0.48
1:B:302:SER:O	6:B:905:HOH:O	2.20	0.48
1:A:331:TYR:C	1:A:331:TYR:CD1	2.92	0.47
1:A:302:SER:O	6:A:805:HOH:O	2.21	0.46
1:B:478:LYS:HD3	6:B:980:HOH:O	2.16	0.45
1:B:595:LYS:HE3	1:B:597:GLU:HG2	1.97	0.45
1:A:381:ILE:HD12	1:A:381:ILE:HA	1.84	0.45
1:A:390:PHE:CZ	1:A:426:ILE:HG23	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:ALA:O	1:B:520:PHE:HA	2.17	0.45
1:B:577:ASN:HD21	1:B:597:GLU:HG3	1.81	0.45
1:B:143:ARG:HD2	1:B:420:THR:HA	1.98	0.44
1:A:351:ALA:O	1:A:520:PHE:HA	2.17	0.44
1:B:179:VAL:HG22	1:B:300:ILE:CD1	2.45	0.44
1:B:331:TYR:CD1	1:B:331:TYR:C	2.95	0.44
1:B:215[A]:HIS:CD2	6:B:1252:HOH:O	2.70	0.44
1:B:179:VAL:HG21	1:B:199:VAL:HG11	2.00	0.43
1:B:580:LYS:HE3	1:B:592:THR:HG21	2.00	0.43
1:B:381:ILE:HD12	1:B:381:ILE:HA	1.91	0.43
1:B:390:PHE:CZ	1:B:426:ILE:HG23	2.54	0.42
1:A:291:PRO:HG2	1:A:293:ASN:OD1	2.20	0.41
1:B:179:VAL:CG2	1:B:199:VAL:HG11	2.50	0.41
1:B:417:GLU:OE2	6:B:1272:HOH:O	2.22	0.40
1:A:334:PHE:CE2	1:A:359:LEU:HD21	2.56	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	479/539 (89%)	471 (98%)	8 (2%)	0	100	100
1	B	491/539 (91%)	483 (98%)	8 (2%)	0	100	100
All	All	970/1078 (90%)	954 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	704	4	32,33,33	1.19	3 (9%)	48,52,52	1.74	7 (14%)
3	DGT	A	702	-	32,33,33	1.43	4 (12%)	48,52,52	1.83	5 (10%)
3	DGT	B	804	-	32,33,33	1.38	5 (15%)	48,52,52	1.86	11 (22%)
3	DGT	B	801	4	32,33,33	1.22	3 (9%)	48,52,52	1.72	8 (16%)
5	DTP	B	805	4	31,32,32	1.28	3 (9%)	46,50,50	1.98	13 (28%)
3	DGT	A	703	4	32,33,33	1.22	3 (9%)	48,52,52	1.77	10 (20%)

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	704	4	-	9/22/34/34	0/3/3/3
3	DGT	A	702	-	-	4/22/34/34	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DGT	B	804	-	-	2/22/34/34	0/3/3/3
3	DGT	B	801	4	-	8/22/34/34	0/3/3/3
5	DTP	B	805	4	-	3/22/34/34	0/3/3/3
3	DGT	A	703	4	-	4/22/34/34	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	DGT	PB-O3A	4.11	1.63	1.59
3	B	804	DGT	PB-O3A	3.30	1.63	1.59
5	B	805	DTP	C5-C4	3.20	1.44	1.39
3	B	804	DGT	PA-O3A	3.09	1.62	1.59
3	A	702	DGT	PA-O3A	3.04	1.62	1.59
3	A	702	DGT	C5-C4	3.00	1.47	1.38
5	B	805	DTP	C8-N7	2.77	1.37	1.31
3	B	801	DGT	C5-C4	2.68	1.46	1.38
3	A	703	DGT	PB-O3A	2.64	1.62	1.59
3	A	703	DGT	C5-N7	-2.63	1.33	1.39
3	A	704	DGT	C5-C4	2.59	1.45	1.38
5	B	805	DTP	C5-N7	-2.51	1.34	1.39
3	A	703	DGT	C5-C4	2.51	1.45	1.38
3	A	704	DGT	C5-N7	-2.48	1.34	1.39
3	B	804	DGT	C5-C4	2.48	1.45	1.38
3	A	702	DGT	C5-N7	-2.41	1.34	1.39
3	B	801	DGT	C5-N7	-2.36	1.34	1.39
3	B	804	DGT	C5-N7	-2.15	1.34	1.39
3	B	801	DGT	PB-O3A	2.07	1.61	1.59
3	A	704	DGT	PB-O3A	2.03	1.61	1.59
3	B	804	DGT	PB-O3B	2.00	1.61	1.59

