



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 26, 2023 – 12:05 PM EST

PDB ID : 4NCA
Title : Structure of *Thermus thermophilus* Argonaute bound to guide DNA 19-mer and target DNA in the presence of Mg²⁺
Authors : Sheng, G.; Zhao, H.; Wang, J.; Rao, Y.; Wang, Y.
Deposited on : 2013-10-24
Resolution : 2.49 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.31.2
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) : 2.31.2

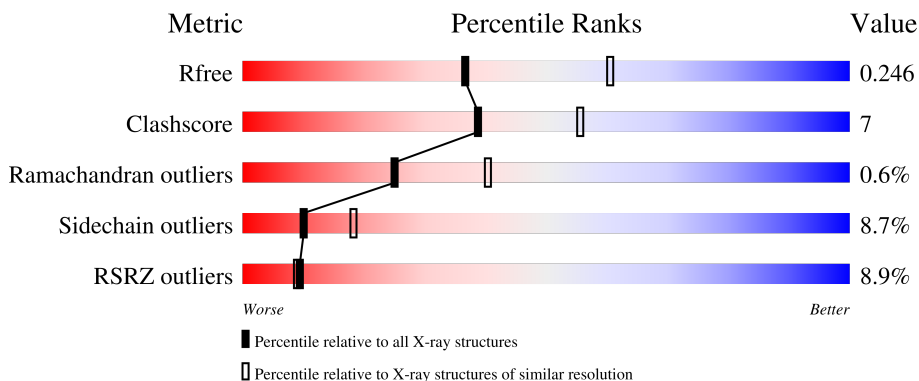
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (2.50-2.46)

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	685	<div style="display: flex; align-items: center;"> <div style="width: 9%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 75%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 22%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 10px;">9% 75% 22% •</p>
1	B	685	<div style="display: flex; align-items: center;"> <div style="width: 9%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 79%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 19%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 10px;">9% 79% 19% ••</p>
2	C	21	<div style="display: flex; align-items: center;"> <div style="width: 48%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 24%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 24%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 10px;">48% 24% 5% 24%</p>
2	E	21	<div style="display: flex; align-items: center;"> <div style="width: 24%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 52%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 24%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 10px;">24% 52% 24%</p>
3	D	10	<div style="display: flex; align-items: center;"> <div style="width: 80%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: orange;"></div> </div> <p style="margin-left: 10px;">80% 10% 10%</p>

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Mol	Chain	Length	Quality of chain
3	F	10	 90% 10%
4	G	6	 67% 33%
4	H	6	 33% 67%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12306 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 Argonaute.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	683	5338	3409	1001	921	7	0	0	0
1	B	678	5289	3383	995	904	7	0	0	0

- Molecule 2 is a DNA chain called 5'-D(P*TP*GP*AP*GP*GP*TP*AP*GP*TP*AP*GP*GP*TP*TP*GP*TP*AP*TP*AP*GP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	C	16	338	160	62	100	16	0	0	0
2	E	16	338	160	62	100	16	0	0	0

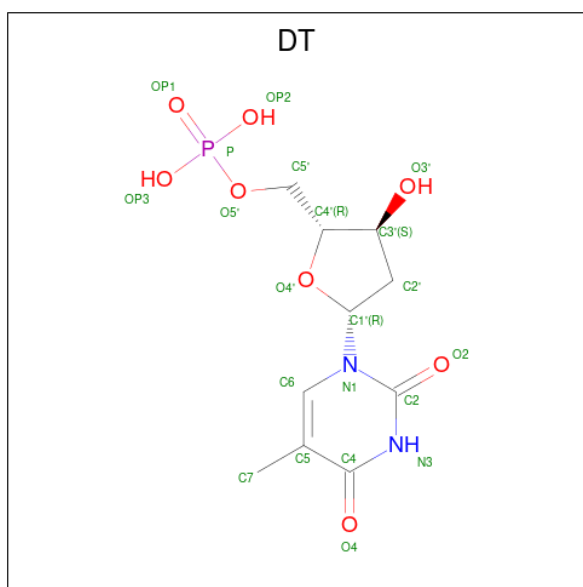
- Molecule 3 is a DNA chain called 5'-D(P*TP*AP*CP*TP*AP*CP*CP*TP*CP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	D	10	200	95	33	62	10	0	0	0
3	F	10	201	96	33	62	10	0	0	0

- Molecule 4 is a DNA chain called 5'-D(*AP*CP*AP*AP*CP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	G	6	117	57	24	31	5	0	0	0
4	H	6	117	57	24	31	5	0	0	0

- Molecule 5 is THYMIDINE-5'-MONOPHOSPHATE (three-letter code: DT) (formula: C₁₀H₁₅N₂O₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			21	10	2	8	1		
5	B	1	Total	C	N	O	P	0	0
			21	10	2	8	1		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		
6	B	2	Total	Mg	0	0
			2	2		
6	C	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		
6	E	1	Total	Mg	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	152	Total	O	0	0
			152	152		
7	B	118	Total	O	0	0
			118	118		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	11	Total O 11 11	0	0
7	D	11	Total O 11 11	0	0
7	E	18	Total O 18 18	0	0
7	F	6	Total O 6 6	0	0
7	G	1	Total O 1 1	0	0
7	H	3	Total O 3 3	0	0

