



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2022 – 06:27 PM EDT

PDB ID : 4TO6  
Title : Structure basis of cellular dNTP regulation, SAMHD1-dGTP-dATP-dTTP/d  
GTP complex  
Authors : Ji, X.; Tang, C.; Zhao, Q.; Wang, W.; Xiong, Y.  
Deposited on : 2014-06-05  
Resolution : 2.33 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 : 2.27  
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) : 2.27

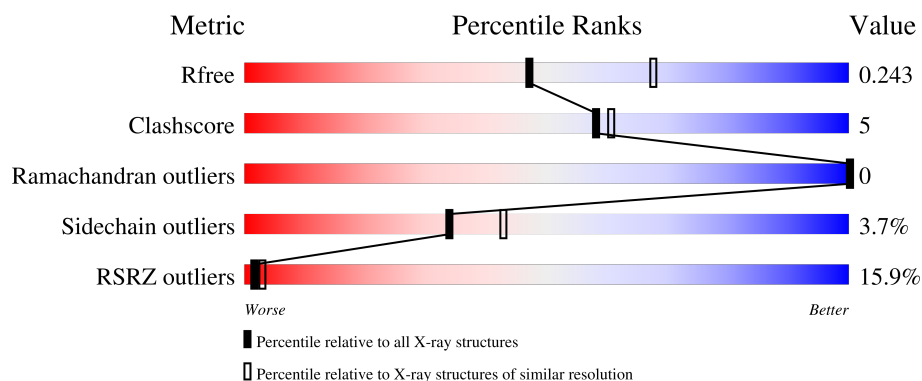
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.33 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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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  $\geq 3$ , 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	514	<div> <div>7%</div> <div> <div></div> <div>82%</div> <div>10%</div> <div>7%</div> </div> </div>
1	B	514	<div> <div>10%</div> <div> <div></div> <div>83%</div> <div>10%</div> <div>7%</div> </div> </div>
1	C	514	<div> <div>23%</div> <div> <div></div> <div>82%</div> <div>11%</div> <div>7%</div> </div> </div>
1	D	514	<div> <div>19%</div> <div> <div></div> <div>82%</div> <div>10%</div> <div>7%</div> </div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16098 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.

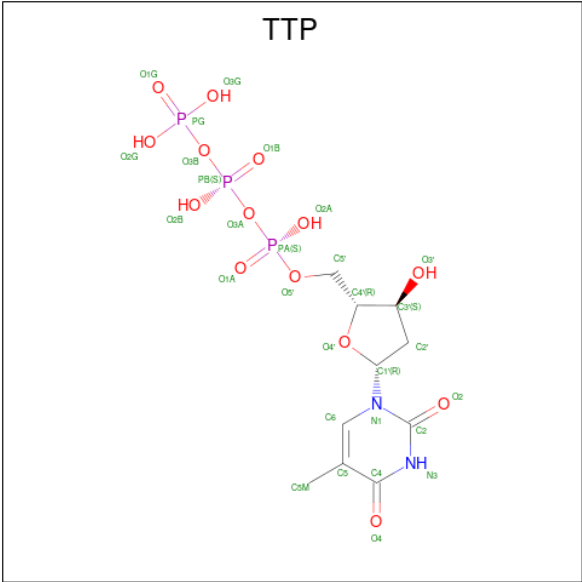
- Molecule 1 is a protein called Deoxynucleoside triphosphate triphosphohydrolase SAMHD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	480	Total	C	N	O	S	0	0	0
			3925	2513	684	708	20			
1	B	480	Total	C	N	O	S	0	0	0
			3925	2513	684	708	20			
1	C	480	Total	C	N	O	S	0	0	0
			3925	2513	684	708	20			
1	D	480	Total	C	N	O	S	0	0	0
			3925	2513	684	708	20			

There are 8 discrepancies between the modelled and reference sequences:

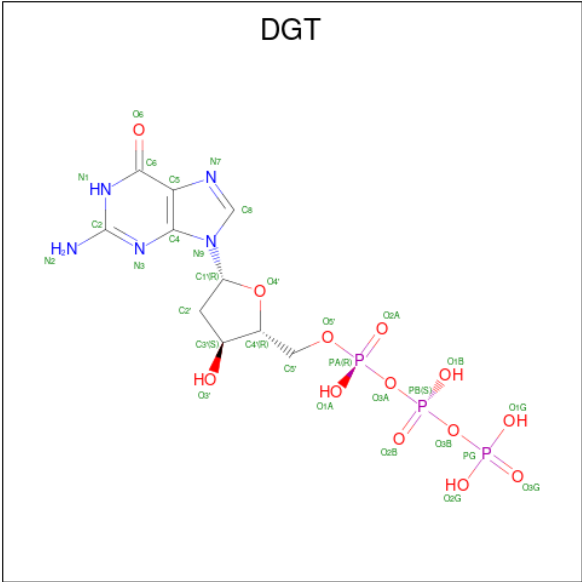
Chain	Residue	Modelled	Actual	Comment	Reference
A	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
A	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
B	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
B	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
C	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
C	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
D	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
D	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3

- Molecule 2 is THYMIDINE-5'-TRIPHOSPHATE (three-letter code: TTP) (formula:  $C_{10}H_{17}N_2O_{14}P_3$ ).



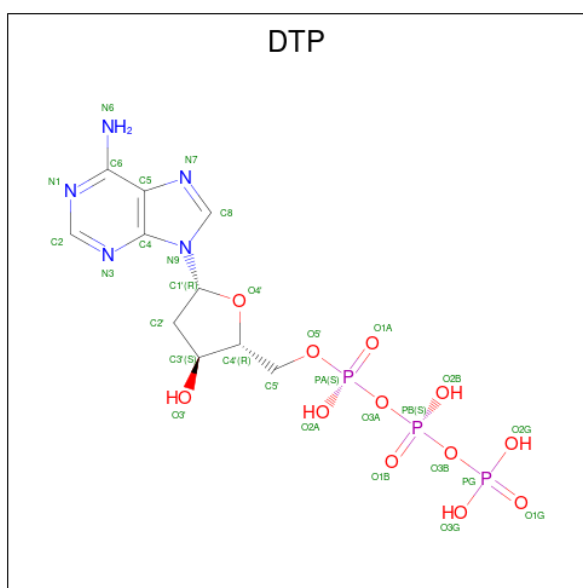
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
2	B	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
2	D	1	Total	C	N	O	P	0	0
			29	10	2	14	3		

- 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		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula:  $C_{10}H_{16}N_5O_{12}P_3$ ).



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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Mg 1	0	0
5	B	1	Total 1	Mg 1	0	0
5	C	1	Total 1	Mg 1	0	0
5	D	1	Total 1	Mg 1	0	0

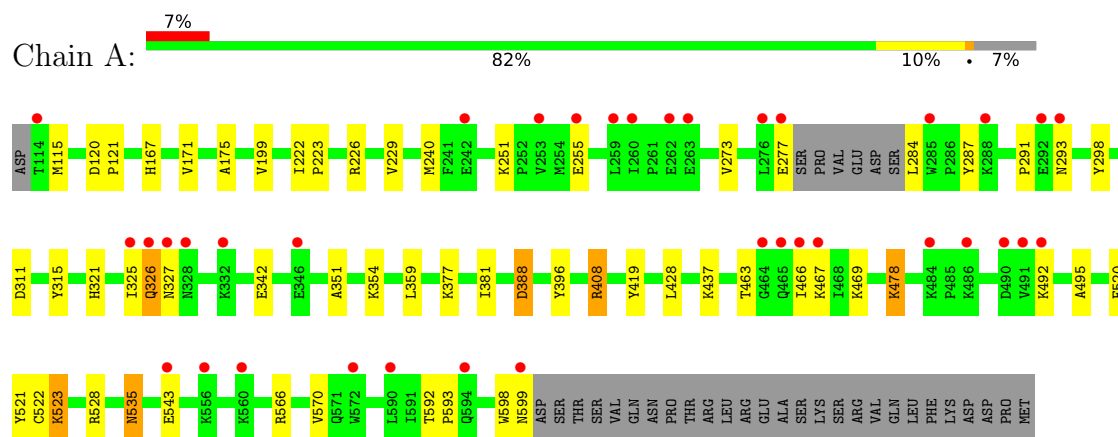
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	16	Total 16	O 16	0	0
6	B	4	Total 4	O 4	0	0
6	C	5	Total 5	O 5	0	0
6	D	7	Total 7	O 7	0	0

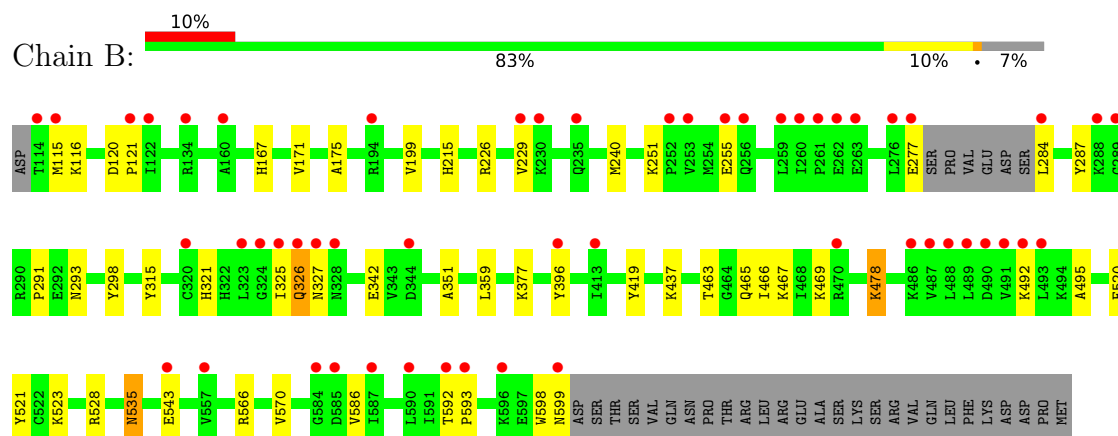
### 3 Residue-property plots

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.

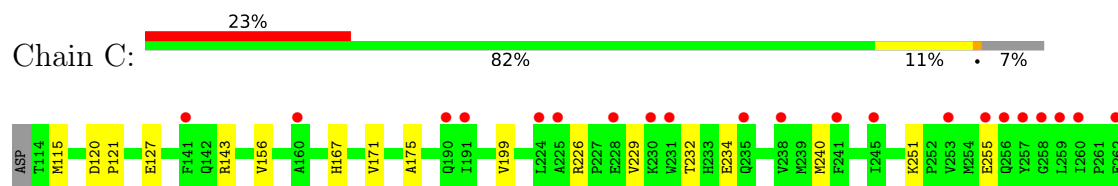
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

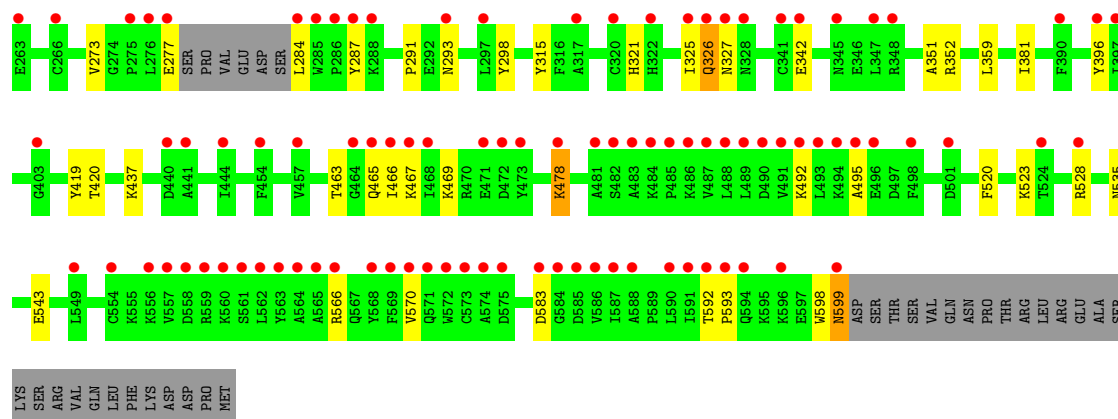


- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

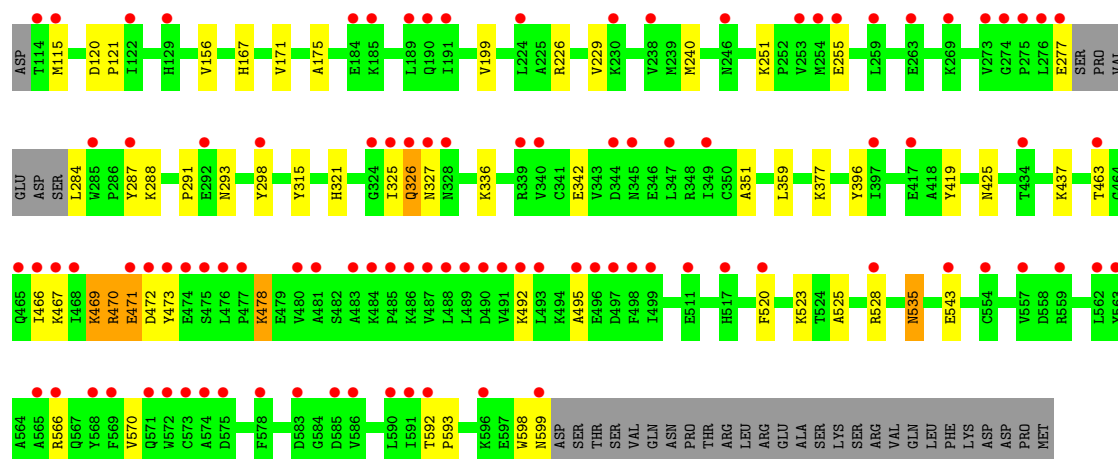
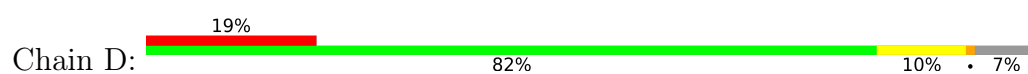


- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1





● Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.59Å 140.81Å 96.90Å 90.00° 114.94° 90.00°	Depositor
Resolution (Å)	50.00 – 2.33 47.89 – 2.33	Depositor EDS
% Data completeness (in resolution range)	99.4 (50.00-2.33) 99.4 (47.89-2.33)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.69 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.225 , 0.244 0.226 , 0.243	Depositor DCC
$R_{free}$ test set	4259 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.5	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 54.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.037 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	16098	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DTP, MG, TTP, 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	0.62	0/4017	0.72	3/5422 (0.1%)
1	B	0.57	0/4017	0.69	0/5422
1	C	0.57	0/4017	0.69	0/5422
1	D	0.56	0/4017	0.68	0/5422
All	All	0.58	0/16068	0.69	3/21688 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	388	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	A	408	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	A	388	ASP	CB-CG-OD1	5.52	123.27	118.30

There are no chirality outliers.

There are no planarity outliers.

### 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	3925	0	3917	37	1
1	B	3925	0	3917	34	2
1	C	3925	0	3917	35	1
1	D	3925	0	3917	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	29	0	13	1	0
2	B	29	0	13	1	0
2	D	29	0	13	0	0
3	A	31	0	12	0	0
3	B	31	0	12	0	0
3	C	62	0	24	5	0
3	D	31	0	12	2	0
4	A	30	0	12	1	0
4	B	30	0	12	2	0
4	C	30	0	12	3	0
4	D	30	0	12	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	16	0	0	1	0
6	B	4	0	0	0	0
6	C	5	0	0	0	0
6	D	7	0	0	1	0
All	All	16098	0	15815	154	2

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 5.