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	DGT	C5-C4-N3	-6.11	118.67	128.39
3	B	804	DGT	C5-C4-N3	-6.08	118.71	128.39
3	B	801	DGT	C5-C4-N3	-5.66	119.38	128.39
3	A	704	DGT	C5-C4-N3	-5.62	119.44	128.39
3	A	702	DGT	C2-N3-C4	5.60	121.94	112.30
3	A	703	DGT	C5-C4-N3	-5.44	119.72	128.39
3	B	804	DGT	C2-N3-C4	5.38	121.56	112.30
5	B	805	DTP	C5-C4-N3	-5.14	119.64	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	801	DGT	C2-N3-C4	5.00	120.92	112.30
3	A	704	DGT	C2-N3-C4	4.95	120.83	112.30
3	A	703	DGT	C2-N3-C4	4.93	120.80	112.30
3	A	702	DGT	N9-C4-N3	4.89	135.72	125.95
3	B	804	DGT	N9-C4-N3	4.78	135.51	125.95
5	B	805	DTP	N3-C2-N1	-4.71	121.45	128.58
3	A	704	DGT	N9-C4-N3	4.51	134.97	125.95
3	B	801	DGT	N9-C4-N3	4.45	134.86	125.95
5	B	805	DTP	N3-C4-N9	4.05	134.05	127.17
3	A	703	DGT	N9-C4-N3	4.01	133.97	125.95
5	B	805	DTP	C2-N3-C4	3.78	121.06	111.83
3	B	804	DGT	O6-C6-C5	-3.62	116.99	126.53
5	B	805	DTP	C4-N9-C8	3.46	109.37	105.74
5	B	805	DTP	N9-C8-N7	-3.40	109.11	113.94
3	A	702	DGT	O6-C6-C5	-3.29	117.83	126.53
3	A	703	DGT	O6-C6-C5	-3.10	118.36	126.53
5	B	805	DTP	C4-C5-N7	-2.99	107.16	110.58
5	B	805	DTP	C5-N7-C8	2.93	108.06	103.45
5	B	805	DTP	O2B-PB-O3A	-2.91	99.41	107.27
3	A	703	DGT	C6-C5-N7	2.85	135.48	130.29
5	B	805	DTP	O2B-PB-O3B	2.82	114.89	107.27
3	A	704	DGT	O2G-PG-O3B	2.81	114.07	104.64
5	B	805	DTP	N6-C6-N1	2.67	124.33	118.38
5	B	805	DTP	C2-N1-C6	2.67	123.12	118.73
3	A	702	DGT	C6-C5-N7	2.65	135.11	130.29
3	A	704	DGT	O6-C6-C5	-2.62	119.62	126.53
3	B	804	DGT	C6-C5-N7	2.59	135.01	130.29
3	B	801	DGT	O6-C6-C5	-2.43	120.11	126.53
3	B	801	DGT	O1A-PA-O3A	2.42	113.82	107.27
3	B	801	DGT	C6-C5-N7	2.40	134.65	130.29
3	A	704	DGT	C6-C5-N7	2.37	134.61	130.29
3	A	703	DGT	O3A-PB-O2B	-2.37	103.57	110.70
3	B	804	DGT	N9-C8-N7	-2.37	109.00	113.40
3	A	703	DGT	N9-C8-N7	-2.28	109.17	113.40
3	B	801	DGT	O2G-PG-O3B	2.28	112.27	104.64
3	A	703	DGT	C4-C5-N7	-2.27	107.08	110.67
3	B	804	DGT	O6-C6-N1	2.25	124.34	120.11
3	A	703	DGT	C8-N7-C5	2.21	108.19	104.26
3	B	804	DGT	C8-N9-C4	2.14	110.04	106.03
3	A	703	DGT	O6-C6-N1	2.14	124.13	120.11
3	B	804	DGT	C4-C5-N7	-2.13	107.29	110.67
3	B	804	DGT	C5-C6-N1	2.12	118.65	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	805	DTP	C5-C6-N6	-2.05	118.20	123.29
3	B	804	DGT	C8-N7-C5	2.03	107.89	104.26
3	B	801	DGT	C4-C5-N7	-2.03	107.46	110.67
3	A	704	DGT	C4-C5-N7	-2.00	107.49	110.67

There are no chirality outliers.

All (30) torsion outliers are listed below:

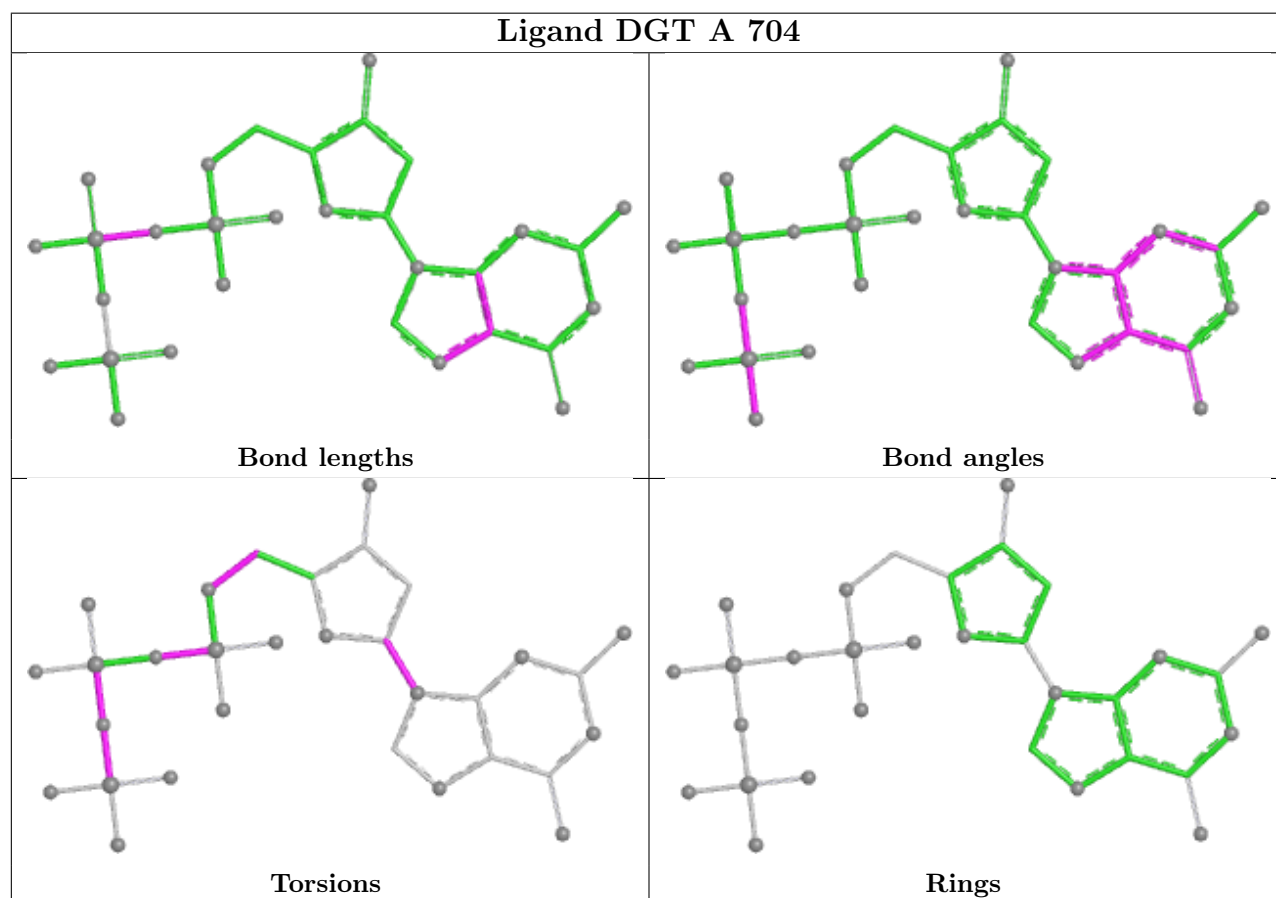
Mol	Chain	Res	Type	Atoms
3	A	702	DGT	PB-O3B-PG-O2G
3	B	804	DGT	PB-O3B-PG-O2G
3	A	704	DGT	PB-O3B-PG-O3G
3	B	801	DGT	PB-O3B-PG-O3G
3	B	804	DGT	PB-O3B-PG-O3G
5	B	805	DTP	PG-O3B-PB-O1B
3	A	704	DGT	PB-O3B-PG-O2G
3	B	801	DGT	PG-O3B-PB-O1B
3	A	704	DGT	C2'-C1'-N9-C8
3	B	801	DGT	C2'-C1'-N9-C8
3	A	704	DGT	PG-O3B-PB-O1B
5	B	805	DTP	PG-O3B-PB-O2B
3	B	801	DGT	C4'-C5'-O5'-PA
3	A	702	DGT	PG-O3B-PB-O2B
3	A	703	DGT	PG-O3B-PB-O2B
3	A	704	DGT	PB-O3A-PA-O1A
3	B	801	DGT	PB-O3A-PA-O1A
3	A	702	DGT	PB-O3B-PG-O1G
3	A	703	DGT	PG-O3B-PB-O1B
3	A	703	DGT	PB-O3A-PA-O2A
3	A	704	DGT	PB-O3A-PA-O2A
3	B	801	DGT	PG-O3B-PB-O2B
3	B	801	DGT	PB-O3A-PA-O2A
3	A	704	DGT	C2'-C1'-N9-C4
3	B	801	DGT	C2'-C1'-N9-C4
3	A	702	DGT	PB-O3B-PG-O3G
3	A	704	DGT	C4'-C5'-O5'-PA
3	A	703	DGT	PB-O3A-PA-O1A
3	A	704	DGT	PG-O3B-PB-O2B
5	B	805	DTP	PB-O3A-PA-O2A