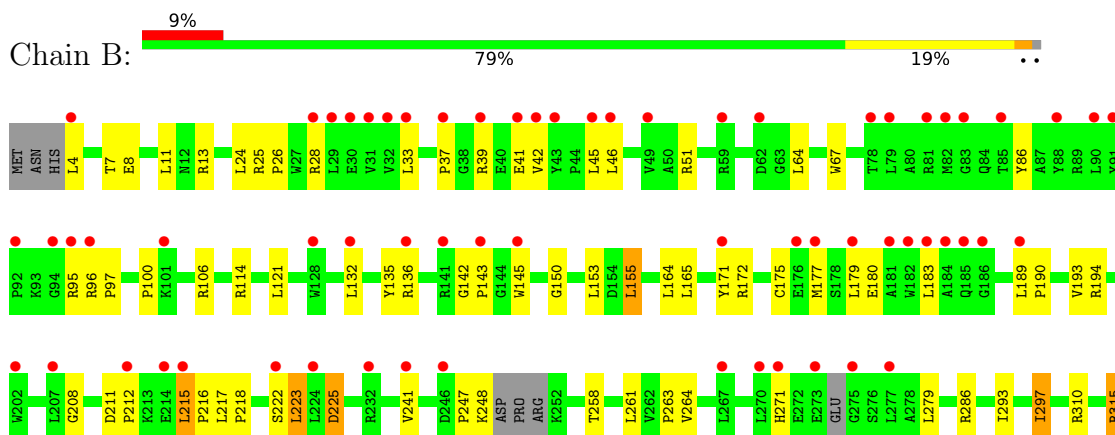
3 Residue-property plots [i](#)

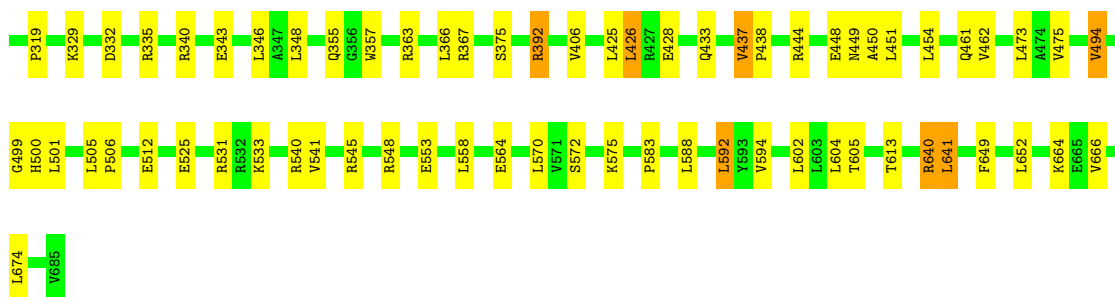
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Argonaute



- Molecule 1: Argonaute





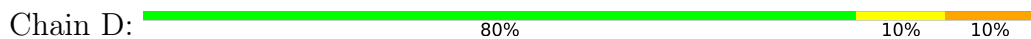
- Molecule 2: 5'-D(P*TP*GP*AP*GP*GP*TP*AP*GP*TP*AP*GP*GP*TP*TP*GP*TP*AP*TP*AP*GP*T)-3'



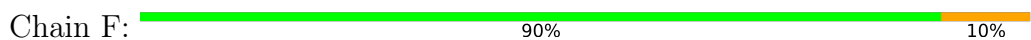
- Molecule 2: 5'-D(P*TP*GP*AP*GP*GP*TP*AP*GP*TP*AP*GP*GP*TP*TP*GP*TP*AP*TP*AP*GP*T)-3'



- Molecule 3: 5'-D(P*TP*AP*CP*TP*AP*CP*CP*TP*CP*G)-3'



- Molecule 3: 5'-D(P*TP*AP*CP*TP*AP*CP*CP*TP*CP*G)-3'

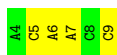


- Molecule 4: 5'-D(*AP*CP*AP*AP*CP*C)-3'



- Molecule 4: 5'-D(*AP*CP*AP*AP*CP*C)-3'





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	110.95Å 117.56Å 160.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.16 – 2.49 49.41 – 2.49	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.16-2.49) 99.4 (49.41-2.49)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 2.48Å)	Xtrriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.200 , 0.245 0.202 , 0.246	Depositor DCC
R_{free} test set	3714 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	46.7	Xtrriage
Anisotropy	0.322	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 61.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12306	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% 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: MG

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	0.26	0/5466	0.47	2/7423 (0.0%)
1	B	0.26	0/5416	0.45	0/7353
2	C	0.73	1/379 (0.3%)	1.28	2/584 (0.3%)
2	E	0.75	1/379 (0.3%)	1.26	4/584 (0.7%)
3	D	0.83	1/222 (0.5%)	1.12	1/337 (0.3%)
3	F	0.82	1/223 (0.4%)	1.11	0/339
4	G	0.50	0/131	1.14	0/199
4	H	0.47	0/131	0.99	0/199
All	All	0.35	4/12347 (0.0%)	0.61	9/17018 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	DT	OP3-P	-10.57	1.48	1.61
2	E	1	DT	OP3-P	-10.56	1.48	1.61
3	F	10	DT	OP3-P	-10.31	1.48	1.61
3	D	10	DT	OP3-P	-10.17	1.49	1.61