All (154) 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:D:469:LYS:HE3	1:D:470:ARG:N	1.62	1.15
1:C:598:TRP:O	1:C:599:ASN:HB2	1.49	1.10
1:D:469:LYS:NZ	1:D:469:LYS:HA	1.73	1.03
1:D:470:ARG:HA	1:D:473:TYR:CE2	1.94	1.03
1:D:469:LYS:HE3	1:D:470:ARG:H	0.86	1.02
1:B:116:LYS:NZ	3:C:704:DGT:O3G	2.02	0.92
1:D:470:ARG:NH1	1:D:471:GLU:HB3	1.87	0.90
1:D:470:ARG:HA	1:D:473:TYR:CZ	2.11	0.86
1:D:469:LYS:HA	1:D:469:LYS:HZ2	1.39	0.85
1:D:469:LYS:HB3	1:D:471:GLU:OE2	1.76	0.84
1:D:469:LYS:CE	1:D:470:ARG:H	1.82	0.84
1:A:523:LYS:NZ	3:C:704:DGT:O1G	2.10	0.83
1:D:470:ARG:NH1	1:D:471:GLU:CB	2.42	0.83
1:C:598:TRP:O	1:C:599:ASN:CB	2.31	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:470:ARG:NH1	1:D:471:GLU:CA	2.47	0.78
1:D:470:ARG:CZ	1:D:471:GLU:HB3	2.15	0.77
1:B:326:GLN:HG2	1:D:326:GLN:HE21	1.51	0.76
1:B:326:GLN:HE21	1:D:326:GLN:HG2	1.51	0.75
1:D:469:LYS:CE	1:D:470:ARG:HG3	2.21	0.69
1:D:470:ARG:HA	1:D:473:TYR:CD2	2.27	0.69
1:D:469:LYS:HA	1:D:469:LYS:CE	2.22	0.68
1:D:469:LYS:HE2	1:D:470:ARG:HG3	1.75	0.68
1:D:470:ARG:NH1	1:D:471:GLU:HA	2.11	0.65
1:D:470:ARG:CA	1:D:473:TYR:CE2	2.78	0.64
1:A:354:LYS:NZ	4:A:703:DTP:O1A	2.30	0.63
1:A:521:TYR:CD1	1:A:521:TYR:O	2.52	0.63
1:D:469:LYS:HD3	1:D:470:ARG:HD3	1.79	0.63
1:D:470:ARG:HH11	1:D:471:GLU:HA	1.61	0.62
1:D:471:GLU:OE2	1:D:471:GLU:N	2.32	0.62
1:A:326:GLN:HE21	1:C:326:GLN:HG2	1.64	0.61
1:A:326:GLN:HG2	1:C:326:GLN:HE21	1.64	0.61
1:D:469:LYS:CE	1:D:469:LYS:CA	2.79	0.61
1:D:291:PRO:HG2	1:D:293:ASN:OD1	2.02	0.60
1:B:521:TYR:O	1:B:521:TYR:CD1	2.53	0.60
1:B:291:PRO:HG2	1:B:293:ASN:OD1	2.02	0.59
1:A:291:PRO:HG2	1:A:293:ASN:OD1	2.02	0.59
1:B:543:GLU:HG3	1:D:543:GLU:HG3	1.84	0.59
1:D:470:ARG:NE	1:D:471:GLU:N	2.50	0.59
1:C:120:ASP:OD1	1:C:121:PRO:HD2	2.02	0.59
1:A:120:ASP:OD1	1:A:121:PRO:HD2	2.01	0.59
1:C:291:PRO:HG2	1:C:293:ASN:OD1	2.03	0.59
1:D:471:GLU:CD	1:D:472:ASP:OD1	2.41	0.58
1:D:120:ASP:OD1	1:D:121:PRO:HD2	2.03	0.58
1:B:120:ASP:OD1	1:B:121:PRO:HD2	2.03	0.58
1:A:175:ALA:HB1	1:A:199:VAL:HG12	1.86	0.57
1:C:463:THR:O	1:C:466:ILE:HG12	2.04	0.57
1:C:175:ALA:HB1	1:C:199:VAL:HG12	1.87	0.57
1:B:463:THR:O	1:B:466:ILE:HG12	2.05	0.56
1:A:463:THR:O	1:A:466:ILE:HG12	2.04	0.56
1:B:175:ALA:HB1	1:B:199:VAL:HG12	1.88	0.56
1:D:175:ALA:HB1	1:D:199:VAL:HG12	1.87	0.56
1:D:463:THR:O	1:D:466:ILE:HG12	2.05	0.56
1:A:522:CYS:SG	1:C:583:ASP:HB3	2.47	0.55
1:A:521:TYR:CD1	1:A:521:TYR:C	2.80	0.55
1:B:521:TYR:CD1	1:B:521:TYR:C	2.80	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:TYR:O	6:A:812:HOH:O	2.18	0.54
1:D:469:LYS:HE3	1:D:470:ARG:HG3	1.89	0.54
1:A:396:TYR:CD1	1:A:437:LYS:HD2	2.44	0.53
1:D:396:TYR:CD1	1:D:437:LYS:HD2	2.43	0.53
1:B:226:ARG:O	1:B:229:VAL:HG12	2.09	0.53
1:B:396:TYR:CD1	1:B:437:LYS:HD2	2.44	0.52
1:C:226:ARG:O	1:C:229:VAL:HG12	2.10	0.52
1:C:396:TYR:CD1	1:C:437:LYS:HD2	2.44	0.52
1:A:377:LYS:NZ	4:C:701:DTP:O1B	2.43	0.52
1:D:226:ARG:O	1:D:229:VAL:HG12	2.09	0.52
1:C:566:ARG:O	1:C:570:VAL:HG23	2.10	0.51
1:D:470:ARG:CZ	1:D:471:GLU:N	2.73	0.51
1:D:470:ARG:HB3	1:D:473:TYR:CE2	2.45	0.51
1:B:566:ARG:O	1:B:570:VAL:HG23	2.10	0.51
1:A:226:ARG:O	1:A:229:VAL:HG12	2.11	0.50
1:D:566:ARG:O	1:D:570:VAL:HG23	2.11	0.50
1:A:566:ARG:O	1:A:570:VAL:HG23	2.11	0.50
1:B:543:GLU:HG2	1:D:543:GLU:HG2	1.92	0.50
1:C:156:VAL:O	3:C:704:DGT:H8	2.12	0.49
1:D:288:LYS:NZ	6:D:801:HOH:O	2.38	0.49
3:C:703:DGT:O1B	3:C:703:DGT:O1A	2.30	0.48
1:C:325:ILE:HG22	1:C:326:GLN:N	2.29	0.48
1:A:251:LYS:O	1:A:255:GLU:HG3	2.14	0.48
4:B:704:DTP:O1B	3:D:704:DGT:H5'A	2.13	0.48
1:B:251:LYS:O	1:B:255:GLU:HG3	2.14	0.48
1:B:351:ALA:O	1:B:520:PHE:HA	2.14	0.47
1:C:167:HIS:O	1:C:171:VAL:HG23	2.14	0.47
1:D:469:LYS:HA	1:D:469:LYS:HZ1	1.69	0.47
1:A:167:HIS:O	1:A:171:VAL:HG23	2.14	0.47
1:A:535:ASN:OD1	1:A:535:ASN:N	2.46	0.47
1:A:592:THR:N	1:A:593:PRO:CD	2.78	0.47
1:D:478:LYS:HE2	1:D:495:ALA:HB1	1.97	0.47
1:D:251:LYS:O	1:D:255:GLU:HG3	2.15	0.47
1:D:287:TYR:CD1	1:D:298:TYR:CE1	3.02	0.47
1:D:592:THR:N	1:D:593:PRO:CD	2.78	0.47
1:A:327:ASN:O	1:C:326:GLN:HB3	2.14	0.47
1:A:478:LYS:HE2	1:A:495:ALA:HB1	1.96	0.47
1:B:592:THR:N	1:B:593:PRO:CD	2.78	0.47
1:C:352:ARG:NH2	4:C:701:DTP:O1G	2.44	0.47
1:D:471:GLU:OE2	1:D:472:ASP:N	2.47	0.47
1:D:167:HIS:O	1:D:171:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:HIS:O	1:B:171:VAL:HG23	2.15	0.46
1:C:478:LYS:HE2	1:C:495:ALA:HB1	1.97	0.46
1:B:326:GLN:HB3	1:D:327:ASN:O	2.16	0.46
1:B:478:LYS:HE2	1:B:495:ALA:HB1	1.98	0.46
1:B:586:VAL:HG11	1:D:525:ALA:HB3	1.98	0.46
1:C:592:THR:N	1:C:593:PRO:CD	2.79	0.46
1:A:351:ALA:O	1:A:520:PHE:HA	2.15	0.46
1:C:287:TYR:CD1	1:C:298:TYR:CE1	3.04	0.46
1:A:325:ILE:HG22	1:A:326:GLN:N	2.30	0.46
1:A:311:ASP:OD2	2:A:701:TTP:O1A	2.34	0.46
1:A:326:GLN:HG2	1:C:326:GLN:HG2	1.97	0.45
1:C:251:LYS:O	1:C:255:GLU:HG3	2.15	0.45
1:C:325:ILE:CG2	1:C:326:GLN:N	2.79	0.45
1:A:287:TYR:CD1	1:A:298:TYR:CE1	3.04	0.45
1:A:326:GLN:HB3	1:C:327:ASN:O	2.17	0.45
1:B:586:VAL:CG1	1:D:525:ALA:HB3	2.46	0.45
1:A:428:LEU:HD13	1:D:425:ASN:HB2	1.98	0.45
1:B:326:GLN:HG2	1:D:326:GLN:HG2	1.98	0.45
1:D:535:ASN:OD1	1:D:535:ASN:N	2.47	0.45
1:A:522:CYS:SG	1:C:583:ASP:CB	3.05	0.45
1:B:325:ILE:HG22	1:B:326:GLN:N	2.31	0.45
1:D:240:MET:CE	1:D:419:TYR:HD2	2.31	0.44
1:B:287:TYR:CD1	1:B:298:TYR:CE1	3.05	0.44
1:D:325:ILE:HG22	1:D:326:GLN:N	2.31	0.44
1:A:325:ILE:CG2	1:A:326:GLN:N	2.80	0.44
1:D:469:LYS:HE3	1:D:469:LYS:CA	2.47	0.44
1:B:325:ILE:CG2	1:B:326:GLN:N	2.81	0.44
1:B:535:ASN:OD1	1:B:535:ASN:N	2.47	0.44
1:C:352:ARG:HH22	4:C:701:DTP:PG	2.40	0.44
1:D:351:ALA:O	1:D:520:PHE:HA	2.18	0.43
1:A:321:HIS:CE1	1:D:321:HIS:CE1	3.06	0.43
1:A:598:TRP:O	1:A:599:ASN:HB2	2.19	0.43
1:C:351:ALA:O	1:C:520:PHE:HA	2.18	0.43
1:A:240:MET:CE	1:A:419:TYR:HD2	2.32	0.43
1:D:156:VAL:O	3:D:704:DGT:H8	2.18	0.43
1:C:143:ARG:HD2	1:C:420:THR:HA	2.01	0.43
1:B:321:HIS:CE1	1:C:321:HIS:CE1	3.06	0.43
1:C:240:MET:CE	1:C:419:TYR:HD2	2.32	0.42
1:C:381:ILE:HD12	1:C:381:ILE:HA	1.87	0.42
1:D:325:ILE:CG2	1:D:326:GLN:N	2.82	0.42
1:D:469:LYS:HZ2	1:D:469:LYS:CA	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:ASN:O	1:D:326:GLN:HB3	2.20	0.42
1:D:470:ARG:CB	1:D:473:TYR:CE2	3.02	0.42
3:C:704:DGT:N3	3:C:704:DGT:H2'A	2.35	0.42
1:C:232:THR:HB	1:C:234:GLU:OE1	2.20	0.41
1:D:598:TRP:O	1:D:599:ASN:HB2	2.19	0.41
1:C:127:GLU:HG3	1:D:336:LYS:HE3	2.02	0.41
1:B:215:HIS:CD2	2:B:701:TTP:C6	3.08	0.41
1:A:222:ILE:HB	1:A:223:PRO:HD3	2.03	0.41
1:A:381:ILE:HD12	1:A:381:ILE:HA	1.88	0.41
1:B:598:TRP:O	1:B:599:ASN:HB2	2.20	0.41
1:A:543:GLU:HG3	1:C:543:GLU:HG3	2.02	0.41
1:C:478:LYS:H	1:C:478:LYS:HD2	1.85	0.41
4:B:704:DTP:O2B	1:D:377:LYS:NZ	2.54	0.40
1:B:543:GLU:CG	1:D:543:GLU:CG	2.99	0.40
1:D:478:LYS:HD2	1:D:478:LYS:H	1.86	0.40
1:B:240:MET:CE	1:B:419:TYR:HD2	2.34	0.40
1:B:377:LYS:NZ	4:D:702:DTP:O2B	2.55	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:ARG:NH2	1:B:478:LYS:CG[1_454]	1.86	0.34
1:B:543:GLU:O	1:C:465:GLN:OE1[1_655]	2.07	0.13

## 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	476/514 (93%)	470 (99%)	6 (1%)	0	100	100
1	B	476/514 (93%)	469 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	476/514 (93%)	470 (99%)	6 (1%)	0	100	100
1	D	476/514 (93%)	471 (99%)	5 (1%)	0	100	100
All	All	1904/2056 (93%)	1880 (99%)	24 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	426/459 (93%)	410 (96%)	16 (4%)	33	41
1	B	426/459 (93%)	411 (96%)	15 (4%)	36	45
1	C	426/459 (93%)	410 (96%)	16 (4%)	33	41
1	D	426/459 (93%)	410 (96%)	16 (4%)	33	41
All	All	1704/1836 (93%)	1641 (96%)	63 (4%)	34	43

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	MET
1	A	273	VAL
1	A	277	GLU
1	A	284	LEU
1	A	315	TYR
1	A	326	GLN
1	A	342	GLU
1	A	359	LEU
1	A	388	ASP
1	A	467	LYS
1	A	469	LYS
1	A	478	LYS
1	A	492	LYS
1	A	523	LYS

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Mol	Chain	Res	Type
1	A	528	ARG
1	A	535	ASN
1	B	115	MET
1	B	277	GLU
1	B	284	LEU
1	B	315	TYR
1	B	326	GLN
1	B	342	GLU
1	B	359	LEU
1	B	465	GLN
1	B	467	LYS
1	B	469	LYS
1	B	478	LYS
1	B	492	LYS
1	B	523	LYS
1	B	528	ARG
1	B	535	ASN
1	C	115	MET
1	C	273	VAL
1	C	277	GLU
1	C	284	LEU
1	C	315	TYR
1	C	326	GLN
1	C	342	GLU
1	C	359	LEU
1	C	467	LYS
1	C	469	LYS
1	C	478	LYS
1	C	492	LYS
1	C	523	LYS
1	C	528	ARG
1	C	535	ASN
1	C	599	ASN
1	D	115	MET
1	D	277	GLU
1	D	284	LEU
1	D	315	TYR
1	D	326	GLN
1	D	342	GLU
1	D	359	LEU
1	D	467	LYS
1	D	469	LYS