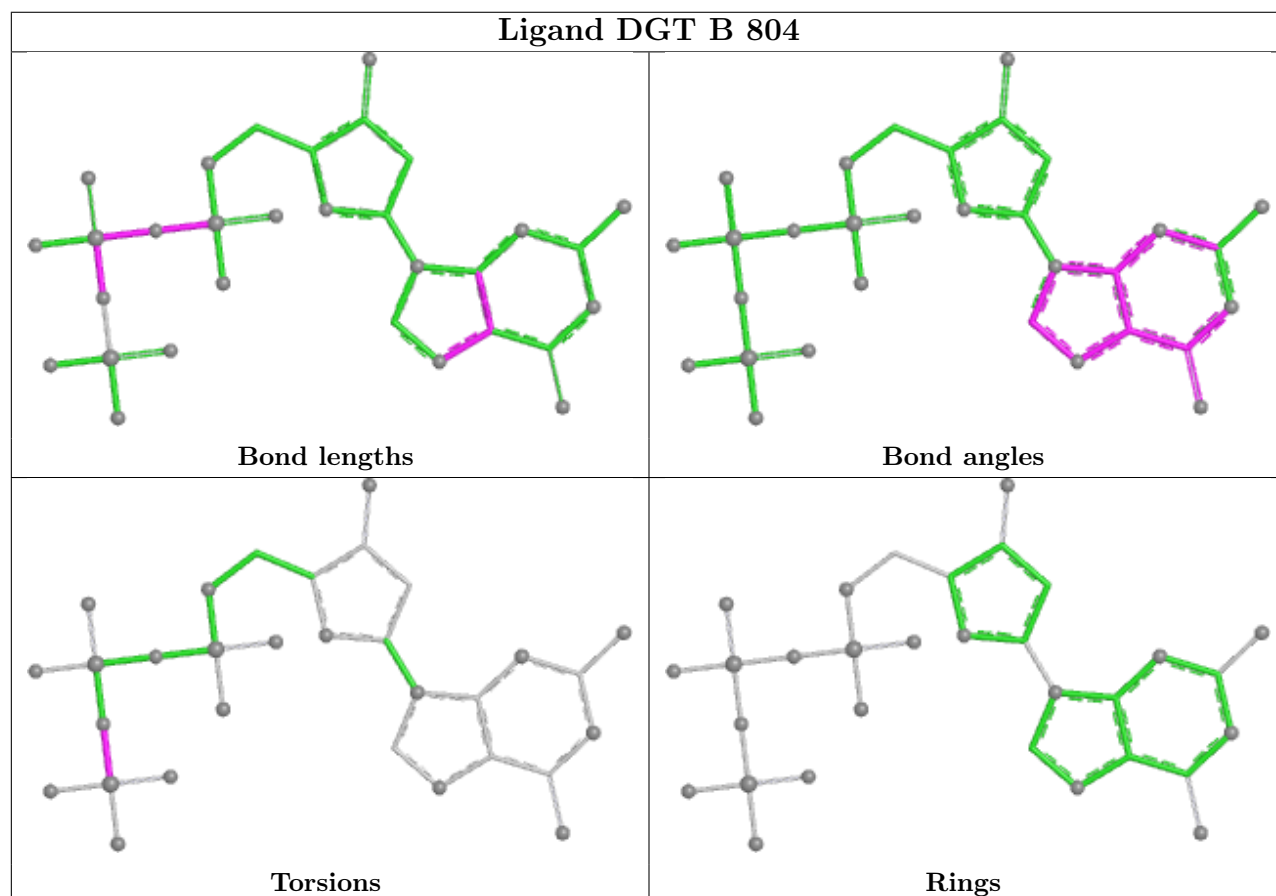
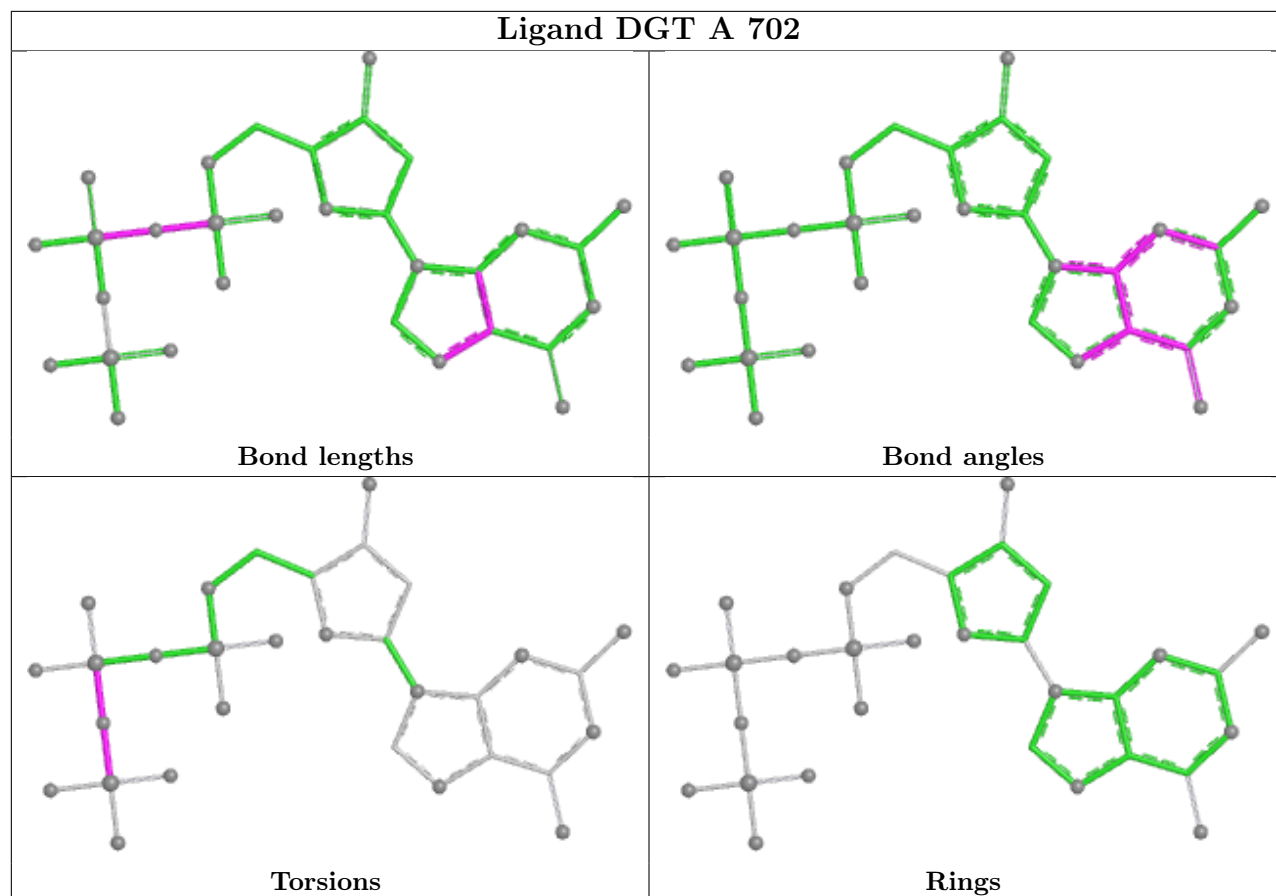
There are no ring outliers.