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	DT	OP1-P-OP2	-8.62	106.67	119.60
2	C	1	DT	OP1-P-OP2	-7.58	108.22	119.60
1	A	247	PRO	N-CA-CB	6.04	110.55	103.30
2	E	11	DG	O4'-C1'-N9	5.66	111.96	108.00
1	A	250	PRO	N-CA-CB	5.60	110.02	103.30
2	E	9	DT	O4'-C1'-N1	5.49	111.84	108.00
2	C	9	DT	N3-C4-O4	5.26	123.05	119.90
3	D	11	DA	O4'-C1'-N9	5.17	111.62	108.00
2	E	13	DT	N3-C4-O4	5.05	122.93	119.90

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	5338	0	5395	95	0
1	B	5289	0	5362	73	0
2	C	338	0	183	5	0
2	E	338	0	183	5	0
3	D	200	0	111	1	0
3	F	201	0	114	1	0
4	G	117	0	67	2	0
4	H	117	0	67	4	0
5	A	21	0	13	4	0
5	B	21	0	13	3	0
6	A	1	0	0	0	0
6	B	2	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	1	0
6	E	1	0	0	0	0
7	A	152	0	0	2	0
7	B	118	0	0	2	0
7	C	11	0	0	0	0
7	D	11	0	0	0	0
7	E	18	0	0	0	0
7	F	6	0	0	0	0
7	G	1	0	0	0	0
7	H	3	0	0	0	0
All	All	12306	0	11508	174	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (174) 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)
2:C:14:DT:H3	4:G:3:DA:H2	1.31	0.78
1:B:494:VAL:HG22	1:B:500:HIS:HB2	1.71	0.72
1:A:129:VAL:HG22	1:A:134:VAL:HG12	1.75	0.69
1:A:136:ARG:NH1	7:A:925:HOH:O	2.26	0.69
1:A:436:ASN:O	1:A:446:ARG:NH2	2.25	0.69
1:A:512:GLU:OE2	1:A:545:ARG:NH2	2.27	0.68
1:A:28:ARG:HE	1:A:96:ARG:HG2	1.59	0.67
1:A:51:ARG:NH2	1:A:118:GLN:OE1	2.28	0.67
1:A:392:ARG:NH1	1:B:525:GLU:OE1	2.28	0.66
1:A:597:GLU:HB3	1:A:600:THR:HG23	1.78	0.65
1:B:25:ARG:O	1:B:95:ARG:NH2	2.30	0.64
1:A:114:ARG:NH2	4:G:4:DA:OP2	2.31	0.64
1:A:583:PRO:HD3	1:A:588:LEU:HD13	1.79	0.64
1:B:8:GLU:OE1	1:B:310:ARG:NH1	2.31	0.63
1:B:190:PRO:HG2	1:B:263:PRO:HB3	1.82	0.62
3:D:10:DT:OP1	6:D:101:MG:MG	1.43	0.62
1:B:28:ARG:HD3	1:B:96:ARG:HB2	1.82	0.61
1:B:548:ARG:NH2	4:H:7:DA:N3	2.50	0.58
1:A:285:GLU:HG3	1:A:288:ARG:HH21	1.68	0.58
1:B:114:ARG:HD3	1:B:132:LEU:HD11	1.86	0.58
1:B:343:GLU:HG3	1:B:375:SER:HB2	1.84	0.58
2:E:6:DT:H2''	2:E:7:DA:H5''	1.85	0.58
1:A:121:LEU:HD22	1:A:134:VAL:HG11	1.84	0.58
1:A:273:GLU:O	1:A:275:GLY:N	2.37	0.58
1:A:319:PRO:HG3	1:A:640:ARG:HD2	1.86	0.57
2:C:3:DA:H2'	2:C:4:DG:C8	2.38	0.57
1:B:136:ARG:NH2	7:B:894:HOH:O	2.36	0.57
1:A:446:ARG:HG3	2:C:2:DG:C8	2.39	0.57
1:A:462:VAL:HG23	1:A:463:VAL:HG13	1.87	0.57
1:B:175:CYS:SG	1:B:263:PRO:HG2	2.45	0.56
1:B:286:ARG:HD2	1:B:613:THR:HG21	1.87	0.56
1:B:594:VAL:HB	1:B:602:LEU:HB2	1.87	0.56
1:A:136:ARG:NH2	1:A:293:ILE:HG23	2.21	0.56
1:B:208:GLY:N	1:B:241:VAL:O	2.39	0.55
1:B:473:LEU:HB3	1:B:541:VAL:HG12	1.89	0.55
1:B:605:THR:O	1:B:640:ARG:NH2	2.40	0.55
1:A:377:ARG:NH1	1:A:401:GLU:O	2.39	0.55
1:A:217:LEU:O	1:A:219:GLY:N	2.40	0.54
1:A:600:THR:HB	1:A:620:VAL:HG22	1.90	0.54
1:A:225:ASP:HA	1:A:228:ALA:HB3	1.89	0.54
1:B:545:ARG:NH1	1:B:553:GLU:OE2	2.40	0.54
1:B:218:PRO:HD2	5:B:701:DT:H3	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:PRO:HG2	1:B:640:ARG:HD2	1.89	0.53
1:A:54:GLY:O	1:A:57:THR:HG23	2.09	0.53