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Mol	Chain	Res	Type
1	D	470	ARG
1	D	471	GLU
1	D	478	LYS
1	D	492	LYS
1	D	523	LYS
1	D	528	ARG
1	D	535	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	235	GLN
1	A	243	HIS
1	A	326	GLN
1	A	364	HIS
1	B	235	GLN
1	B	243	HIS
1	B	326	GLN
1	C	215	HIS
1	C	235	GLN
1	C	243	HIS
1	C	322	HIS
1	C	326	GLN
1	D	235	GLN
1	D	243	HIS
1	D	326	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 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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	702	5	26,33,33	1.07	2 (7%)	32,52,52	2.29	10 (31%)
4	DTP	B	704	5	26,32,32	0.97	1 (3%)	30,50,50	1.77	6 (20%)
4	DTP	D	702	5	26,32,32	1.15	1 (3%)	30,50,50	1.48	5 (16%)
3	DGT	D	704	5	26,33,33	1.18	2 (7%)	32,52,52	2.26	11 (34%)
2	TTP	D	703	-	23,30,30	1.12	1 (4%)	29,47,47	2.01	6 (20%)
4	DTP	A	703	5	26,32,32	1.14	2 (7%)	30,50,50	1.80	7 (23%)
2	TTP	A	701	-	23,30,30	1.18	1 (4%)	29,47,47	1.85	6 (20%)
2	TTP	B	701	-	23,30,30	1.16	1 (4%)	29,47,47	1.91	7 (24%)
4	DTP	C	701	5	26,32,32	1.05	2 (7%)	30,50,50	1.72	7 (23%)
3	DGT	C	704	5	26,33,33	1.12	1 (3%)	32,52,52	2.17	10 (31%)
3	DGT	C	703	-	26,33,33	1.48	2 (7%)	32,52,52	2.17	11 (34%)
3	DGT	B	702	5	26,33,33	1.09	2 (7%)	32,52,52	2.19	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	A	702	5	-	4/18/34/34	0/3/3/3
4	DTP	B	704	5	-	3/18/34/34	0/3/3/3
4	DTP	D	702	5	-	4/18/34/34	0/3/3/3
3	DGT	D	704	5	-	5/18/34/34	0/3/3/3
2	TTP	D	703	-	-	4/19/34/34	0/2/2/2
4	DTP	A	703	5	-	8/18/34/34	0/3/3/3
2	TTP	A	701	-	-	4/19/34/34	0/2/2/2
2	TTP	B	701	-	-	4/19/34/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DTP	C	701	5	-	5/18/34/34	0/3/3/3
3	DGT	C	704	5	-	4/18/34/34	0/3/3/3
3	DGT	C	703	-	-	10/18/34/34	0/3/3/3
3	DGT	B	702	5	-	4/18/34/34	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	703	DGT	C5-C6	5.48	1.50	1.41
2	B	701	TTP	C5-C4	4.49	1.51	1.41
2	A	701	TTP	C5-C4	4.27	1.50	1.41
2	D	703	TTP	C5-C4	4.23	1.50	1.41
3	C	704	DGT	C5-C6	4.01	1.48	1.41
3	D	704	DGT	C5-C6	3.42	1.47	1.41
3	B	702	DGT	C5-C6	3.36	1.47	1.41
3	A	702	DGT	C5-C6	3.22	1.46	1.41
3	C	703	DGT	C5-C4	3.12	1.49	1.40
4	C	701	DTP	C2-N3	3.01	1.37	1.32
3	D	704	DGT	C5-C4	2.59	1.47	1.40
4	A	703	DTP	C2-N3	2.59	1.36	1.32
4	D	702	DTP	C2-N3	2.46	1.36	1.32
4	C	701	DTP	C5-C4	2.45	1.47	1.40
3	A	702	DGT	C5-C4	2.37	1.47	1.40
4	A	703	DTP	O4'-C4'	-2.17	1.40	1.45
4	B	704	DTP	C5-C4	2.11	1.46	1.40
3	B	702	DGT	C5-C4	2.06	1.46	1.40

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	TTP	C2-N3-C4	6.22	120.40	115.14
3	C	704	DGT	C2-N3-C4	6.04	122.25	115.36
3	A	702	DGT	C5-C6-N1	-5.57	115.81	123.43
2	A	701	TTP	C2-N3-C4	5.47	119.76	115.14
2	D	703	TTP	C2-N3-C4	5.34	119.65	115.14
4	B	704	DTP	N3-C2-N1	-5.13	120.65	128.68
2	D	703	TTP	PB-O3B-PG	-5.12	115.25	132.83
3	B	702	DGT	C2-N3-C4	5.00	121.07	115.36
4	A	703	DTP	N3-C2-N1	-4.99	120.89	128.68
3	B	702	DGT	C4-C5-C6	-4.89	116.13	120.80
3	A	702	DGT	C2-N1-C6	4.65	123.31	115.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	704	DGT	C5-C6-N1	-4.58	117.16	123.43
3	C	703	DGT	C4-C5-C6	-4.56	116.44	120.80
3	D	704	DGT	C2-N1-C6	4.56	123.17	115.93
3	A	702	DGT	PA-O3A-PB	-4.56	117.19	132.83
2	D	703	TTP	PB-O3A-PA	-4.54	117.23	132.83
3	C	704	DGT	C4-C5-C6	-4.53	116.47	120.80
3	B	702	DGT	PA-O3A-PB	-4.52	117.33	132.83
3	D	704	DGT	C2-N3-C4	4.41	120.40	115.36
3	C	703	DGT	C2-N3-C4	4.33	120.30	115.36
4	C	701	DTP	N3-C2-N1	-4.31	121.94	128.68
3	C	703	DGT	PB-O3B-PG	-4.30	118.05	132.83
2	B	701	TTP	PB-O3B-PG	-4.10	118.75	132.83
3	C	704	DGT	N3-C2-N1	-4.09	121.77	127.22
3	D	704	DGT	O2G-PG-O1G	4.08	123.22	107.64
3	D	704	DGT	PB-O3B-PG	-4.07	118.87	132.83
3	B	702	DGT	C2-N1-C6	4.06	122.38	115.93
3	B	702	DGT	N3-C2-N1	-4.04	121.83	127.22
3	C	703	DGT	PA-O3A-PB	-3.87	119.53	132.83
3	A	702	DGT	C4-C5-N7	-3.83	105.40	109.40
2	A	701	TTP	PB-O3B-PG	-3.83	119.69	132.83
2	B	701	TTP	PB-O3A-PA	-3.77	119.87	132.83
3	C	703	DGT	C2-N1-C6	3.76	121.91	115.93
4	A	703	DTP	PB-O3B-PG	-3.75	119.96	132.83
2	A	701	TTP	PB-O3A-PA	-3.72	120.05	132.83
4	D	702	DTP	C4-C5-N7	-3.71	105.54	109.40
3	C	703	DGT	C5-C6-N1	-3.63	118.46	123.43
4	B	704	DTP	PB-O3B-PG	-3.59	120.52	132.83
4	C	701	DTP	O3B-PG-O1G	-3.51	91.70	111.19
3	D	704	DGT	C4-C5-C6	-3.49	117.46	120.80
3	C	704	DGT	PB-O3B-PG	-3.47	120.92	132.83
3	C	704	DGT	C2-N1-C6	3.45	121.41	115.93
3	A	702	DGT	O1G-PG-O3G	3.43	124.09	110.68
4	B	704	DTP	C2-N1-C6	3.42	124.61	118.75
2	D	703	TTP	C5-C6-N1	-3.42	118.51	122.19
2	A	701	TTP	C5-C6-N1	-3.40	118.53	122.19
4	C	701	DTP	PB-O3B-PG	-3.40	121.17	132.83
3	C	704	DGT	PA-O3A-PB	-3.37	121.25	132.83
3	A	702	DGT	O5'-PA-O2A	-3.34	96.00	109.07
3	B	702	DGT	C5-C6-N1	-3.31	118.90	123.43
3	A	702	DGT	C2-N3-C4	3.24	119.06	115.36
3	D	704	DGT	N3-C2-N1	-3.21	122.94	127.22
3	A	702	DGT	PB-O3B-PG	-3.19	121.89	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	702	DTP	N3-C2-N1	-3.15	123.76	128.68
3	C	704	DGT	C5-C6-N1	-3.12	119.16	123.43
3	C	703	DGT	O2G-PG-O1G	3.11	119.53	107.64
4	A	703	DTP	PA-O3A-PB	-3.10	122.19	132.83
2	D	703	TTP	O3G-PG-O2G	3.06	119.35	107.64
4	C	701	DTP	PA-O3A-PB	-3.02	122.48	132.83
4	B	704	DTP	PA-O3A-PB	-2.98	122.59	132.83
4	A	703	DTP	C4-C5-N7	-2.93	106.34	109.40
4	D	702	DTP	PB-O3B-PG	-2.88	122.94	132.83
3	B	702	DGT	PB-O3B-PG	-2.86	123.00	132.83
3	A	702	DGT	N3-C2-N1	-2.82	123.46	127.22
3	C	703	DGT	N3-C2-N1	-2.82	123.47	127.22
3	C	704	DGT	C4-C5-N7	-2.78	106.50	109.40
3	D	704	DGT	C4-C5-N7	-2.74	106.54	109.40
3	B	702	DGT	O2G-PG-O3G	2.74	121.41	110.68
3	C	703	DGT	C4-C5-N7	-2.73	106.55	109.40
3	D	704	DGT	PA-O3A-PB	-2.72	123.48	132.83
2	A	701	TTP	O3G-PG-O2G	2.72	118.05	107.64
4	A	703	DTP	O3G-PG-O2G	2.72	118.04	107.64
3	C	703	DGT	C2'-C3'-C4'	2.68	108.34	102.76
3	C	703	DGT	O2G-PG-O3B	-2.65	95.74	104.64
4	A	703	DTP	C2'-C3'-C4'	2.62	108.23	102.76
2	B	701	TTP	C5-C6-N1	-2.61	119.38	122.19
3	C	704	DGT	O2G-PG-O1G	2.50	117.18	107.64
3	A	702	DGT	O1A-PA-O2A	2.48	124.49	112.24
4	C	701	DTP	C2-N1-C6	2.47	122.97	118.75
4	D	702	DTP	O3G-PG-O2G	2.34	116.58	107.64
2	A	701	TTP	O2B-PB-O1B	2.30	123.60	112.24
3	D	704	DGT	O1A-PA-O2A	2.27	123.46	112.24
2	B	701	TTP	C2'-C3'-C4'	2.26	107.48	102.76
4	B	704	DTP	C4-C5-N7	-2.26	107.05	109.40
2	D	703	TTP	O2B-PB-O1B	2.23	123.26	112.24
3	D	704	DGT	O4'-C1'-C2'	-2.20	102.09	106.25
4	A	703	DTP	N6-C6-N1	2.19	123.11	118.57
4	C	701	DTP	N6-C6-N1	2.18	123.10	118.57
3	C	704	DGT	N2-C2-N1	2.14	120.58	117.25
4	B	704	DTP	C2'-C3'-C4'	2.14	107.21	102.76
2	B	701	TTP	O3G-PG-O2G	2.12	115.74	107.64
4	C	701	DTP	C4-C5-N7	-2.08	107.23	109.40
2	B	701	TTP	O2A-PA-O1A	2.05	122.37	112.24
4	D	702	DTP	O3B-PG-O1G	-2.02	100.01	111.19

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	TTP	C5'-O5'-PA-O1A
2	A	701	TTP	C5'-O5'-PA-O2A
2	B	701	TTP	PB-O3A-PA-O5'
2	D	703	TTP	C5'-O5'-PA-O1A
2	D	703	TTP	C5'-O5'-PA-O2A
3	B	702	DGT	PB-O3B-PG-O1G
3	C	703	DGT	C5'-O5'-PA-O3A
3	D	704	DGT	C5'-O5'-PA-O2A
4	A	703	DTP	PB-O3B-PG-O3G
4	A	703	DTP	C5'-O5'-PA-O1A
4	A	703	DTP	C5'-O5'-PA-O2A
4	A	703	DTP	C5'-O5'-PA-O3A
4	A	703	DTP	O4'-C4'-C5'-O5'
4	C	701	DTP	PB-O3B-PG-O3G
4	D	702	DTP	PB-O3B-PG-O3G
4	A	703	DTP	C3'-C4'-C5'-O5'
3	C	703	DGT	C3'-C4'-C5'-O5'
3	C	703	DGT	PA-O3A-PB-O2B
3	D	704	DGT	C4'-C5'-O5'-PA
2	A	701	TTP	C5'-O5'-PA-O3A
2	A	701	TTP	PA-O3A-PB-O1B
4	B	704	DTP	PG-O3B-PB-O1B
4	C	701	DTP	PG-O3B-PB-O2B
4	C	701	DTP	PB-O3A-PA-O2A
2	B	701	TTP	C4'-C5'-O5'-PA
3	C	704	DGT	C4'-C5'-O5'-PA
3	C	703	DGT	C5'-O5'-PA-O1A
3	C	703	DGT	C5'-O5'-PA-O2A
3	A	702	DGT	PB-O3B-PG-O3G
4	C	701	DTP	PB-O3B-PG-O1G
3	C	703	DGT	O4'-C4'-C5'-O5'
3	A	702	DGT	PG-O3B-PB-O1B
3	A	702	DGT	PB-O3A-PA-O1A
3	C	703	DGT	PA-O3A-PB-O1B
3	D	704	DGT	PG-O3B-PB-O1B
4	B	704	DTP	PB-O3A-PA-O2A
4	D	702	DTP	PB-O3A-PA-O2A
3	A	702	DGT	C4'-C5'-O5'-PA
2	D	703	TTP	C3'-C4'-C5'-O5'
2	B	701	TTP	PG-O3B-PB-O1B
3	C	703	DGT	PG-O3B-PB-O1B
4	B	704	DTP	PB-O3A-PA-O1A

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Mol	Chain	Res	Type	Atoms
3	B	702	DGT	PB-O3B-PG-O3G
4	D	702	DTP	PB-O3B-PG-O1G
4	A	703	DTP	PB-O3B-PG-O2G
4	D	702	DTP	PB-O3B-PG-O2G
2	D	703	TTP	C5'-O5'-PA-O3A
3	D	704	DGT	C5'-O5'-PA-O3A
2	B	701	TTP	PG-O3B-PB-O2B
3	B	702	DGT	PG-O3B-PB-O1B
3	C	703	DGT	PB-O3A-PA-O1A
3	C	703	DGT	PB-O3A-PA-O2A
3	C	704	DGT	PB-O3A-PA-O1A
3	C	704	DGT	PB-O3A-PA-O2A
3	D	704	DGT	PG-O3B-PB-O2B
4	A	703	DTP	PG-O3B-PB-O1B
4	C	701	DTP	PB-O3A-PA-O1A
3	B	702	DGT	C4'-C5'-O5'-PA
3	C	704	DGT	C5'-O5'-PA-O2A

There are no ring outliers.