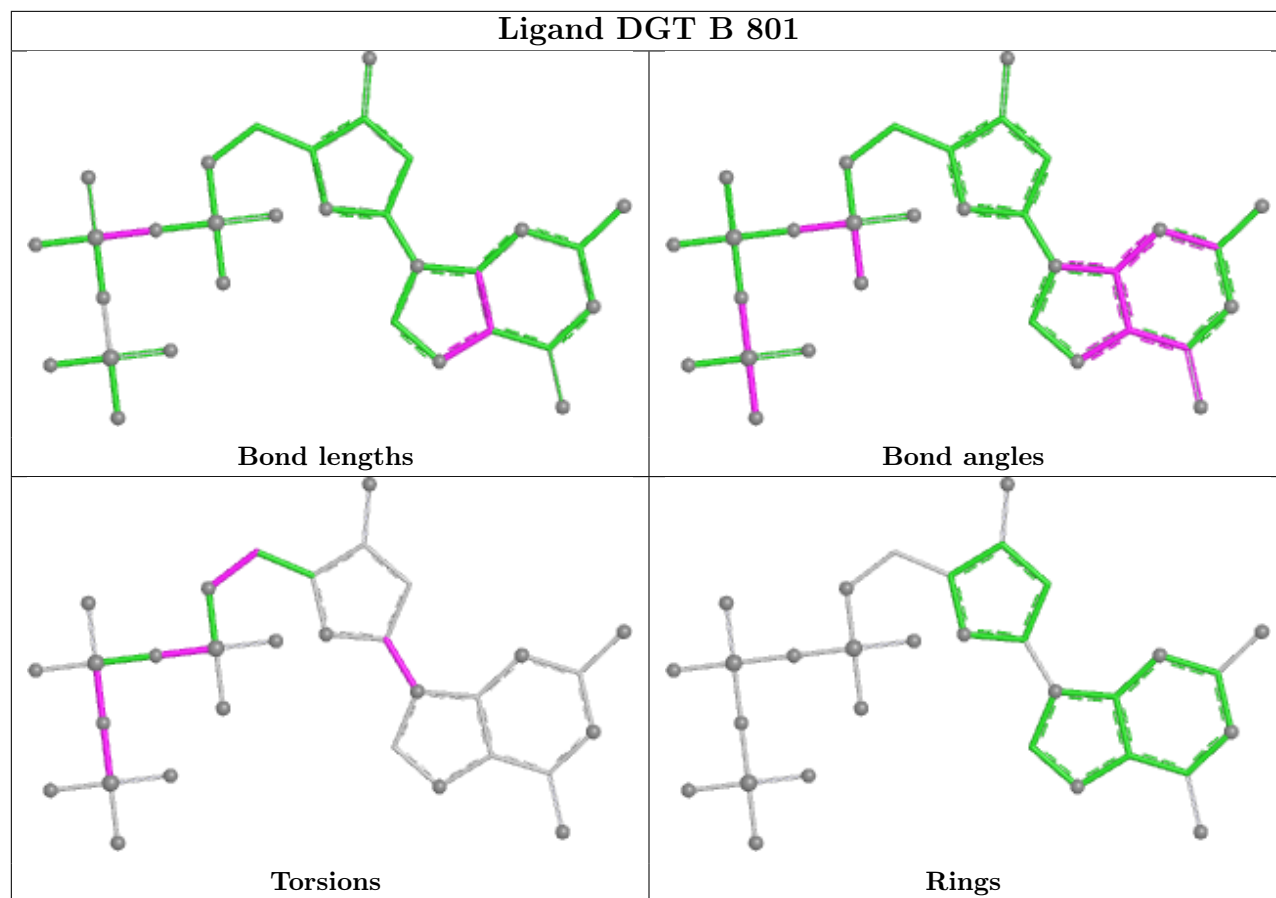
1 monomer is involved in 2 short contacts:

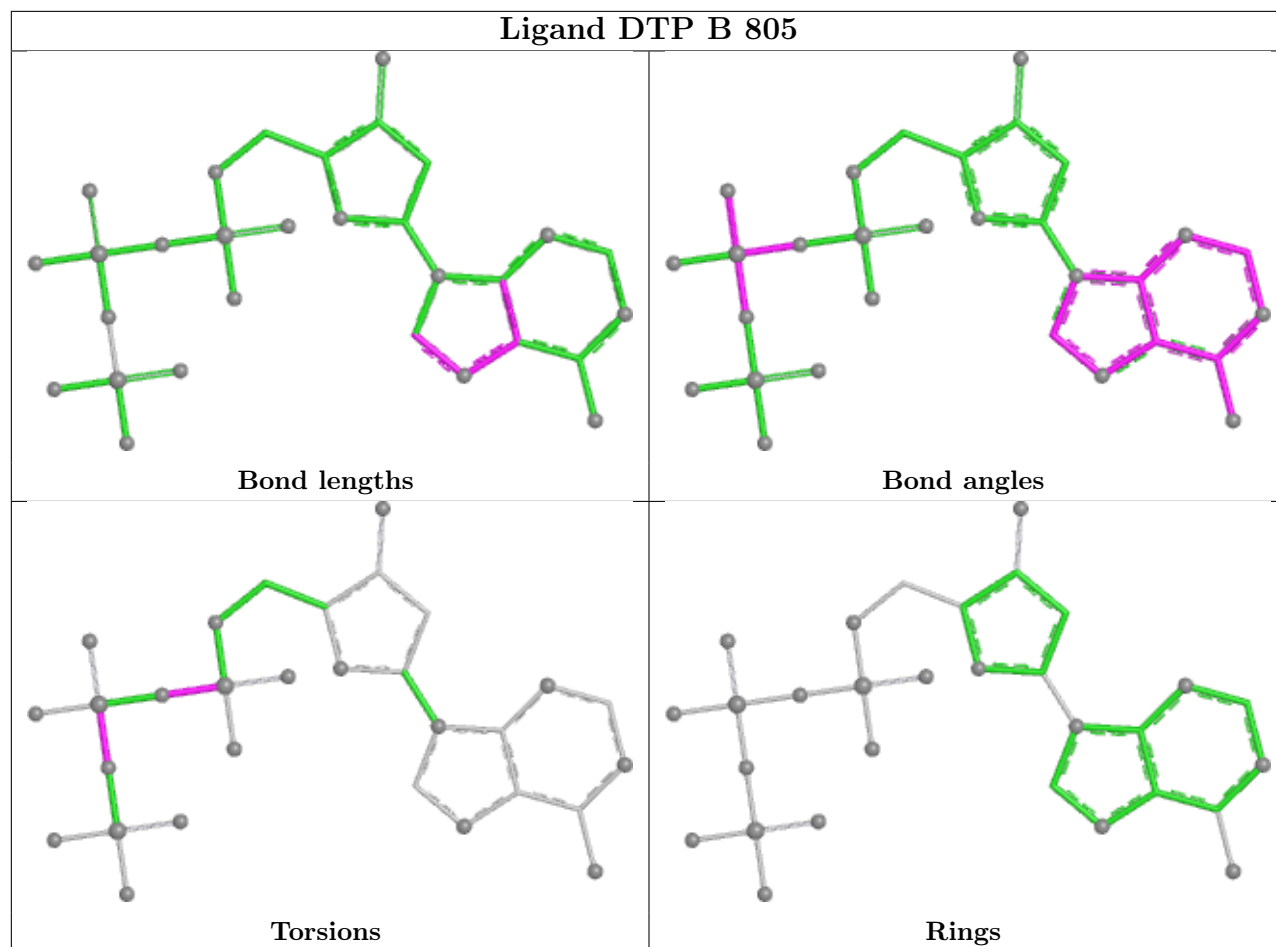
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	703	DGT	2	0

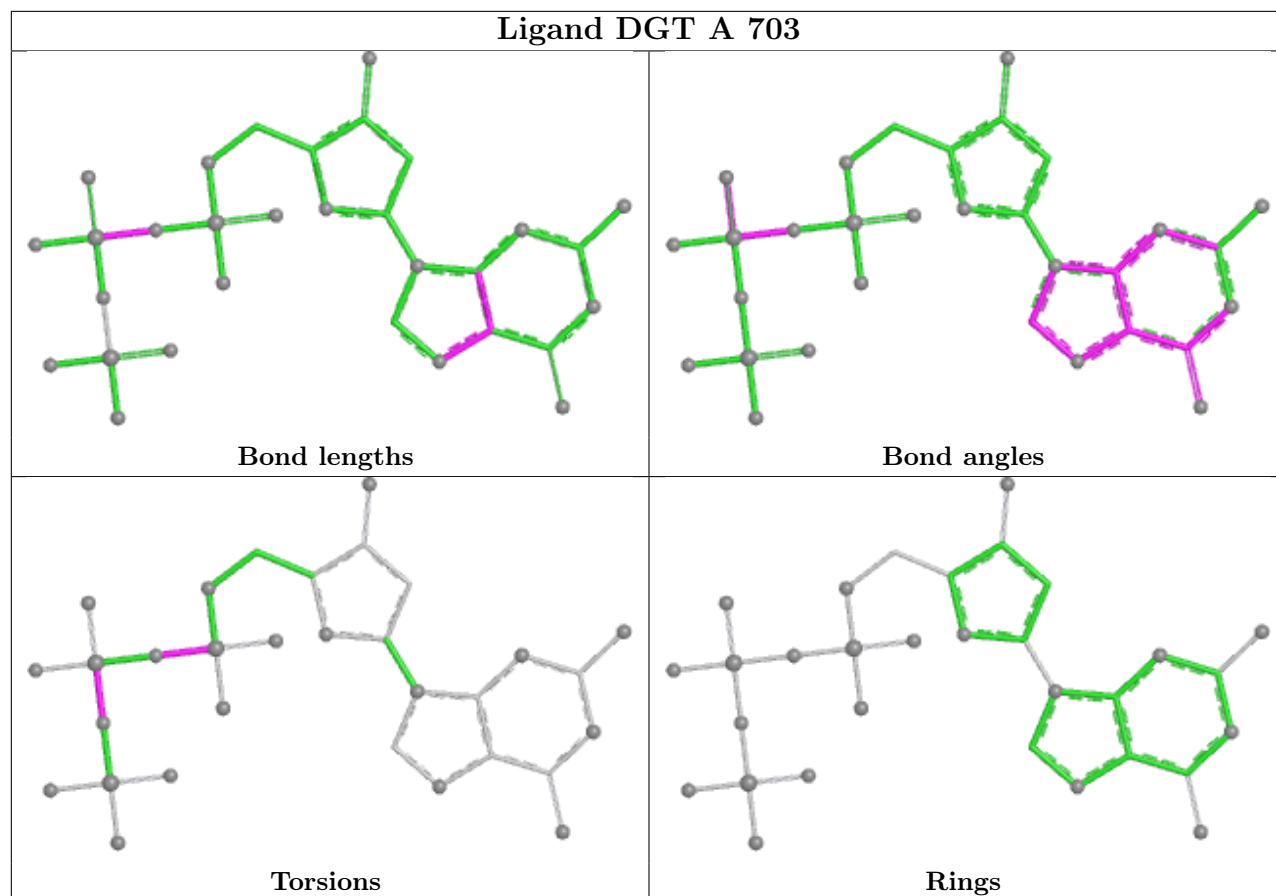
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	481/539 (89%)	0.65	60 (12%) 8 6	6, 22, 52, 77	2 (0%)
1	B	493/539 (91%)	0.25	29 (5%) 28 27	4, 17, 40, 81	2 (0%)
All	All	974/1078 (90%)	0.45	89 (9%) 15 13	4, 19, 46, 81	4 (0%)