1:B:100:PRO:O	1:B:106:ARG:NH1	2.38	0.53
1:B:506:PRO:HG2	1:B:666:VAL:HG21	1.91	0.53
1:B:583:PRO:HD3	1:B:588:LEU:HD13	1.91	0.53
1:B:41:GLU:O	1:B:45:LEU:HB2	2.09	0.52
1:A:605:THR:O	1:A:640:ARG:NH2	2.42	0.52
1:A:212:PRO:O	1:A:222:SER:OG	2.28	0.52
1:A:180:GLU:HG2	1:A:258:THR:OG1	2.09	0.52
3:F:10:DT:OP2	4:H:9:DC:O3'	2.28	0.52
1:B:193:VAL:HG11	1:B:261:LEU:HD13	1.92	0.52
2:E:3:DA:H2'	2:E:4:DG:C8	2.46	0.51
1:A:221:LEU:HD13	1:A:226:TYR:HB2	1.92	0.51
1:A:410:THR:O	1:A:436:ASN:HA	2.10	0.51
1:B:363:ARG:O	1:B:367:ARG:HG3	2.10	0.51
1:A:48:GLN:HG2	1:A:79:LEU:HD22	1.93	0.51
1:B:33:LEU:HD13	1:B:45:LEU:HD23	1.91	0.51
1:A:217:LEU:HD21	1:A:223:LEU:HG	1.93	0.50
1:A:39:ARG:HD3	5:B:701:DT:C2	2.46	0.50
1:A:340:ARG:NH1	1:A:499:GLY:O	2.35	0.50
1:A:461:GLN:NE2	1:A:498:GLY:O	2.44	0.50
1:A:461:GLN:HG3	1:A:499:GLY:O	2.12	0.50
1:A:362:ARG:NH1	7:A:872:HOH:O	2.36	0.50
1:A:393:GLU:OE2	1:A:396:ARG:NH2	2.36	0.50
1:B:293:ILE:O	1:B:297:ILE:HG12	2.11	0.50
1:B:437:VAL:HG22	1:B:438:PRO:HA	1.92	0.50
1:A:114:ARG:HD2	1:A:132:LEU:HD11	1.94	0.50
1:B:512:GLU:OE2	1:B:545:ARG:NH2	2.45	0.49
1:A:440:ARG:HB2	1:A:442:GLU:HG2	1.93	0.49
1:B:461:GLN:HG3	1:B:499:GLY:O	2.11	0.49
1:B:222:SER:HB2	1:B:225:ASP:HB2	1.93	0.49
1:A:319:PRO:CG	1:A:640:ARG:HD2	2.43	0.49
1:B:335:ARG:NH2	1:B:448:GLU:OE2	2.46	0.49
1:B:501:LEU:HD21	1:B:641:LEU:HD13	1.94	0.49
1:A:45:LEU:HD12	1:A:45:LEU:HA	1.69	0.49
1:A:200:ARG:NH1	5:A:701:DT:OP1	2.42	0.49
1:B:4:LEU:HB3	1:B:315:ARG:O	2.12	0.49
1:A:395:LEU:HD11	1:A:425:LEU:HD22	1.94	0.49
1:A:472:GLU:OE2	1:A:536:ARG:NH2	2.28	0.48
5:A:701:DT:C2	1:B:39:ARG:HB2	2.47	0.48
1:B:180:GLU:HG2	1:B:258:THR:OG1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:14:DT:H3	4:H:6:DA:H2	1.60	0.48
1:A:341:ALA:HA	1:A:460:LEU:HD22	1.95	0.48
1:A:37:PRO:HB3	1:A:45:LEU:HD23	1.95	0.48
1:B:37:PRO:HB2	1:B:41:GLU:HG3	1.95	0.48
1:A:444:ARG:HA	1:A:447:TRP:NE1	2.28	0.48
1:A:558:LEU:HG	1:A:568:TYR:CZ	2.49	0.48
1:A:125:GLU:HA	1:A:126:GLY:HA2	1.64	0.47
1:A:142:GLY:HA3	1:A:145:TRP:CE2	2.49	0.47
1:A:350:ARG:HD2	1:A:352:ASP:OD1	2.14	0.47
1:B:217:LEU:HD11	1:B:223:LEU:HA	1.97	0.47
1:B:335:ARG:HH21	1:B:444:ARG:HE	1.63	0.47
1:B:392:ARG:NH2	1:B:428:GLU:OE2	2.47	0.47
1:B:135:TYR:HA	1:B:150:GLY:HA3	1.97	0.47
1:A:210:GLU:N	1:A:210:GLU:OE1	2.47	0.46
1:B:121:LEU:HD11	1:B:153:LEU:HD12	1.98	0.46
1:A:296:TRP:HE3	1:A:299:ARG:HH21	1.63	0.46
1:B:51:ARG:NE	4:H:5:DC:OP1	2.48	0.46
1:B:548:ARG:HA	1:B:572:SER:OG	2.15	0.46
1:A:666:VAL:HG22	1:A:674:LEU:HD11	1.97	0.46
1:B:142:GLY:HA3	1:B:145:TRP:CE2	2.50	0.46
1:A:506:PRO:HG2	1:A:666:VAL:HG21	1.97	0.45
1:A:225:ASP:OD1	1:A:225:ASP:N	2.46	0.45
1:A:640:ARG:HG3	1:A:649:PHE:CD2	2.52	0.45
1:A:179:LEU:HD12	1:A:258:THR:HG22	1.98	0.45
1:A:494:VAL:HG22	1:A:500:HIS:HB2	1.99	0.45
1:B:171:TYR:CG	1:B:279:LEU:HD22	2.52	0.45
1:B:329:LYS:NZ	1:B:332:ASP:OD1	2.50	0.45
1:B:575:LYS:HD3	1:B:652:LEU:HD11	1.99	0.45
1:B:666:VAL:HG22	1:B:674:LEU:HD11	1.99	0.45