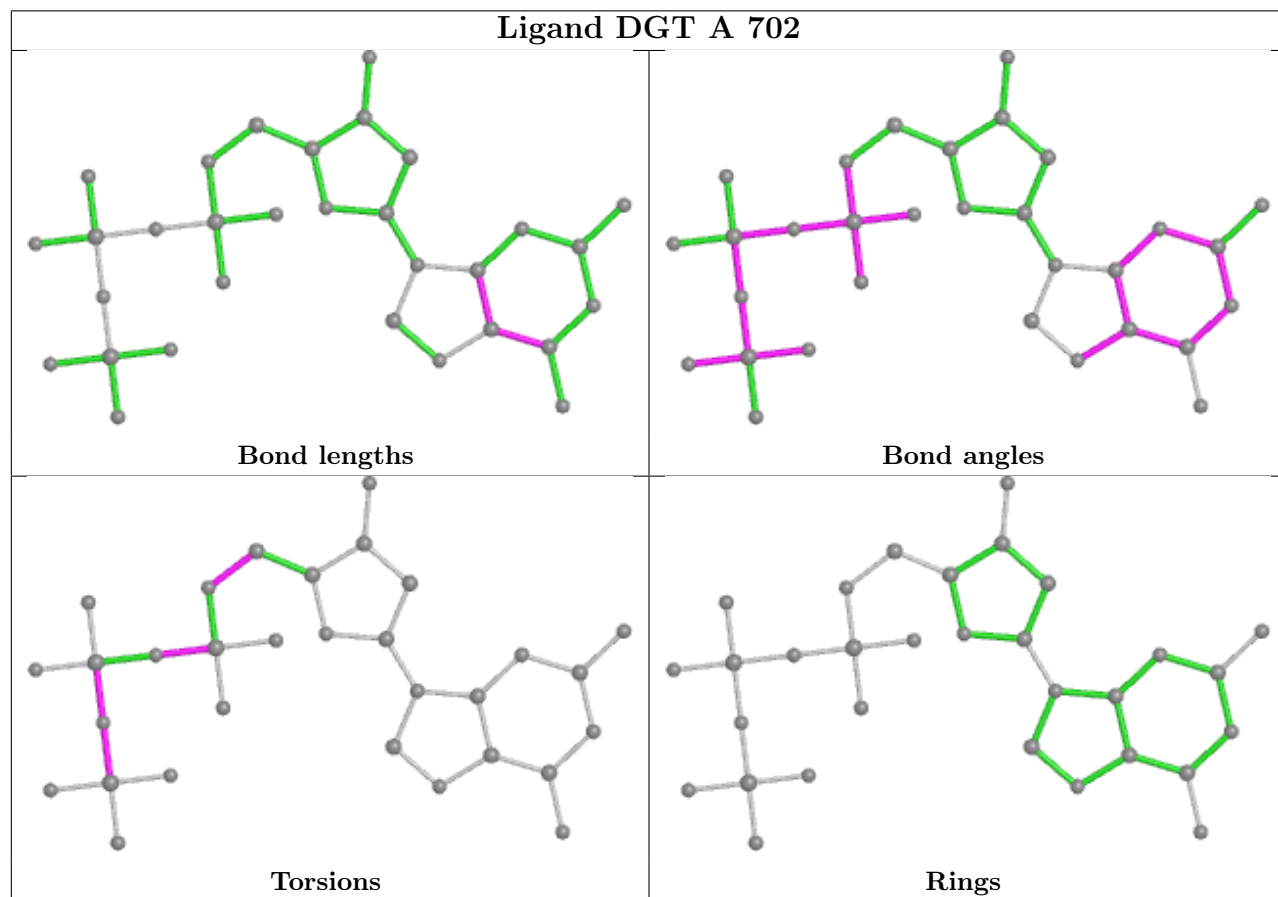
9 monomers are involved in 15 short contacts:

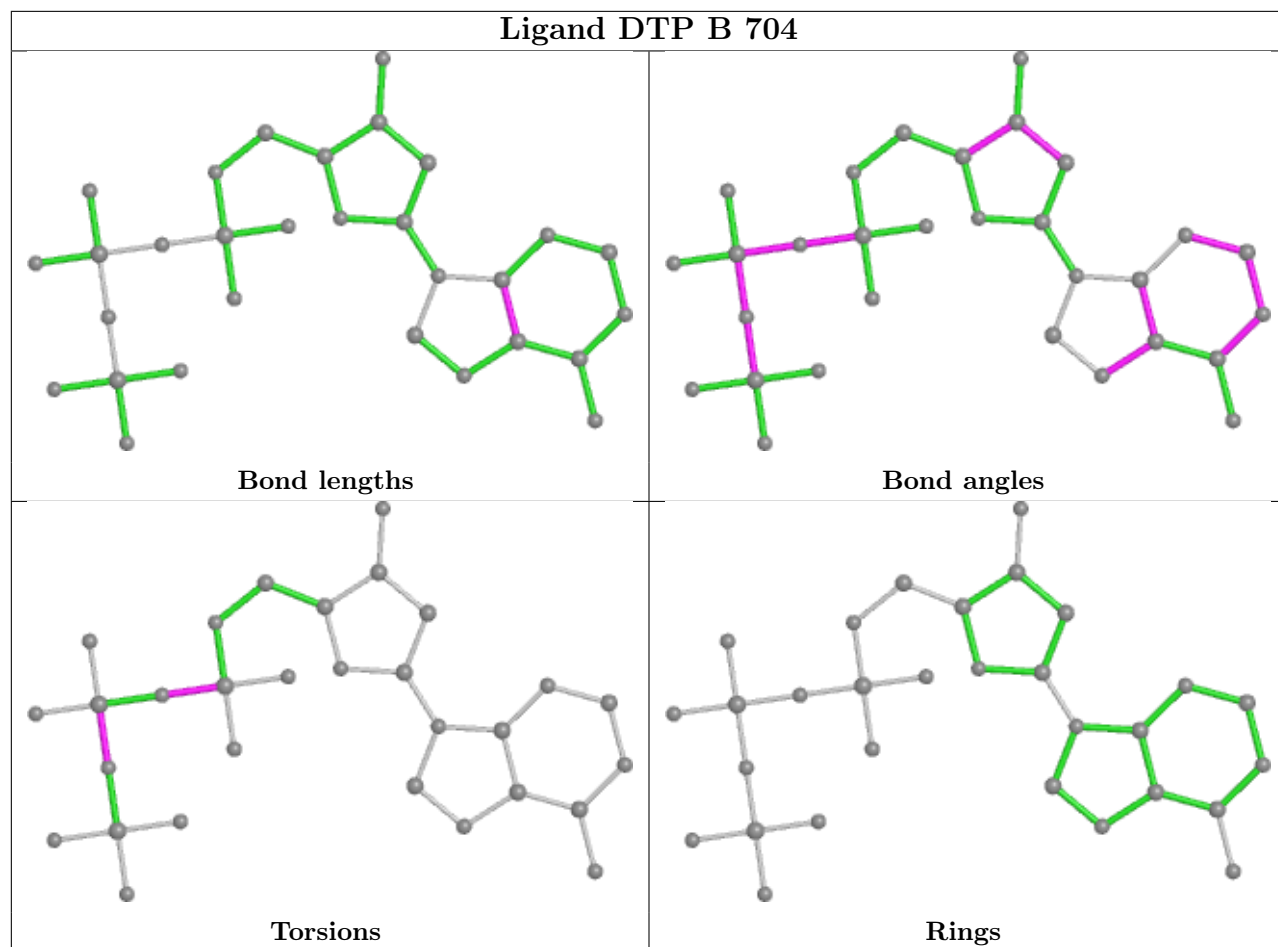
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	704	DTP	2	0
4	D	702	DTP	1	0
3	D	704	DGT	2	0
4	A	703	DTP	1	0
2	A	701	TTP	1	0
2	B	701	TTP	1	0
4	C	701	DTP	3	0
3	C	704	DGT	4	0
3	C	703	DGT	1	0

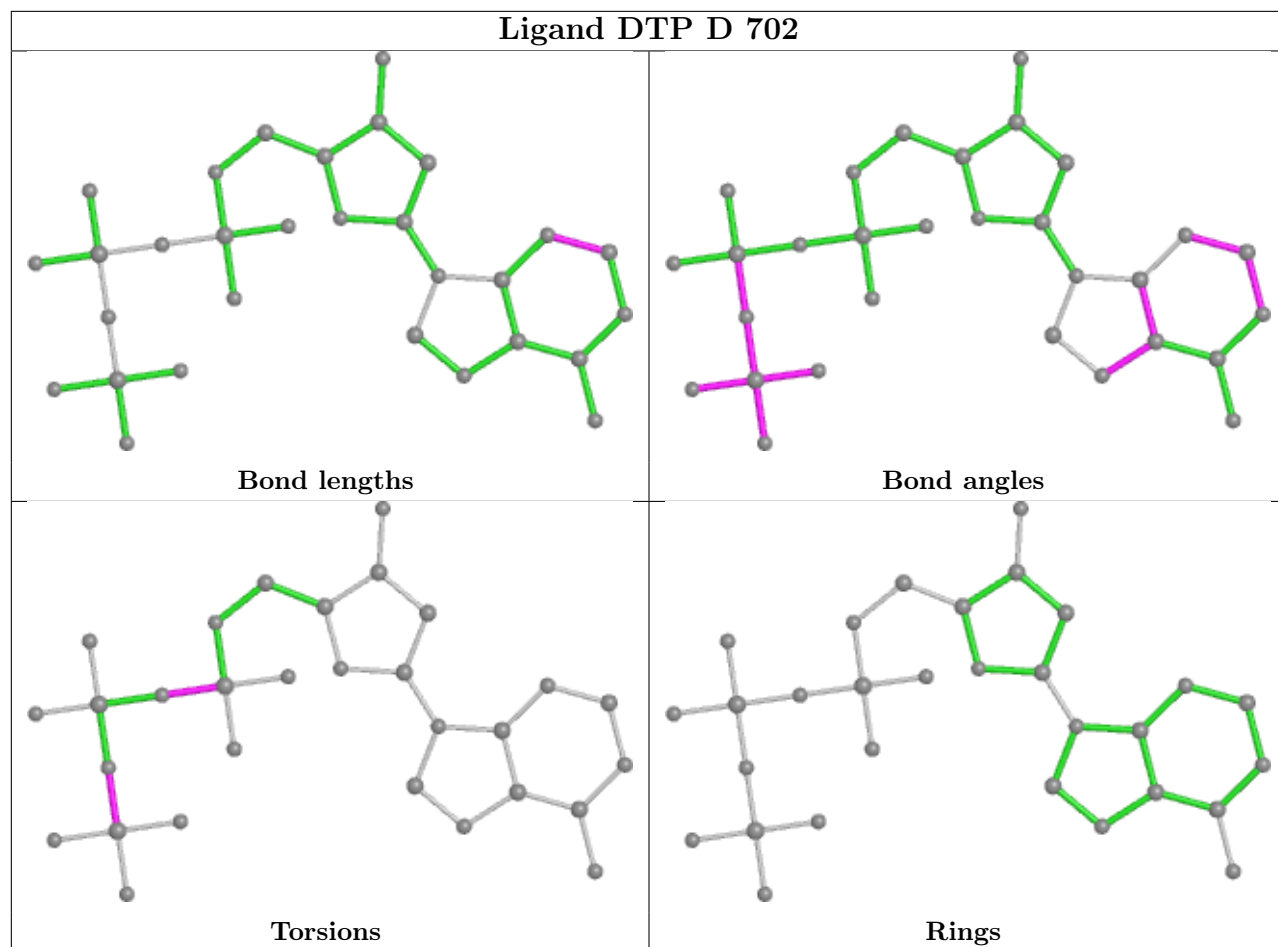
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

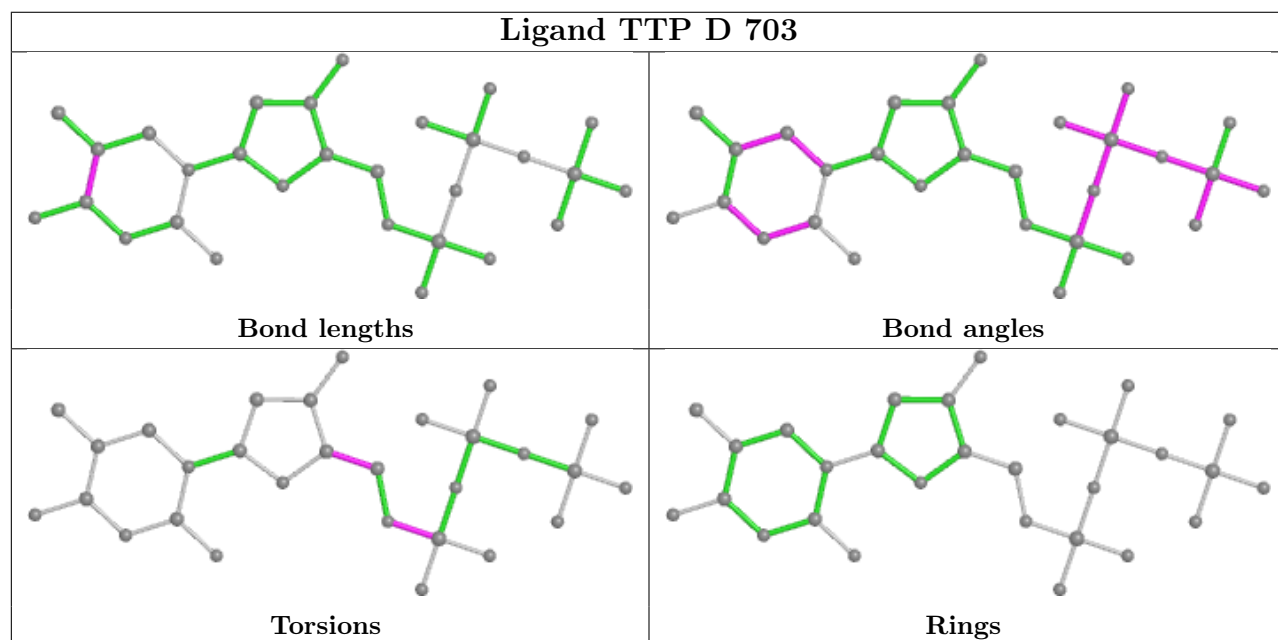
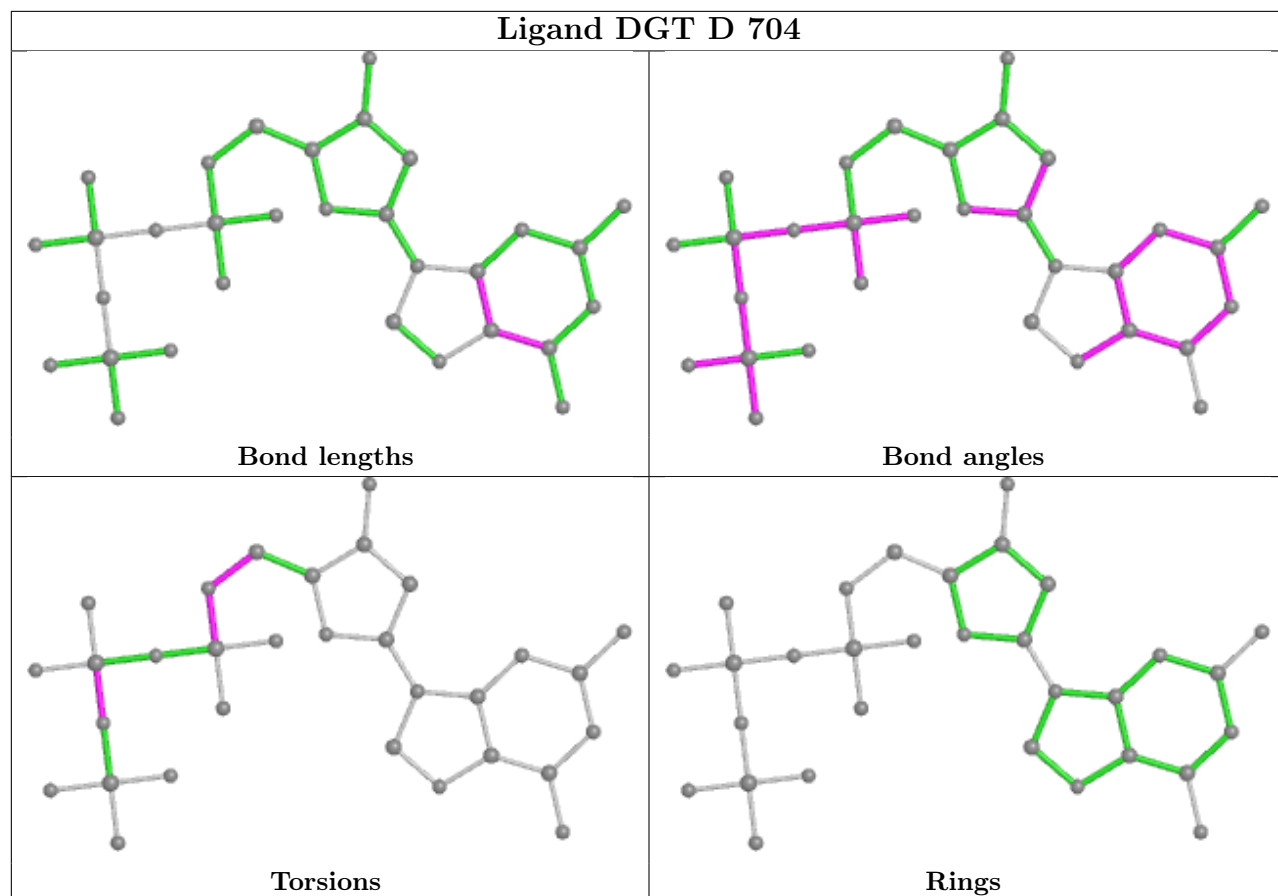