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	284	LEU	5.8
1	A	488	LEU	5.7
1	A	466	ILE	5.7
1	A	489	LEU	4.9
1	B	111	HIS	4.7
1	A	487	VAL	4.7
1	B	284	LEU	4.5
1	A	491	VAL	4.4
1	B	110	ILE	4.4
1	B	112	VAL	4.2
1	A	464	GLY	3.8
1	B	328	ASN	3.8
1	A	285	TRP	3.7
1	A	590	LEU	3.7
1	A	593	PRO	3.7
1	B	113	ASP	3.6
1	A	598	TRP	3.6
1	A	574	ALA	3.6
1	B	114	THR	3.5
1	A	114	THR	3.5
1	B	403	GLY	3.5
1	A	577	ASN	3.3
1	A	592	THR	3.2
1	A	535	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	278	SER	3.2
1	A	328	ASN	3.1
1	A	230	LYS	3.0
1	A	403	GLY	3.0
1	A	468	ILE	3.0
1	B	104	TYR	3.0
1	A	470	ARG	2.9
1	B	102	ASN	2.9
1	B	593	PRO	2.9
1	A	496	GLU	2.9
1	A	345	ASN	2.8
1	A	595	LYS	2.8
1	A	277	GLU	2.8
1	A	344	ASP	2.8
1	A	599	ASN	2.8
1	B	466	ILE	2.8
1	B	230	LYS	2.7
1	A	594	GLN	2.7
1	B	115	MET	2.7
1	A	591	ILE	2.7
1	A	113	ASP	2.6
1	B	535	ASN	2.6
1	A	485	PRO	2.6
1	B	277	GLU	2.6
1	A	557	VAL	2.6
1	A	463	THR	2.6
1	A	490	ASP	2.5
1	B	490	ASP	2.5
1	A	587	ILE	2.5
1	B	491	VAL	2.4
1	A	486	LYS	2.4
1	A	596	LYS	2.4
1	A	562	LEU	2.4
1	A	471	GLU	2.4
1	A	556	LYS	2.4
1	A	291	PRO	2.3
1	A	229	VAL	2.3
1	A	326	GLN	2.3
1	A	473	TYR	2.3
1	A	563	TYR	2.3
1	A	467	LYS	2.3
1	A	327	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	467	LYS	2.3
1	A	483	ALA	2.3
1	A	543	GLU	2.3
1	B	345	ASN	2.3
1	B	103	LEU	2.3
1	A	559	ARG	2.2
1	A	465	GLN	2.2
1	B	107	GLY	2.2
1	B	464	GLY	2.2
1	A	115	MET	2.2
1	B	599	ASN	2.2
1	A	405	LYS	2.2
1	A	564	ALA	2.2
1	B	406	LYS	2.2
1	A	568	TYR	2.1
1	B	397	ILE	2.1
1	A	584	GLY	2.1
1	A	474	GLU	2.1
1	A	527	ASN	2.1
1	A	481	ALA	2.1
1	B	474	GLU	2.0
1	A	404	GLY	2.0
1	B	594	GLN	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](#)

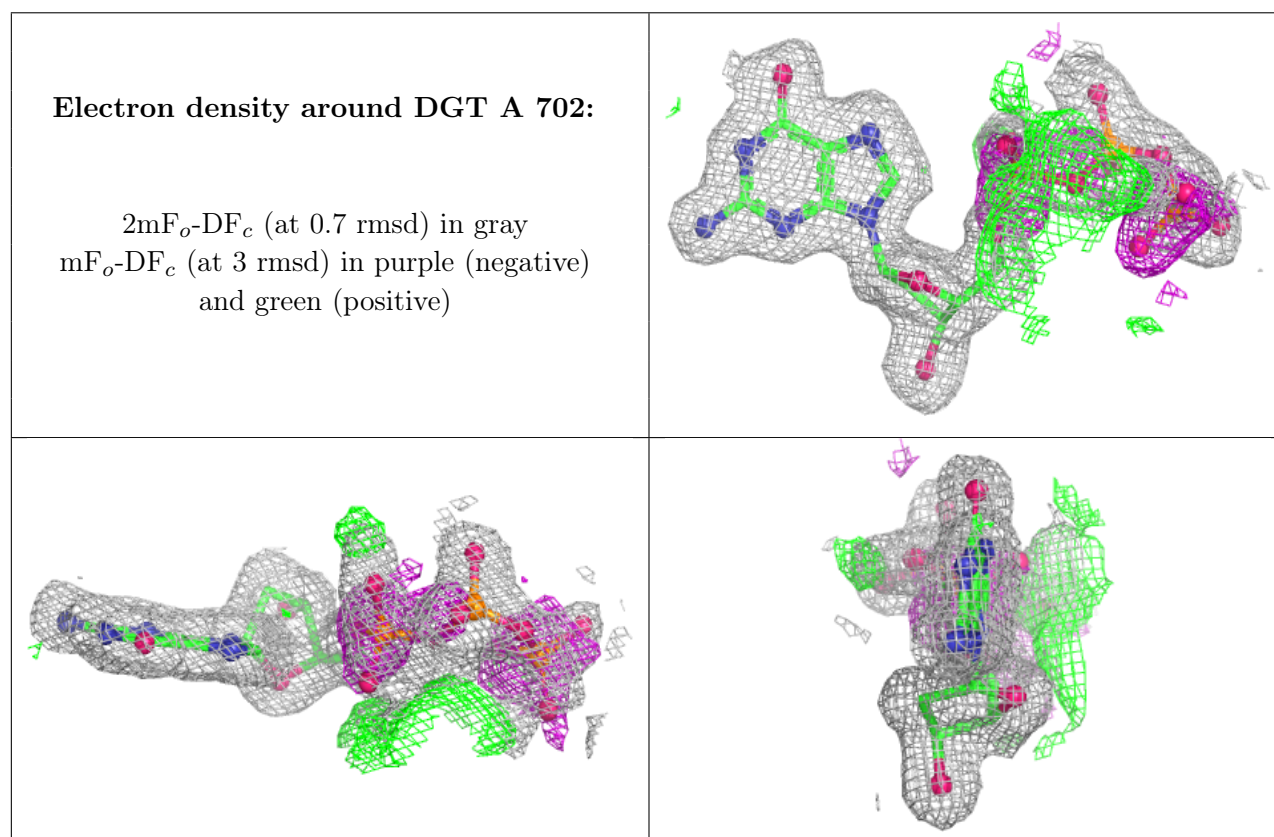
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