1:A:409:LEU:HD23	1:A:435:LEU:HB3	1.98	0.45
1:A:136:ARG:HH22	1:A:293:ILE:HA	1.82	0.44
1:A:350:ARG:NH2	1:A:352:ASP:OD2	2.50	0.44
1:A:329:LYS:NZ	1:A:332:ASP:OD1	2.50	0.44
1:A:120:ARG:NH1	1:A:301:LEU:O	2.51	0.44
1:A:558:LEU:HG	1:A:568:TYR:CE2	2.53	0.44
1:B:26:PRO:HB3	1:B:67:TRP:CD1	2.53	0.44
1:B:640:ARG:HG3	1:B:649:PHE:CD2	2.53	0.44
1:A:135:TYR:HA	1:A:150:GLY:HA3	1.99	0.44
1:A:392:ARG:NH2	1:A:428:GLU:OE2	2.48	0.43
1:A:177:MET:HB2	1:A:181:ALA:HB3	2.01	0.43
1:B:592:LEU:HD12	1:B:592:LEU:HA	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:LEU:HA	1:A:46:LEU:HD12	1.80	0.43
1:B:41:GLU:OE1	1:B:86:TYR:OH	2.37	0.43
1:B:433:GLN:HG2	1:B:450:ALA:O	2.18	0.43
1:A:39:ARG:NH1	5:B:701:DT:O2	2.52	0.43
1:A:102:ASP:HA	1:A:103:PRO:HD3	1.82	0.43
1:A:433:GLN:HG2	1:A:450:ALA:O	2.19	0.43
1:A:96:ARG:HA	1:A:97:PRO:HD3	1.88	0.42
1:B:545:ARG:HA	1:B:545:ARG:HD2	1.89	0.42
1:A:22:GLU:OE1	1:A:95:ARG:NH1	2.52	0.42
1:A:639:THR:HG21	1:A:640:ARG:HH21	1.83	0.42
1:A:348:LEU:HB2	1:A:357:TRP:CE2	2.54	0.42
1:B:348:LEU:HB2	1:B:357:TRP:CE2	2.54	0.42
1:A:255:PRO:O	5:A:701:DT:H2''	2.19	0.42
1:B:449:ASN:ND2	2:E:2:DG:H21	2.18	0.42
1:A:190:PRO:HG3	1:A:263:PRO:HB3	2.01	0.42
1:A:217:LEU:HB2	1:A:221:LEU:O	2.20	0.42
1:A:348:LEU:HB2	1:A:357:TRP:CZ2	2.55	0.42
1:A:305:THR:HA	1:A:306:PRO:HD3	1.85	0.42
5:A:701:DT:N3	1:B:39:ARG:HB2	2.35	0.42
1:A:505:LEU:HD23	1:A:505:LEU:HA	1.89	0.41
1:A:575:LYS:HB3	1:A:651:ARG:HH22	1.85	0.41
1:A:434:ILE:O	2:C:1:DT:H4'	2.20	0.41
1:A:449:ASN:ND2	2:C:2:DG:H21	2.19	0.41
1:B:340:ARG:NH2	1:B:499:GLY:O	2.44	0.41
1:A:20:ASN:HB2	1:A:21:PRO:HD2	2.03	0.41
1:A:608:ARG:HB2	1:A:611:ARG:HG3	2.01	0.41
1:B:37:PRO:HB3	1:B:45:LEU:HD22	2.02	0.41
1:A:14:PHE:HB3	1:A:306:PRO:HB3	2.02	0.41
1:A:46:LEU:O	1:A:49:VAL:HG12	2.21	0.41
1:A:254:ILE:HA	1:A:255:PRO:HD3	1.95	0.41
1:A:7:THR:OG1	1:A:8:GLU:N	2.52	0.41
1:B:155:LEU:HD23	1:B:164:LEU:O	2.21	0.41
1:B:183:LEU:HD21	1:B:189:LEU:HD23	2.03	0.41
1:B:664:LYS:HE2	1:B:664:LYS:HB2	1.67	0.41
1:B:211:ASP:HA	1:B:212:PRO:HD2	1.93	0.41
1:B:426:LEU:HD13	7:B:872:HOH:O	2.20	0.41
1:A:533:LYS:HD3	1:A:533:LYS:HA	1.79	0.41
1:B:264:VAL:HG11	2:E:10:DA:H5'	2.03	0.41
1:A:171:TYR:CG	1:A:279:LEU:HD22	2.56	0.40
1:A:473:LEU:HB3	1:A:541:VAL:HG12	2.02	0.40
1:B:11:LEU:C	1:B:13:ARG:H	2.24	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:LEU:HD13	1:B:164:LEU:HA	1.97	0.40
1:A:101:LYS:HD3	1:A:101:LYS:HA	1.91	0.40
1:A:331:ALA:HA	1:A:452:LEU:HD11	2.03	0.40
1:B:193:VAL:HG21	1:B:261:LEU:HB3	2.03	0.40
1:B:640:ARG:HG3	1:B:649:PHE:CG	2.55	0.40
1:A:57:THR:HG22	1:A:66:SER:OG	2.21	0.40
1:B:215:LEU:HA	1:B:216:PRO:HD3	1.84	0.40
1:B:335:ARG:NH2	1:B:444:ARG:HH21	2.19	0.40
1:B:25:ARG:CZ	1:B:97:PRO:HG3	2.52	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	681/685 (99%)	643 (94%)	32 (5%)	6 (1%)	17	29
1	B	672/685 (98%)	654 (97%)	16 (2%)	2 (0%)	41	59
All	All	1353/1370 (99%)	1297 (96%)	48 (4%)	8 (1%)	25	40