The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

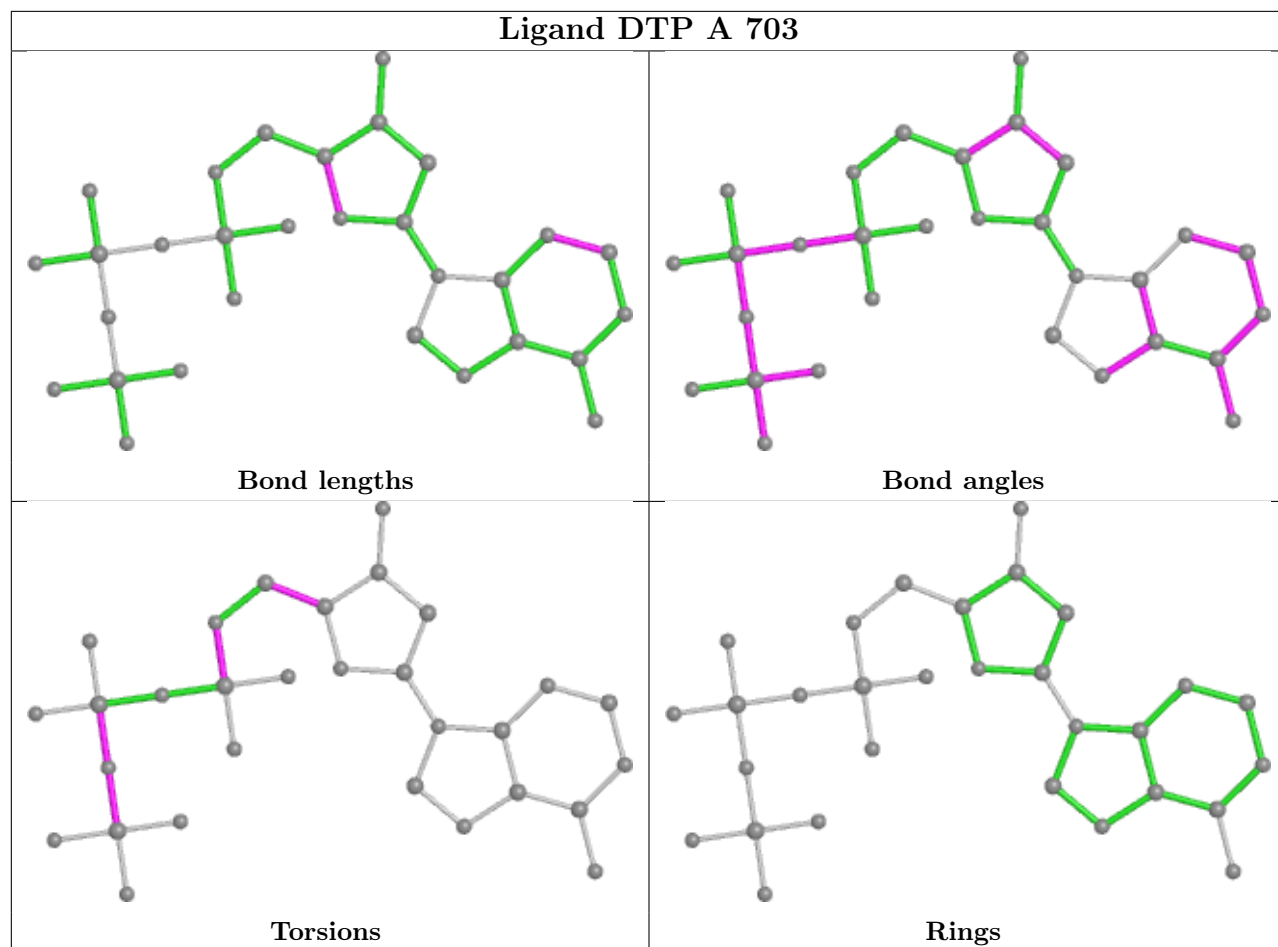




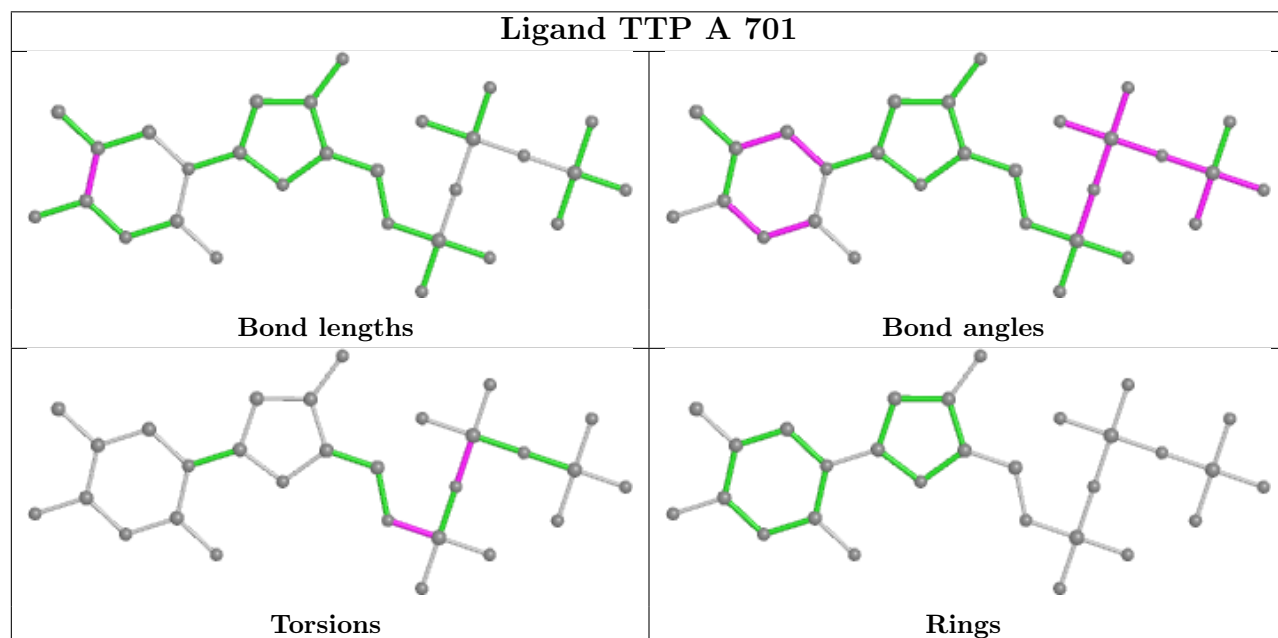




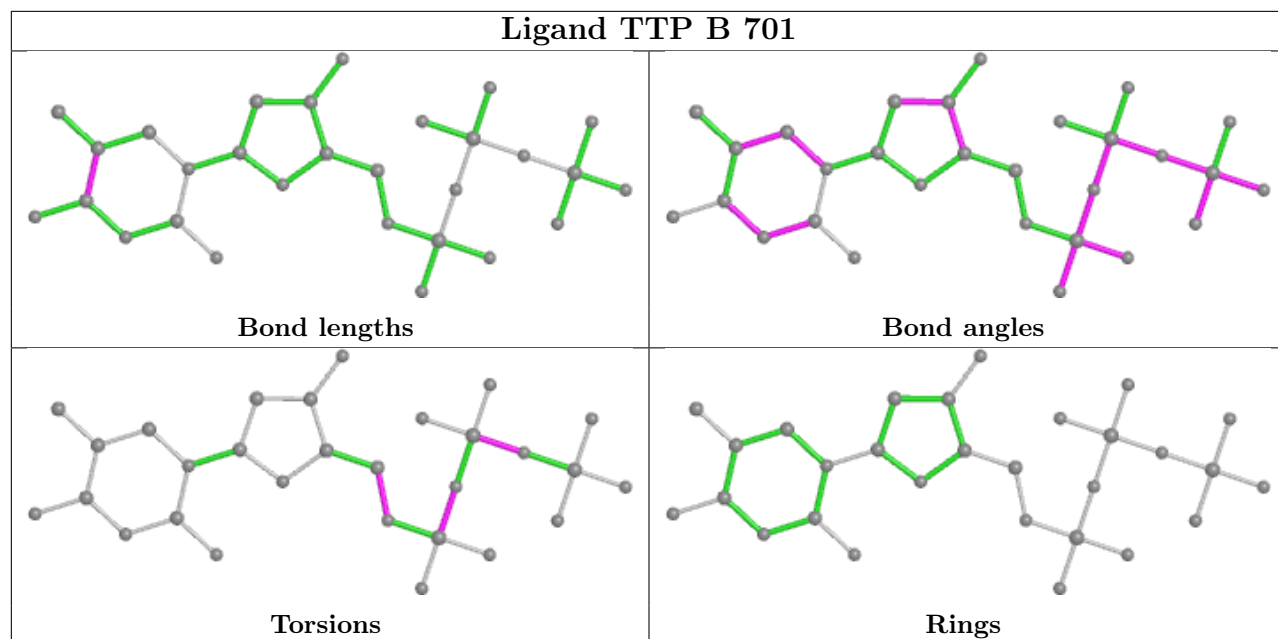
## Ligand DTP A 703



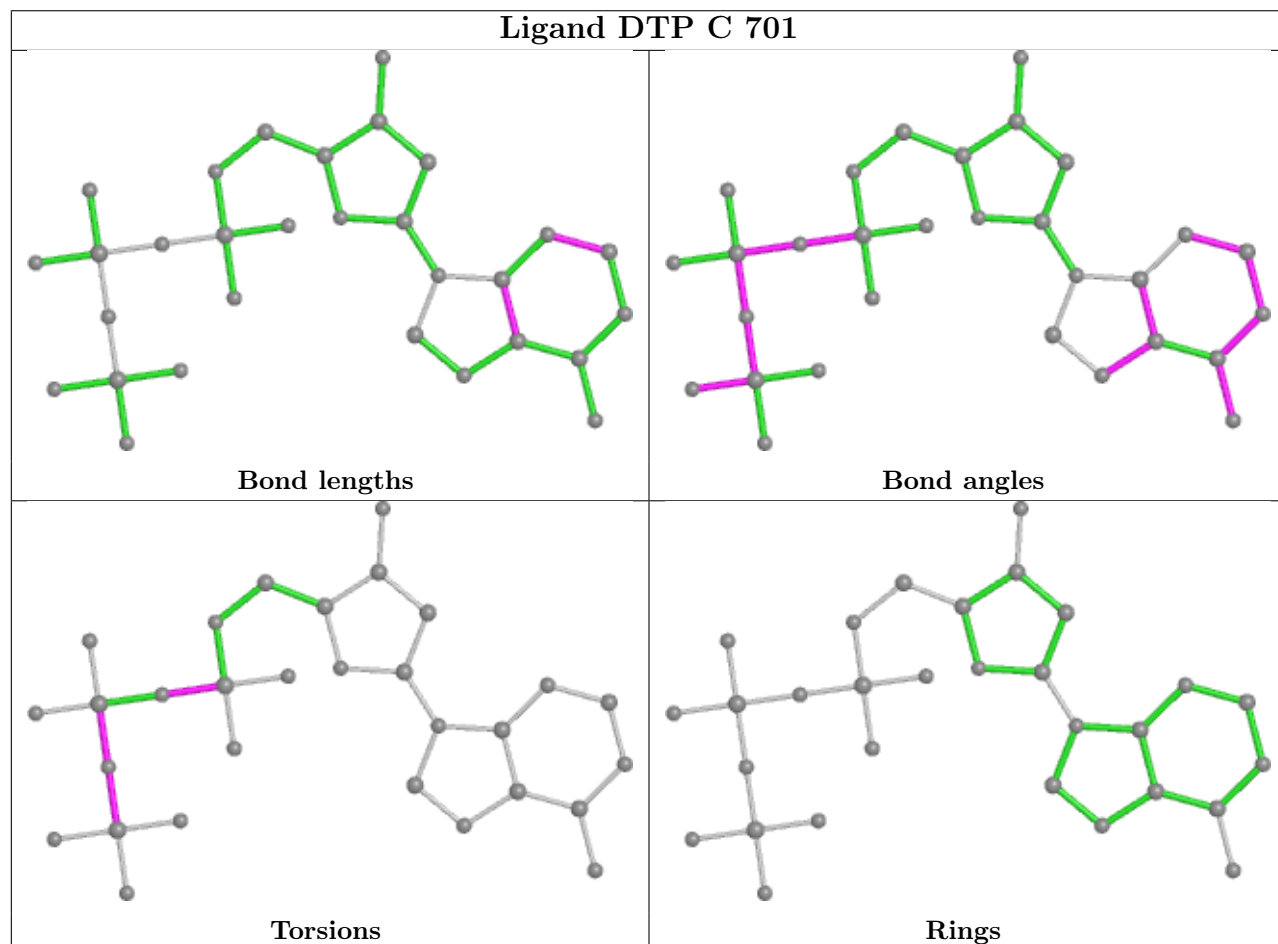
## Ligand TTP A 701

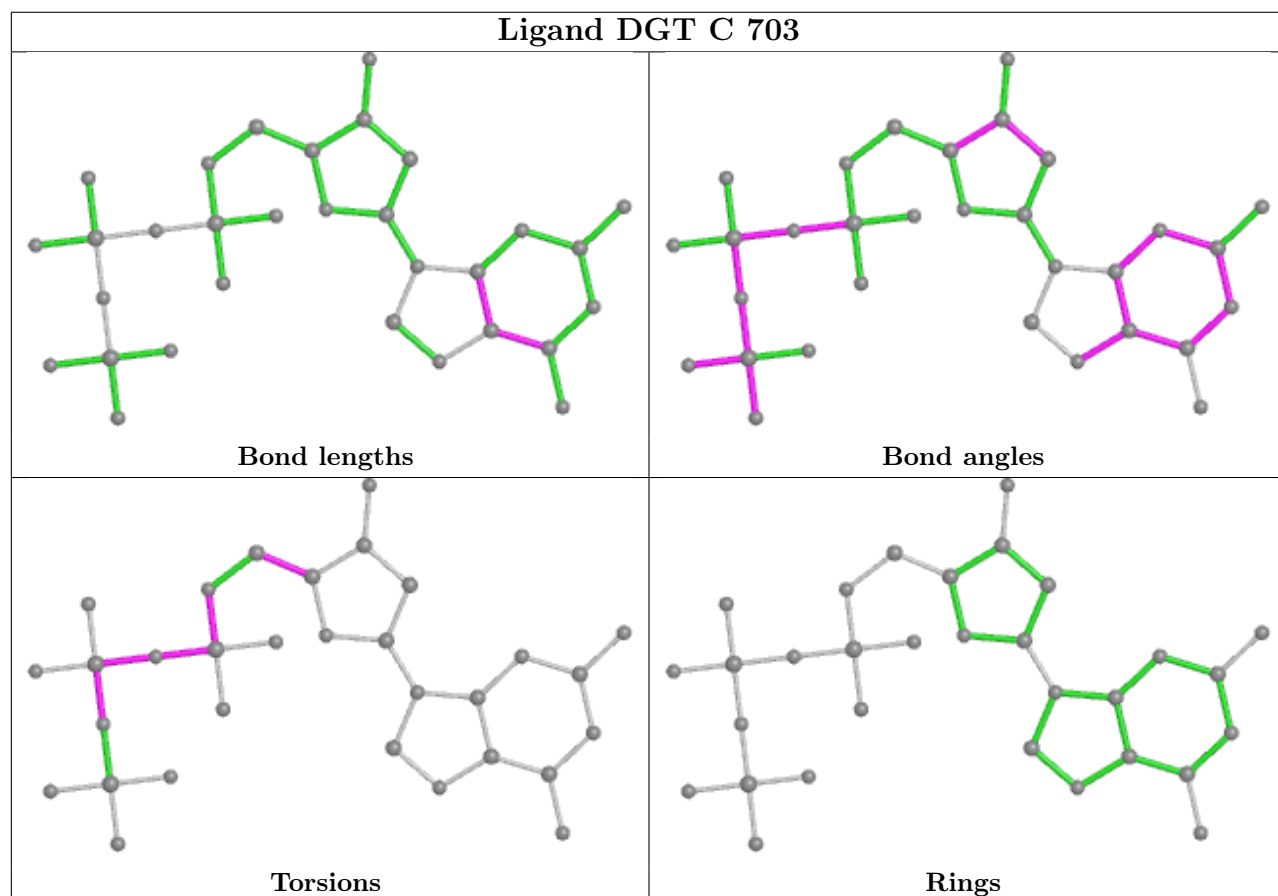
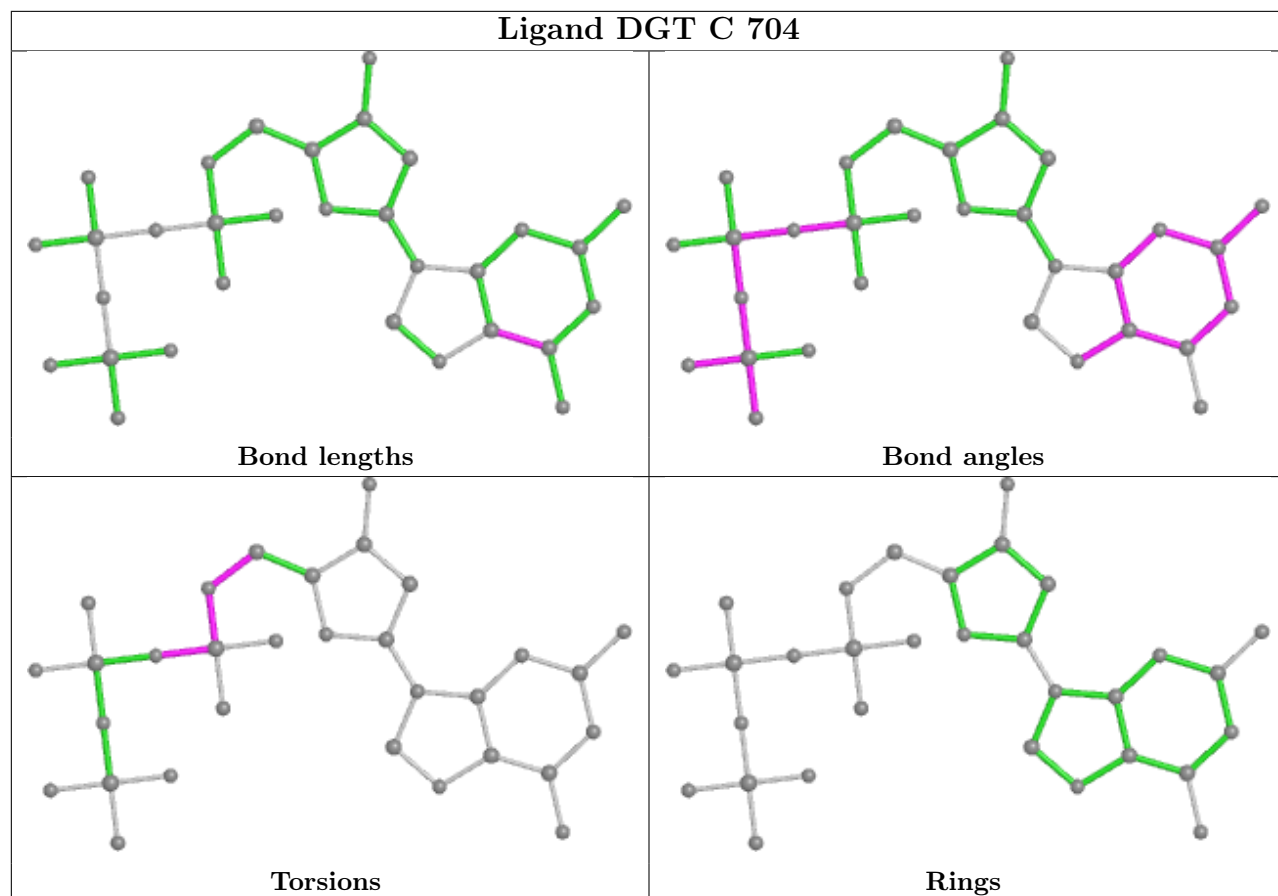


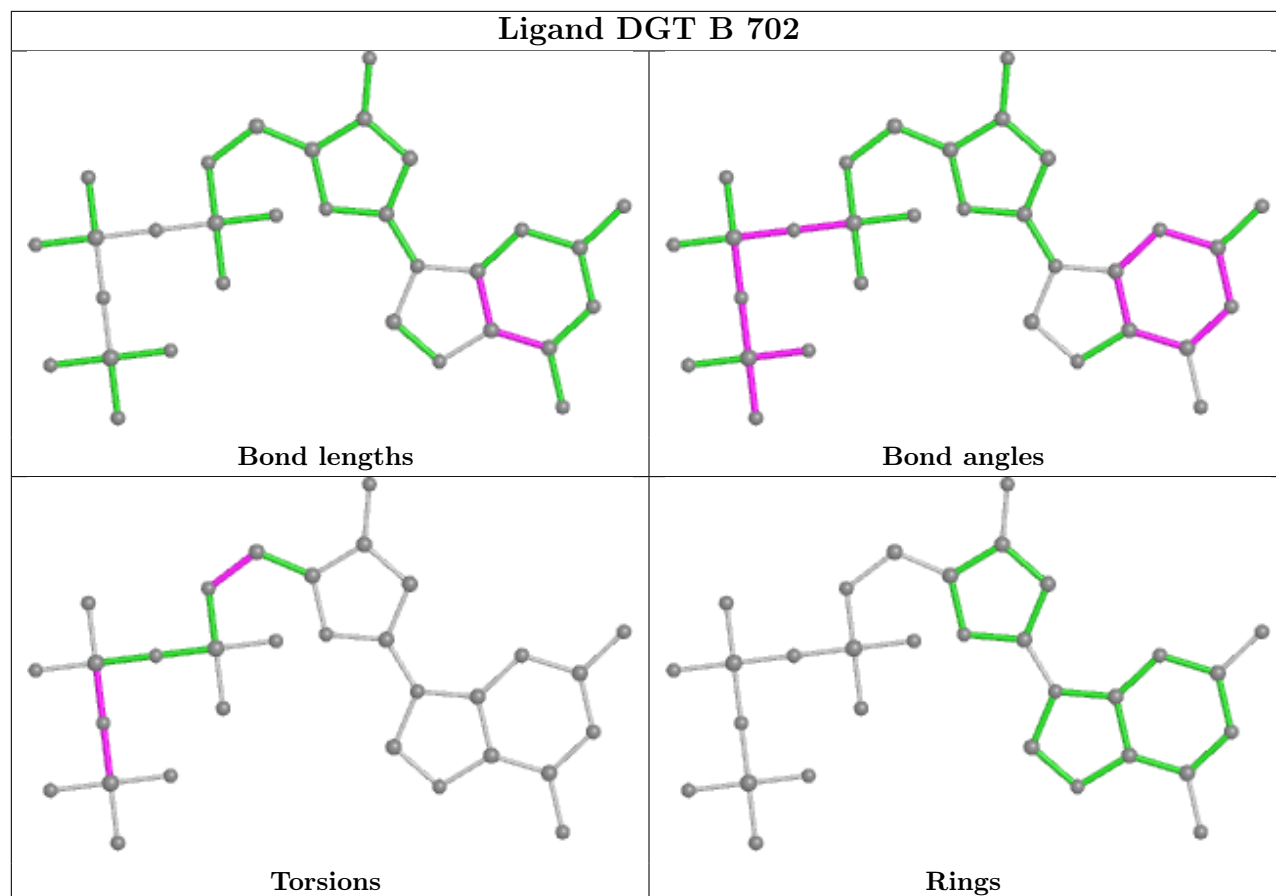
## Ligand TTP B 701



## Ligand DTP C 701







## 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, 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	480/514 (93%)	0.59	36 (7%) 14 21	29, 59, 94, 136	0
1	B	480/514 (93%)	0.82	53 (11%) 5 9	33, 66, 103, 133	0
1	C	480/514 (93%)	1.31	117 (24%) 0 1	35, 80, 129, 171	0
1	D	480/514 (93%)	1.28	100 (20%) 1 1	33, 77, 134, 176	0
All	All	1920/2056 (93%)	1.00	306 (15%) 1 3	29, 70, 119, 176	0

All (306) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	489	LEU	14.3
1	D	489	LEU	12.2
1	D	562	LEU	11.3
1	C	496	GLU	10.1
1	C	488	LEU	10.0
1	C	486	LYS	9.6
1	D	490	ASP	8.2
1	D	590	LEU	8.1
1	D	491	VAL	7.7
1	D	466	ILE	7.7
1	B	488	LEU	7.7
1	D	274	GLY	7.1
1	D	487	VAL	7.0
1	C	285	TRP	6.4
1	D	465	GLN	6.4
1	D	493	LEU	6.3
1	C	498	PHE	6.2
1	D	481	ALA	6.0
1	C	557	VAL	5.7
1	D	473	TYR	5.7
1	D	592	THR	5.6

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Mol	Chain	Res	Type	RSRZ
1	C	466	ILE	5.6
1	C	263	GLU	5.6
1	B	599	ASN	5.5
1	D	488	LEU	5.5
1	D	497	ASP	5.4
1	B	489	LEU	5.3
1	C	590	LEU	5.3
1	C	255	GLU	5.3
1	C	584	GLY	5.3
1	D	345	ASN	5.3
1	D	599	ASN	5.3
1	D	486	LYS	5.1
1	C	403	GLY	5.0
1	B	487	VAL	5.0
1	C	478	LYS	5.0
1	B	277	GLU	5.0
1	B	262	GLU	5.0
1	B	276	LEU	4.9
1	A	466	ILE	4.9
1	D	472	ASP	4.9
1	D	287	TYR	4.9
1	C	483	ALA	4.8
1	C	276	LEU	4.7
1	D	563	TYR	4.7
1	D	483	ALA	4.6
1	C	284	LEU	4.6
1	D	573	CYS	4.6
1	B	490	ASP	4.6
1	D	568	TYR	4.6
1	B	326	GLN	4.5
1	D	476	LEU	4.5
1	D	275	PRO	4.4
1	D	277	GLU	4.4
1	C	554	CYS	4.4
1	C	586	VAL	4.3
1	D	586	VAL	4.3
1	C	592	THR	4.3
1	C	563	TYR	4.3
1	C	465	GLN	4.3
1	D	467	LYS	4.2
1	B	229	VAL	4.2
1	C	253	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	495	ALA	4.1
1	A	255	GLU	4.1
1	D	326	GLN	4.1
1	D	569	PHE	4.1
1	C	341	CYS	4.0
1	D	496	GLU	4.0
1	A	260	ILE	4.0
1	B	492	LYS	4.0
1	C	596	LYS	4.0
1	B	328	ASN	4.0
1	C	561	SER	4.0
1	D	263	GLU	4.0
1	D	498	PHE	3.9
1	B	587	ILE	3.9
1	C	484	LYS	3.9
1	C	568	TYR	3.9
1	B	590	LEU	3.9
1	C	473	TYR	3.9
1	C	573	CYS	3.8
1	B	253	VAL	3.8
1	C	490	ASP	3.8
1	C	594	GLN	3.8
1	D	273	VAL	3.8
1	B	596	LYS	3.8
1	C	493	LEU	3.8
1	D	596	LYS	3.8
1	A	263	GLU	3.8
1	C	228	GLU	3.7
1	C	258	GLY	3.7
1	D	492	LYS	3.7
1	C	562	LEU	3.6
1	C	287	TYR	3.6
1	C	591	ILE	3.6
1	C	275	PRO	3.6
1	C	558	ASP	3.6
1	D	115	MET	3.6
1	D	189	LEU	3.6
1	D	468	ILE	3.5
1	B	230	LYS	3.5
1	B	114	THR	3.5
1	C	231	TRP	3.5
1	A	560	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	565	ALA	3.5
1	C	326	GLN	3.5
1	C	571	GLN	3.5
1	D	480	VAL	3.4
1	D	528	ARG	3.4
1	D	191	ILE	3.4
1	B	557	VAL	3.4
1	B	396	TYR	3.4
1	A	277	GLU	3.4
1	A	543	GLU	3.4
1	D	511	GLU	3.3
1	D	485	PRO	3.3
1	A	486	LYS	3.3
1	B	134	ARG	3.3
1	D	475	SER	3.3
1	C	293	ASN	3.3
1	D	572	TRP	3.3
1	C	467	LYS	3.3
1	A	590	LEU	3.3
1	C	191	ILE	3.3
1	D	471	GLU	3.2
1	C	570	VAL	3.2