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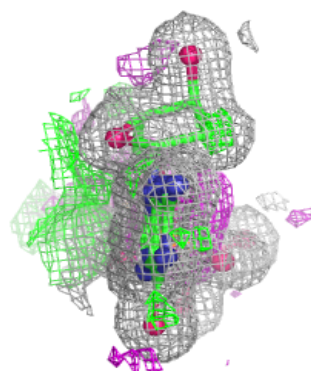
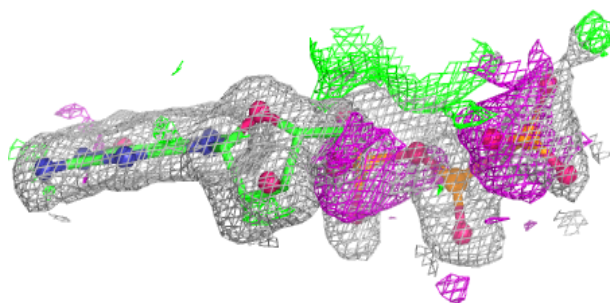
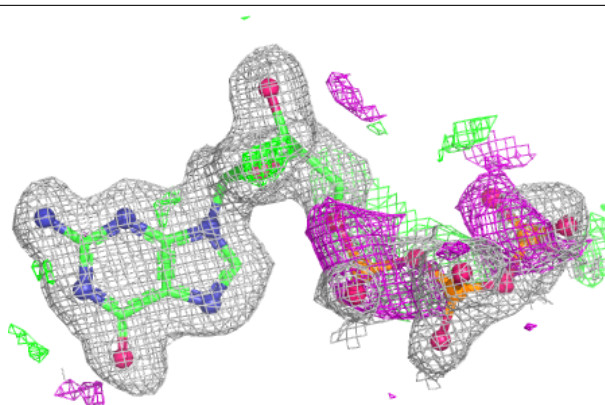
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	DGT	A	702	31/31	0.87	0.13	10,17,43,47	0
3	DGT	B	804	31/31	0.89	0.12	7,13,38,39	0
4	MG	A	705	1/1	0.96	0.08	16,16,16,16	0
4	MG	B	802	1/1	0.96	0.08	19,19,19,19	0
3	DGT	B	801	31/31	0.97	0.05	9,11,20,22	0
3	DGT	A	703	31/31	0.98	0.05	8,11,15,17	0
3	DGT	A	704	31/31	0.98	0.04	8,9,15,16	0
5	DTP	B	805	30/30	0.98	0.04	6,8,11,12	0
2	ZN	A	701	1/1	0.99	0.03	14,14,14,14	0
2	ZN	B	803	1/1	0.99	0.03	11,11,11,11	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.

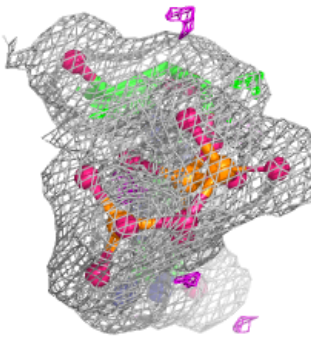
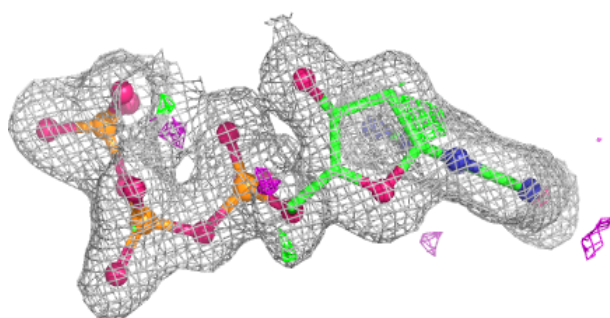
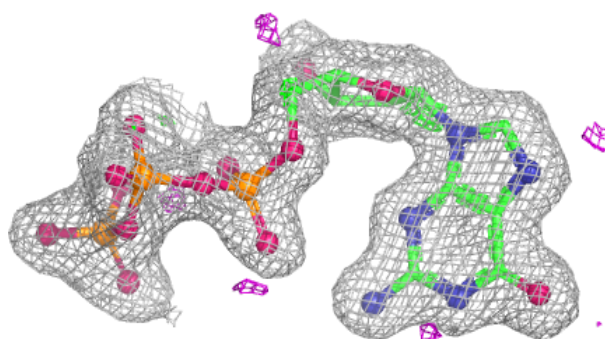


Electron density around DGT B 804:

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

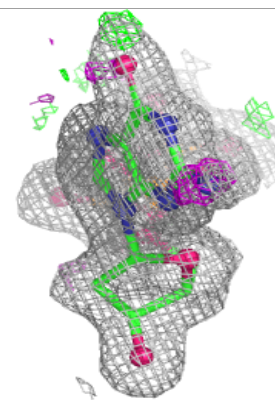
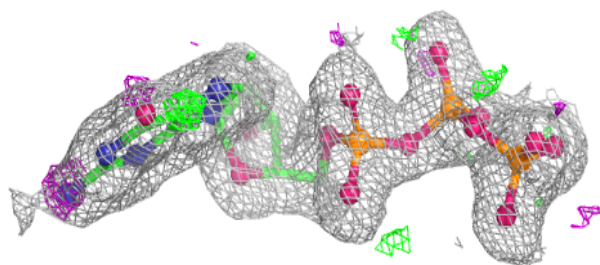
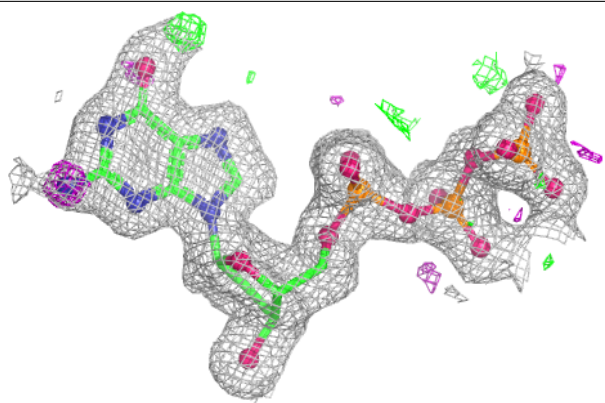
**Electron density around DGT B 801:**