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	247	PRO
1	A	274	GLU
1	A	275	GLY
1	A	585	GLN
1	B	143	PRO
1	A	218	PRO
1	A	219	GLY
1	A	355	GLN

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	529/549 (96%)	480 (91%)	49 (9%)	9 15
1	B	522/549 (95%)	480 (92%)	42 (8%)	12 21
All	All	1051/1098 (96%)	960 (91%)	91 (9%)	10 18

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	45	LEU
1	A	46	LEU
1	A	51	ARG
1	A	57	THR
1	A	96	ARG
1	A	98	LEU
1	A	114	ARG
1	A	155	LEU
1	A	165	LEU
1	A	172	ARG
1	A	185	GLN
1	A	221	LEU
1	A	223	LEU
1	A	236	ARG
1	A	273	GLU
1	A	277	LEU
1	A	289	ARG
1	A	321	LEU
1	A	335	ARG
1	A	342	GLN
1	A	346	LEU
1	A	366	LEU
1	A	381	LEU
1	A	392	ARG
1	A	420	ARG
1	A	425	LEU

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Mol	Chain	Res	Type
1	A	426	LEU
1	A	437	VAL
1	A	440	ARG
1	A	442	GLU
1	A	451	LEU
1	A	454	LEU
1	A	462	VAL
1	A	475	VAL
1	A	505	LEU
1	A	531	ARG
1	A	543	LEU
1	A	545	ARG
1	A	558	LEU
1	A	559	GLU
1	A	570	LEU
1	A	598	ASP
1	A	600	THR
1	A	604	LEU
1	A	609	ASP
1	A	639	THR
1	A	640	ARG
1	A	641	LEU
1	B	7	THR
1	B	24	LEU
1	B	42	VAL
1	B	46	LEU
1	B	64	LEU
1	B	155	LEU
1	B	165	LEU
1	B	172	ARG
1	B	177	MET
1	B	179	LEU
1	B	194	ARG
1	B	215	LEU
1	B	223	LEU
1	B	225	ASP
1	B	248	LYS
1	B	271	HIS
1	B	297	ILE
1	B	315	ARG
1	B	346	LEU
1	B	355	GLN

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Mol	Chain	Res	Type
1	B	366	LEU
1	B	392	ARG
1	B	406	VAL
1	B	425	LEU
1	B	426	LEU
1	B	437	VAL
1	B	451	LEU
1	B	454	LEU
1	B	462	VAL
1	B	475	VAL
1	B	494	VAL
1	B	505	LEU
1	B	531	ARG
1	B	533	LYS
1	B	540	ARG
1	B	558	LEU
1	B	564	GLU
1	B	570	LEU
1	B	592	LEU
1	B	604	LEU
1	B	640	ARG
1	B	641	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	461	GLN
1	B	312	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 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
5	DT	B	701	-	22,22,22	0.64	0	33,33,33	0.99	2 (6%)
5	DT	A	701	-	22,22,22	0.59	0	33,33,33	0.87	2 (6%)

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
5	DT	B	701	-	-	1/10/22/22	0/2/2/2
5	DT	A	701	-	-	3/10/22/22	0/2/2/2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
5	B	701	DT	O4-C4-C5	-2.87	121.58	124.90
5	B	701	DT	OP2-P-OP3	2.66	117.81	107.64
5	A	701	DT	O4-C4-C5	-2.62	121.86	124.90
5	A	701	DT	OP2-P-OP1	2.09	118.87	110.68

There are no chirality outliers.

All (4) torsion outliers are listed below:

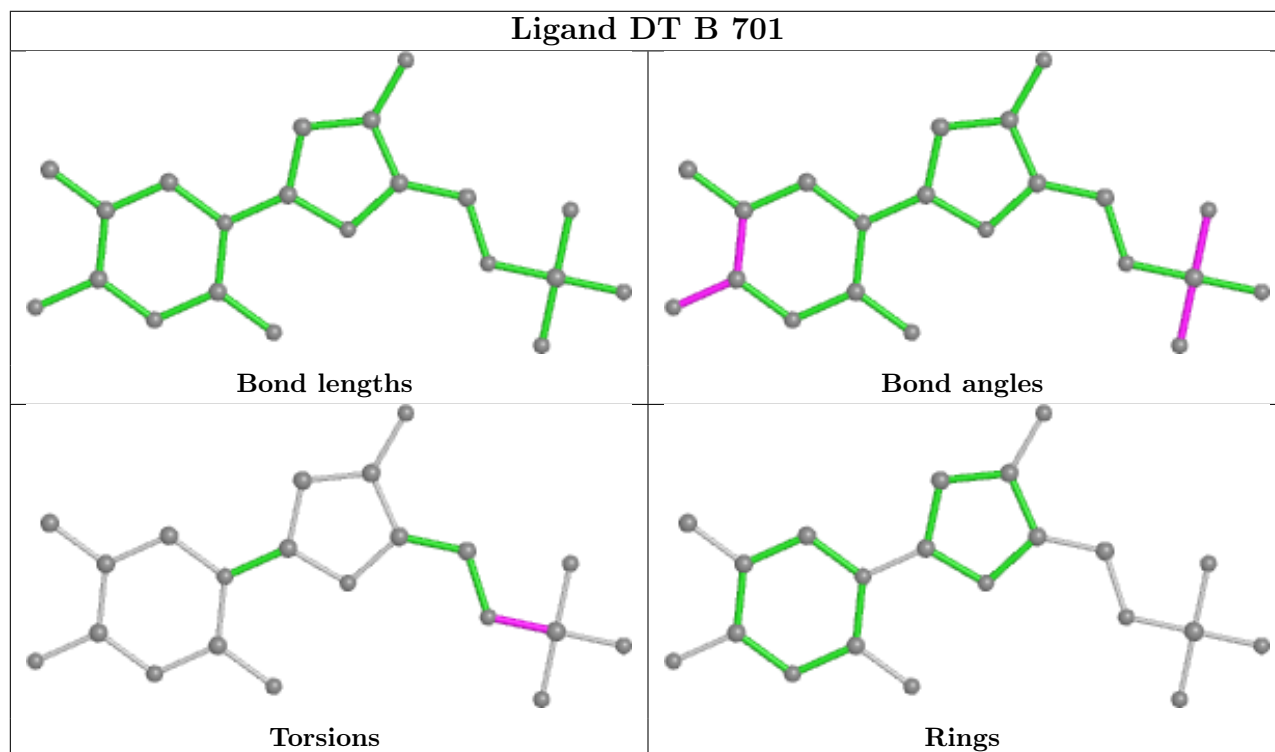
Mol	Chain	Res	Type	Atoms
5	A	701	DT	C5'-O5'-P-OP3
5	A	701	DT	C5'-O5'-P-OP1
5	A	701	DT	C5'-O5'-P-OP2
5	B	701	DT	C5'-O5'-P-OP1