1	D	554	CYS	3.2
1	C	345	ASN	3.2
1	D	591	ILE	3.2
1	C	494	LYS	3.2
1	B	592	THR	3.2
1	B	263	GLU	3.2
1	B	260	ILE	3.1
1	A	327	ASN	3.1
1	B	288	LYS	3.1
1	B	327	ASN	3.1
1	C	593	PRO	3.1
1	A	490	ASP	3.1
1	D	575	ASP	3.1
1	A	465	GLN	3.1
1	C	347	LEU	3.1
1	C	572	TRP	3.1
1	C	492	LYS	3.1
1	D	292	GLU	3.1
1	B	284	LEU	3.0
1	D	578	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	114	THR	3.0
1	C	560	LYS	3.0
1	D	254	MET	3.0
1	C	262	GLU	3.0
1	D	190	GLN	3.0
1	C	440	ASP	3.0
1	D	543	GLU	2.9
1	D	565	ALA	2.9
1	C	241	PHE	2.9
1	C	277	GLU	2.9
1	C	564	ALA	2.9
1	B	491	VAL	2.9
1	C	396	TYR	2.9
1	B	325	ILE	2.9
1	C	556	LYS	2.9
1	C	569	PHE	2.9
1	D	253	VAL	2.9
1	D	585	ASP	2.9
1	C	390	PHE	2.8
1	C	259	LEU	2.8
1	D	276	LEU	2.8
1	D	495	ALA	2.8
1	C	491	VAL	2.8
1	D	559	ARG	2.8
1	D	259	LEU	2.8
1	C	471	GLU	2.8
1	A	262	GLU	2.8
1	A	325	ILE	2.8
1	C	325	ILE	2.8
1	C	444	ILE	2.8
1	A	259	LEU	2.8
1	C	528	ARG	2.7
1	D	477	PRO	2.7
1	A	556	LYS	2.7
1	B	585	ASP	2.7
1	C	297	LEU	2.7
1	D	255	GLU	2.7
1	D	463	THR	2.7
1	C	472	ASP	2.6
1	A	328	ASN	2.6
1	C	468	ILE	2.6
1	C	588	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	289	GLY	2.6
1	B	252	PRO	2.6
1	C	587	ILE	2.6
1	A	285	TRP	2.6
1	B	543	GLU	2.6
1	C	454	PHE	2.6
1	D	557	VAL	2.6
1	B	261	PRO	2.6
1	C	230	LYS	2.6
1	C	225	ALA	2.6
1	A	464	GLY	2.6
1	C	441	ALA	2.6
1	A	332	LYS	2.6
1	A	253	VAL	2.5
1	C	238	VAL	2.5
1	B	593	PRO	2.5
1	A	484	LYS	2.5
1	A	326	GLN	2.5
1	D	327	ASN	2.5
1	A	288	LYS	2.5
1	B	320	CYS	2.5
1	C	266	CYS	2.5
1	C	566	ARG	2.5
1	C	575	ASP	2.5
1	D	230	LYS	2.4
1	C	501	ASP	2.4
1	D	484	LYS	2.4
1	A	293	ASN	2.4
1	D	574	ALA	2.4
1	B	470	ARG	2.4
1	C	288	LYS	2.4
1	B	413	ILE	2.4
1	C	260	ILE	2.4
1	B	323	LEU	2.4
1	C	559	ARG	2.4
1	C	485	PRO	2.4
1	C	327	ASN	2.4
1	D	285	TRP	2.4
1	A	292	GLU	2.4
1	B	235	GLN	2.4
1	A	594	GLN	2.3
1	D	417	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	346	GLU	2.3
1	D	122	ILE	2.3
1	C	257	TYR	2.3
1	C	585	ASP	2.3
1	D	566	ARG	2.3
1	D	224	LEU	2.3
1	B	584	GLY	2.3
1	C	141	PHE	2.3
1	C	574	ALA	2.3
1	C	224	LEU	2.3
1	A	491	VAL	2.3
1	C	487	VAL	2.3
1	D	325	ILE	2.3
1	A	242	GLU	2.2
1	C	342	GLU	2.2
1	C	397	ILE	2.2
1	B	324	GLY	2.2
1	C	464	GLY	2.2
1	D	114	THR	2.2
1	A	599	ASN	2.2
1	C	457	VAL	2.2
1	A	492	LYS	2.2
1	D	269	LYS	2.2
1	D	129	HIS	2.2
1	B	121	PRO	2.2
1	D	520	PHE	2.2
1	D	184	GLU	2.2
1	D	583	ASP	2.2
1	C	160	ALA	2.2
1	A	572	TRP	2.2
1	B	486	LYS	2.2
1	C	481	ALA	2.2
1	D	499	ILE	2.2
1	D	347	LEU	2.2
1	D	298	TYR	2.1
1	C	245	ILE	2.1
1	B	259	LEU	2.1
1	D	339	ARG	2.1
1	D	517	HIS	2.1
1	B	160	ALA	2.1
1	D	185	LYS	2.1
1	D	340	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	434	THR	2.1
1	C	190	GLN	2.1
1	D	571	GLN	2.1
1	B	194	ARG	2.1
1	C	348	ARG	2.1
1	B	256	GLN	2.1
1	C	524	THR	2.1
1	D	238	VAL	2.1
1	D	397	ILE	2.1
1	C	549	LEU	2.1
1	C	322	HIS	2.1
1	C	235	GLN	2.1
1	C	256	GLN	2.1
1	C	320	CYS	2.1
1	D	328	ASN	2.1
1	D	349	ILE	2.1
1	D	474	GLU	2.1
1	C	583	ASP	2.0
1	B	122	ILE	2.0
1	D	324	GLY	2.0
1	B	255	GLU	2.0
1	B	344	ASP	2.0
1	C	286	PRO	2.0
1	D	344	ASP	2.0
1	C	328	ASN	2.0
1	C	599	ASN	2.0
1	D	246	ASN	2.0
1	A	276	LEU	2.0
1	B	493	LEU	2.0
1	B	115	MET	2.0
1	A	467	LYS	2.0
1	C	482	SER	2.0
1	C	317	ALA	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.