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

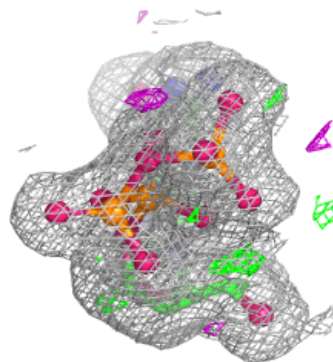
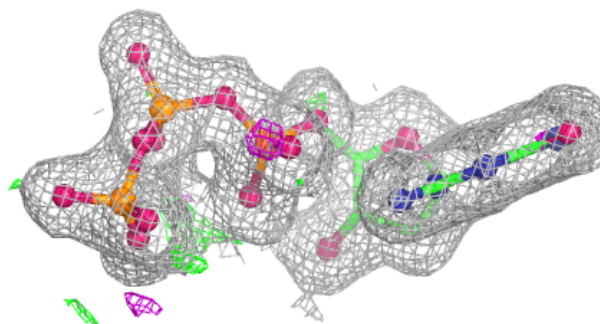
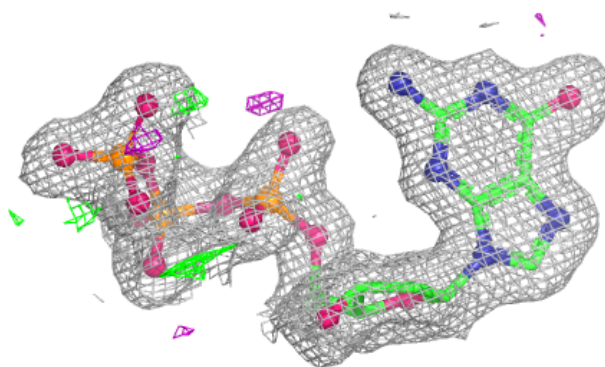


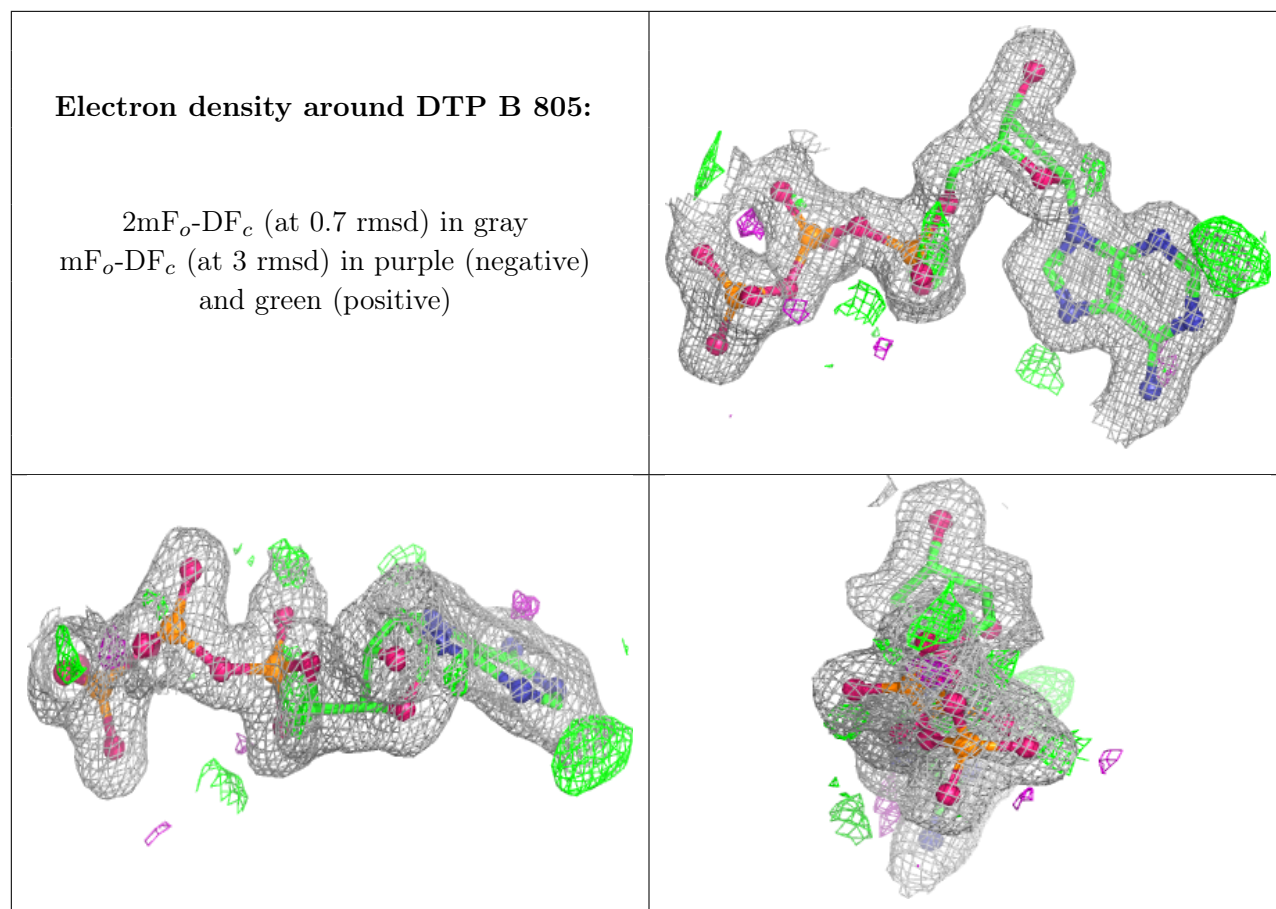
Electron density around DGT A 703:

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

**Electron density around DGT A 704:**

$2mF_o-DF_c$ (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.