## 6.4 Ligands

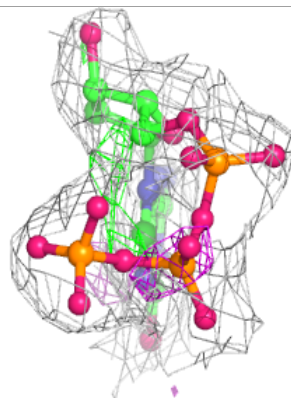
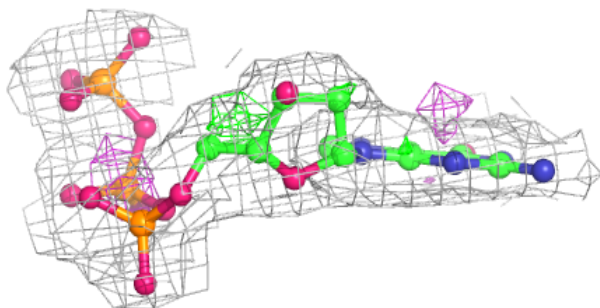
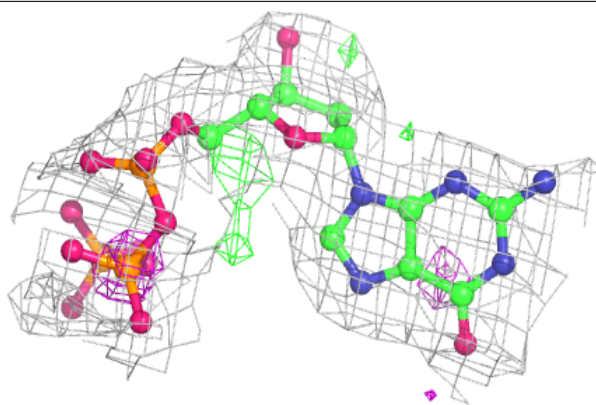
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	DGT	C	703	31/31	0.86	0.18	66,83,98,110	0
5	MG	A	704	1/1	0.86	0.09	59,59,59,59	0
2	TTP	A	701	29/29	0.92	0.14	37,55,81,89	0
2	TTP	D	703	29/29	0.92	0.14	58,73,91,100	0
2	TTP	B	701	29/29	0.94	0.13	58,68,79,81	0
5	MG	D	701	1/1	0.95	0.10	50,50,50,50	0
3	DGT	C	704	31/31	0.97	0.13	47,54,69,71	0
3	DGT	D	704	31/31	0.97	0.14	37,41,50,51	0
3	DGT	B	702	31/31	0.97	0.14	39,44,49,49	0
3	DGT	A	702	31/31	0.97	0.13	38,43,49,52	0
4	DTP	C	701	30/30	0.98	0.16	33,36,39,41	0
4	DTP	D	702	30/30	0.98	0.15	32,39,42,44	0
4	DTP	A	703	30/30	0.98	0.14	42,45,56,56	0
5	MG	B	703	1/1	0.98	0.10	55,55,55,55	0
4	DTP	B	704	30/30	0.98	0.15	34,39,46,49	0
5	MG	C	702	1/1	0.99	0.09	47,47,47,47	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.

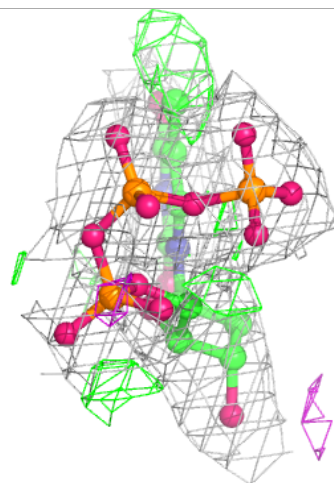
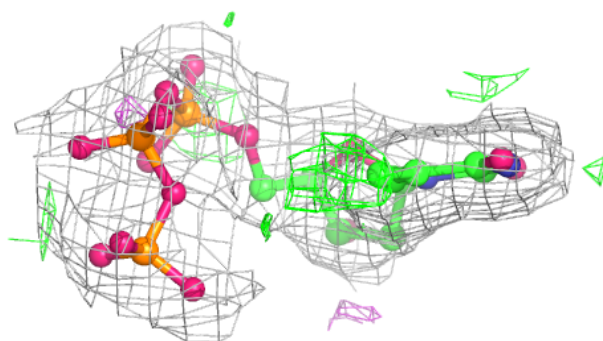
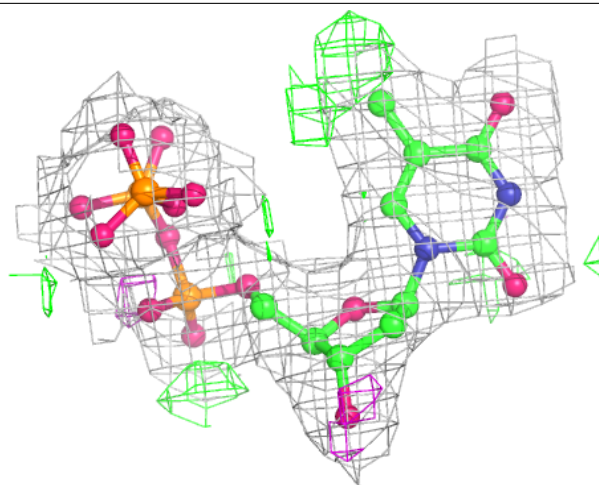
**Electron density around DGT C 703:**

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



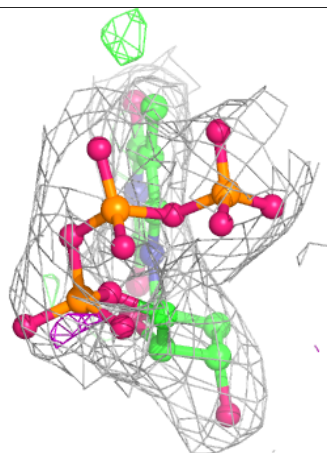
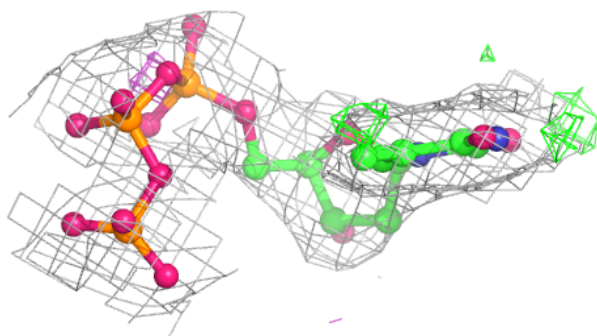
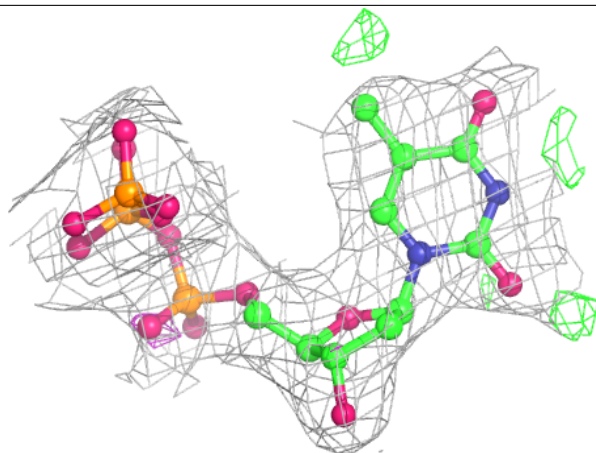
**Electron density around TTP A 701:**

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



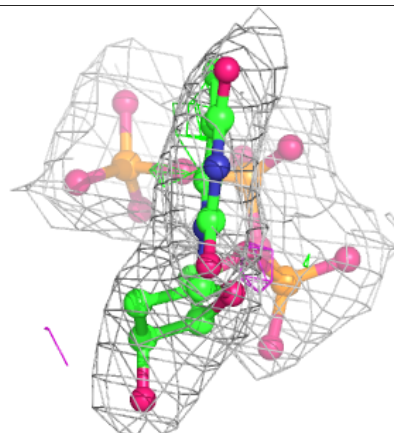
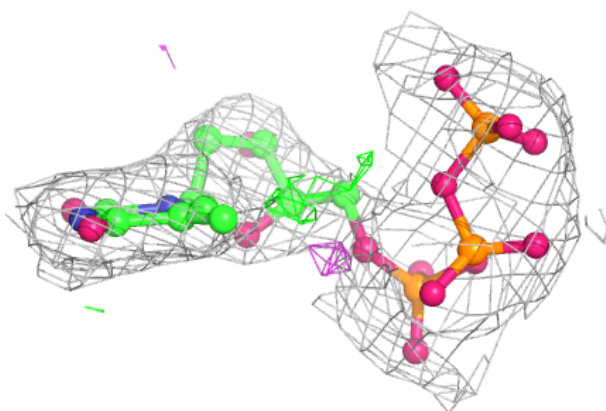
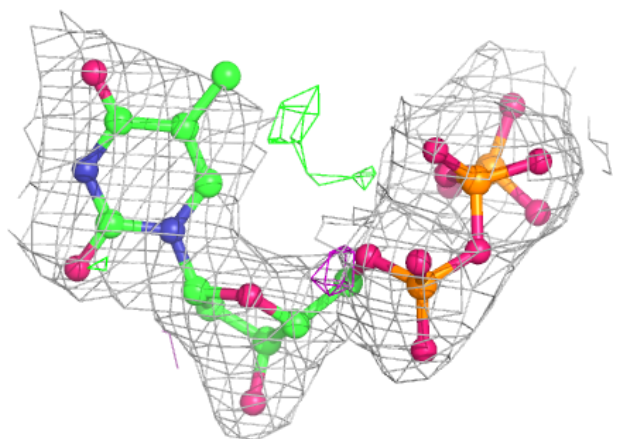
**Electron density around TTP D 703:**

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

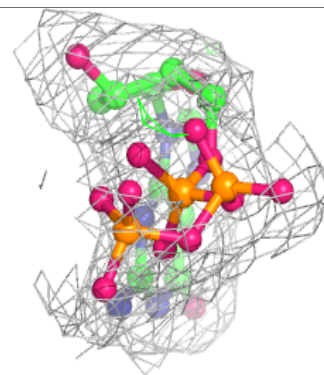
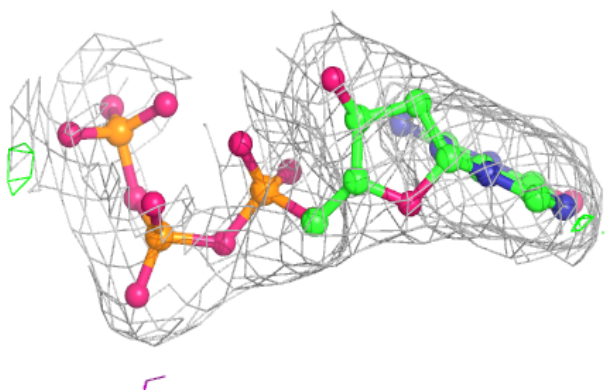
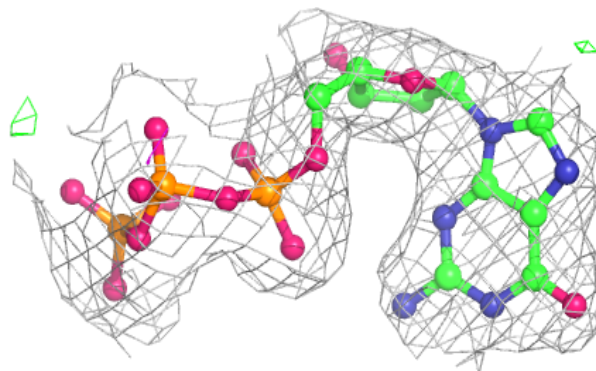


**Electron density around TTP B 701:**

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

**Electron density around DGT C 704:**

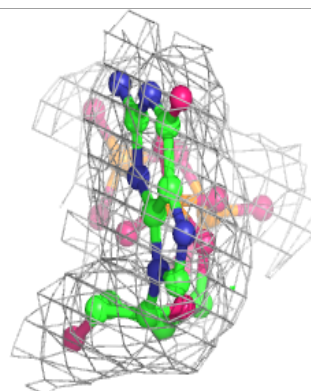
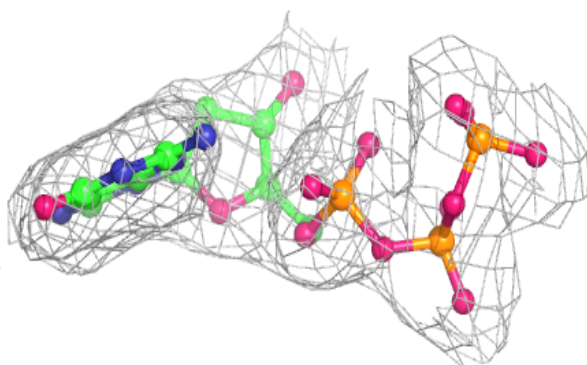
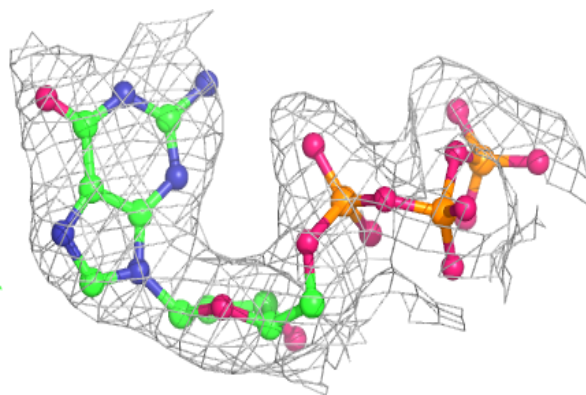
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



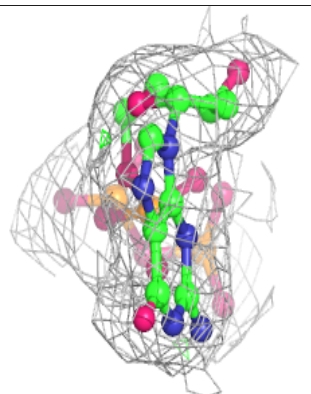
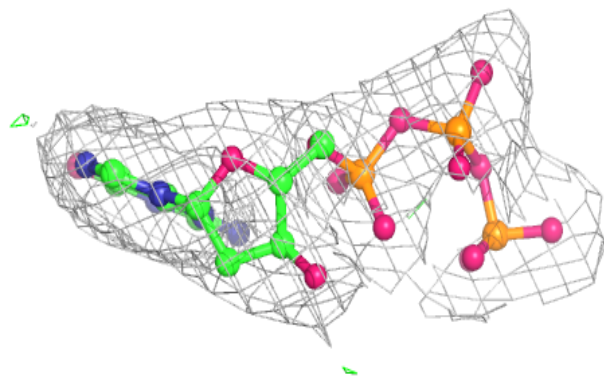
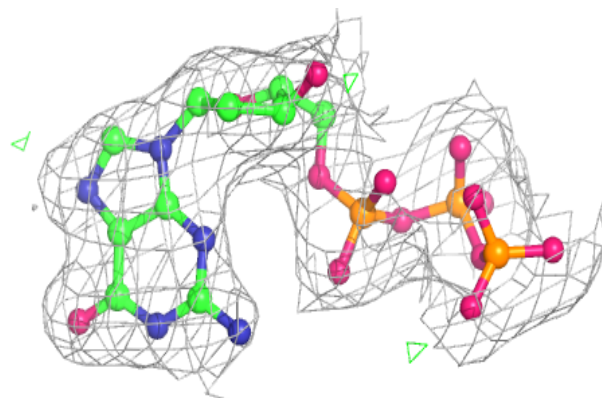


**Electron density around DGT D 704:**

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

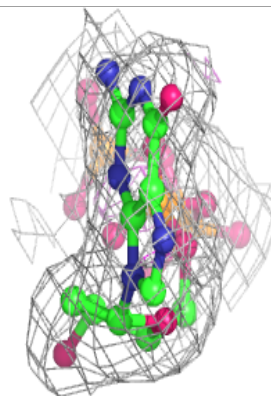
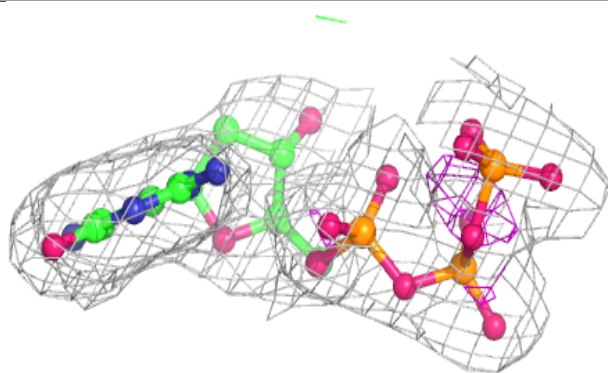
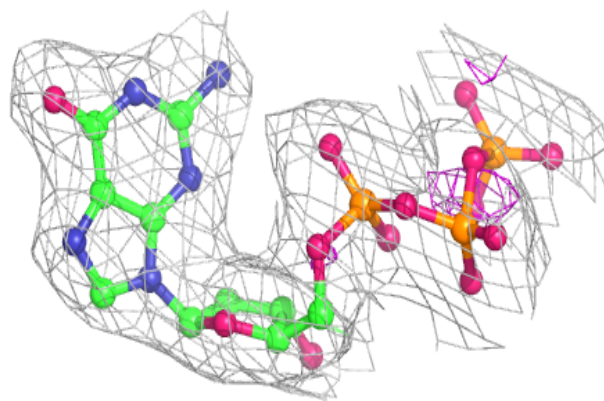
**Electron density around DGT B 702:**

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

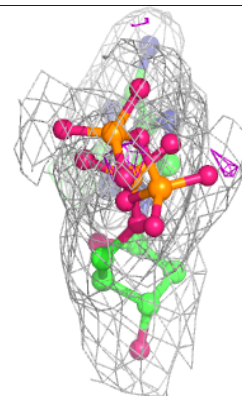
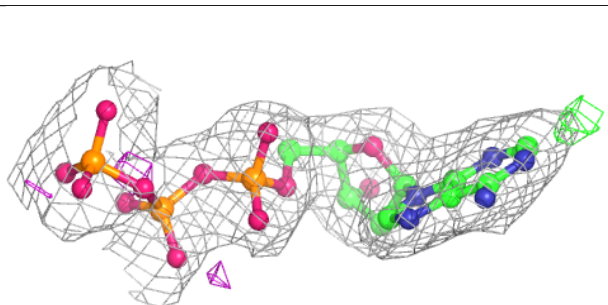
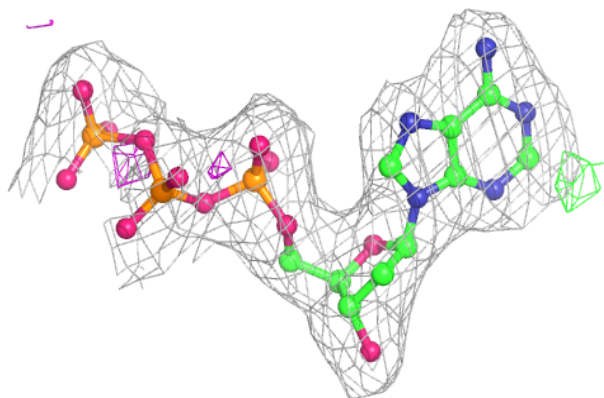


**Electron density around DGT A 702:**

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and green (positive)

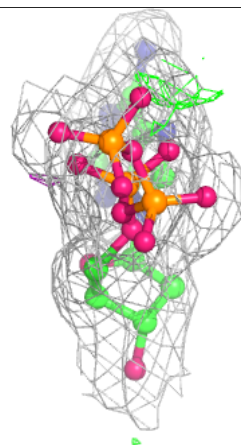
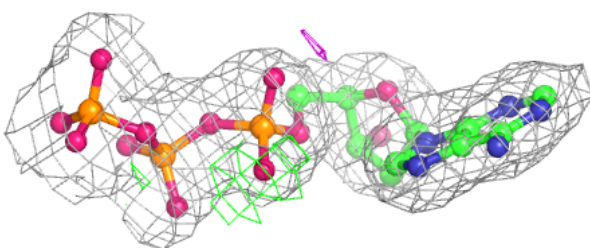
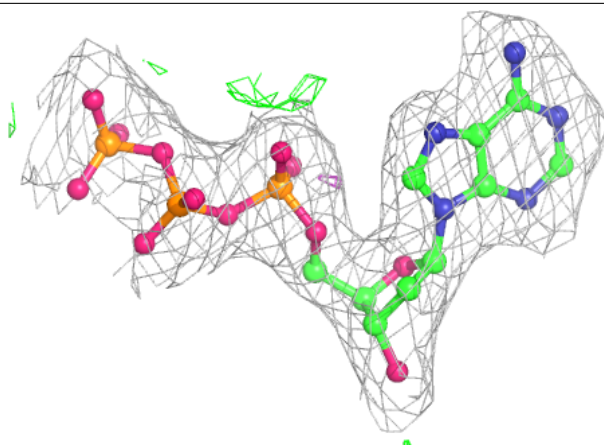
**Electron density around DTP C 701:**

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

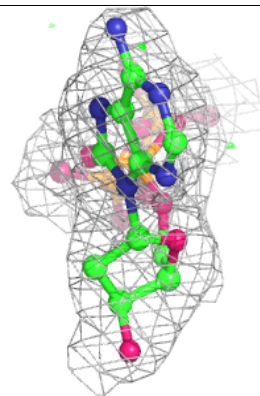
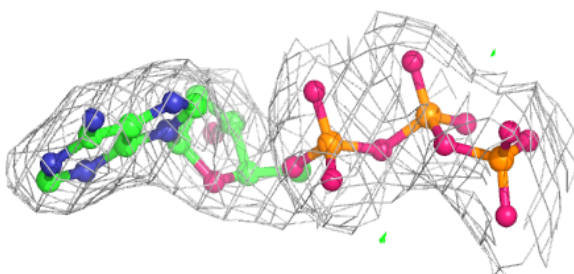
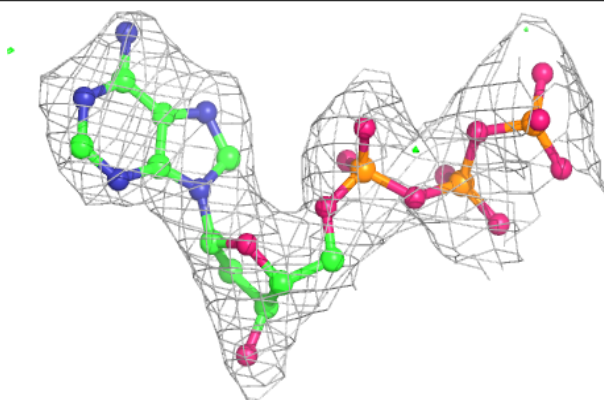


**Electron density around DTP D 702:**

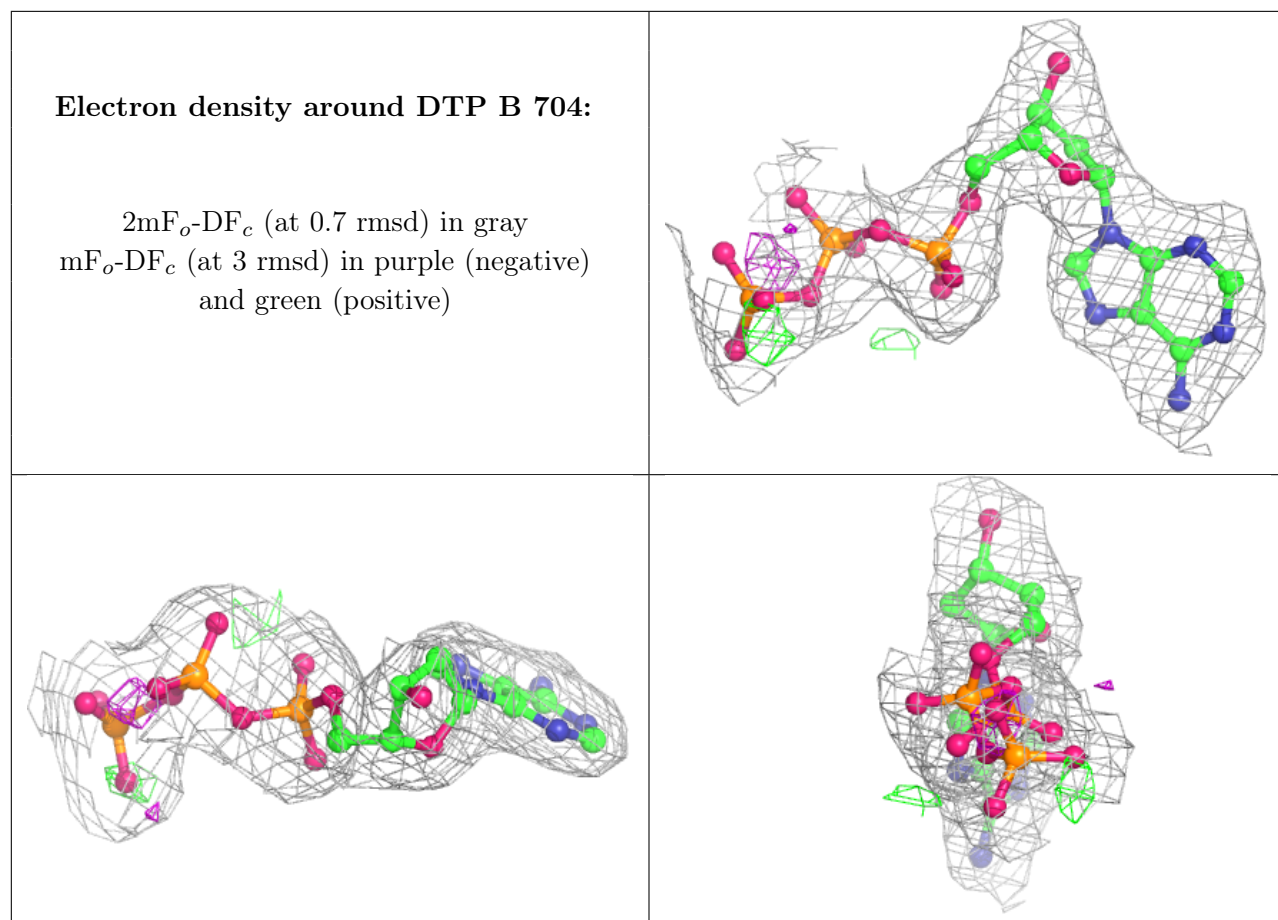
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around DTP 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)







## 6.5 Other polymers [i](#)

There are no such residues in this entry.