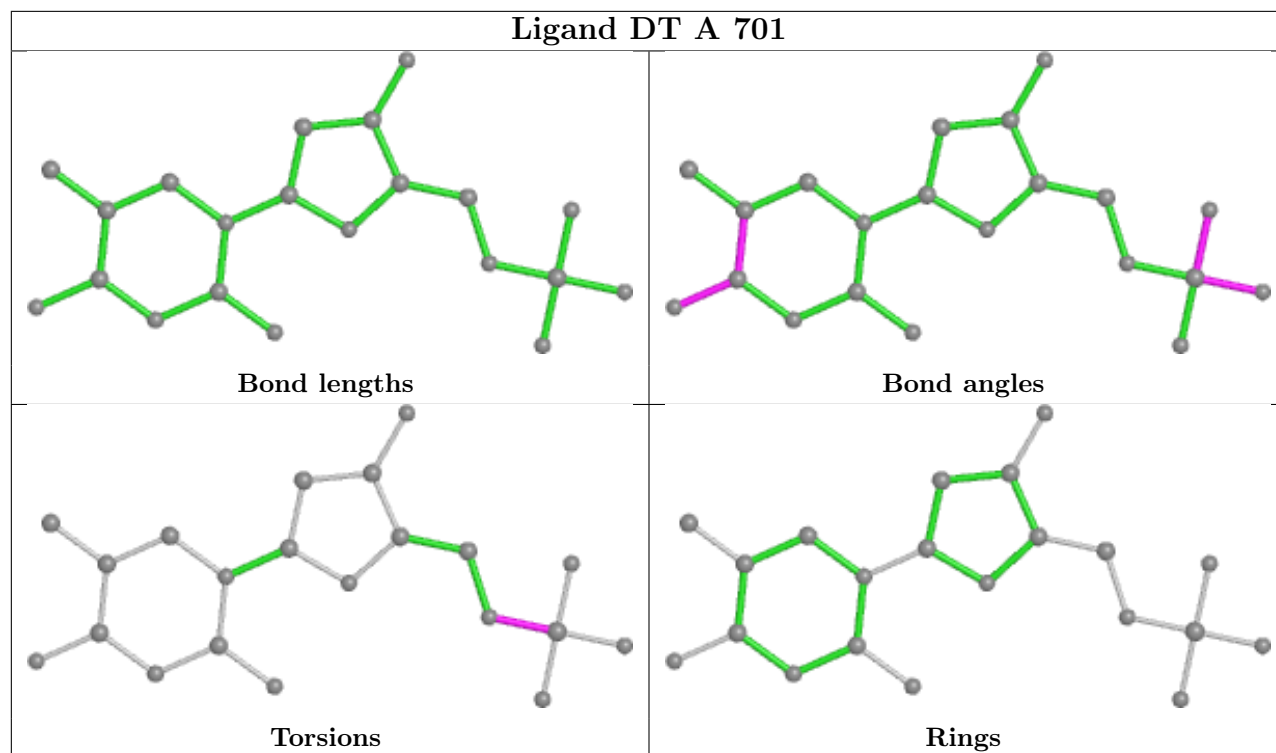
There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	701	DT	3	0
5	A	701	DT	4	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	683/685 (99%)	0.50	63 (9%) 9 8	31, 56, 106, 142	0
1	B	678/685 (98%)	0.49	64 (9%) 8 8	36, 59, 99, 160	0
2	C	16/21 (76%)	-0.29	0 100 100	50, 56, 71, 90	0
2	E	16/21 (76%)	-0.34	0 100 100	46, 57, 73, 95	0
3	D	10/10 (100%)	-0.26	0 100 100	53, 65, 73, 76	0
3	F	10/10 (100%)	-0.36	0 100 100	52, 62, 69, 72	0
4	G	6/6 (100%)	-0.14	0 100 100	53, 67, 85, 99	0
4	H	6/6 (100%)	-0.02	0 100 100	50, 70, 93, 94	0
All	All	1425/1444 (98%)	0.46	127 (8%) 9 9	31, 57, 101, 160	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	277	LEU	7.6
1	A	251	ARG	6.5
1	A	136	ARG	6.3
1	A	207	LEU	6.3
1	A	183	LEU	5.9
1	A	275	GLY	5.8
1	A	212	PRO	5.6
1	A	223	LEU	5.5
1	A	216	PRO	4.9
1	A	184	ALA	4.8
1	A	221	LEU	4.7
1	A	276	SER	4.7
1	A	270	LEU	4.6
1	A	272	GLU	4.6
1	A	182	TRP	4.6
1	A	249	ASP	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	278	ALA	4.5
1	A	247	PRO	4.4
1	A	205	LEU	4.4
1	A	271	HIS	4.1
1	A	217	LEU	4.1
1	B	94	GLY	4.1
1	A	238	GLY	4.0
1	B	37	PRO	4.0
1	B	83	GLY	4.0
1	A	250	PRO	4.0
1	A	243	TRP	3.9
1	B	267	LEU	3.8
1	B	270	LEU	3.8
1	A	208	GLY	3.7
1	B	275	GLY	3.7
1	A	236	ARG	3.7
1	A	233	LEU	3.7
1	A	248	LYS	3.6
1	A	235	GLY	3.6
1	B	96	ARG	3.6
1	A	204	LEU	3.6
1	B	246	ASP	3.6
1	B	29	LEU	3.5
1	B	241	VAL	3.5
1	B	45	LEU	3.5
1	B	42	VAL	3.4
1	B	189	LEU	3.3
1	B	43	TYR	3.3
1	A	219	GLY	3.3
1	B	90	LEU	3.2
1	A	242	ALA	3.2
1	B	271	HIS	3.2
1	A	209	GLU	3.2
1	A	241	VAL	3.1
1	A	240	ARG	3.1
1	A	224	LEU	3.1
1	A	226	TYR	3.1
1	B	91	TYR	3.0
1	B	145	TRP	3.0
1	B	176	GLU	3.0
1	A	222	SER	3.0
1	B	101	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	212	PRO	3.0
1	B	182	TRP	2.9
1	B	186	GLY	2.9
1	B	202	TRP	2.9
1	B	82	MET	2.8
1	B	277	LEU	2.8
1	B	179	LEU	2.8
1	B	28	ARG	2.8
1	A	177	MET	2.8
1	B	273	GLU	2.8
1	A	186	GLY	2.8
1	B	32	VAL	2.7
1	B	185	GLN	2.7
1	A	220	GLY	2.7
1	A	437	VAL	2.7
1	A	267	LEU	2.7
1	A	187	HIS	2.7
1	B	46	LEU	2.7
1	A	232	ARG	2.7
1	A	96	ARG	2.6
1	A	143	PRO	2.6
1	A	200	ARG	2.6
1	B	79	LEU	2.6
1	A	213	LYS	2.6
1	B	39	ARG	2.6
1	B	143	PRO	2.6
1	A	257	LEU	2.6
1	B	184	ALA	2.5
1	A	179	LEU	2.5
1	B	132	LEU	2.5
1	B	30	GLU	2.5
1	B	49	VAL	2.5
1	B	62	ASP	2.5
1	B	183	LEU	2.5
1	B	33	LEU	2.4
1	B	215	LEU	2.4
1	A	244	VAL	2.4
1	A	189	LEU	2.4
1	B	207	LEU	2.4
1	B	59	ARG	2.4
1	B	214	GLU	2.3
1	A	180	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	181	ALA	2.3
1	B	128	TRP	2.3
1	A	206	ARG	2.2
1	B	31	VAL	2.2
1	A	215	LEU	2.2
1	A	185	GLN	2.2
1	B	224	LEU	2.2
1	A	197	TYR	2.2
1	B	88	TYR	2.2
1	B	171	TYR	2.2
1	B	78	THR	2.2
1	A	234	GLN	2.2
1	B	177	MET	2.2
1	B	41	GLU	2.1
1	A	214	GLU	2.1
1	A	254	ILE	2.1
1	B	141	ARG	2.1
1	A	341	ALA	2.1
1	B	4	LEU	2.1
1	B	85	THR	2.0
1	B	222	SER	2.0
1	B	232	ARG	2.0
1	A	227	HIS	2.0
1	B	81	ARG	2.0
1	B	95	ARG	2.0
1	B	136	ARG	2.0
1	B	92	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

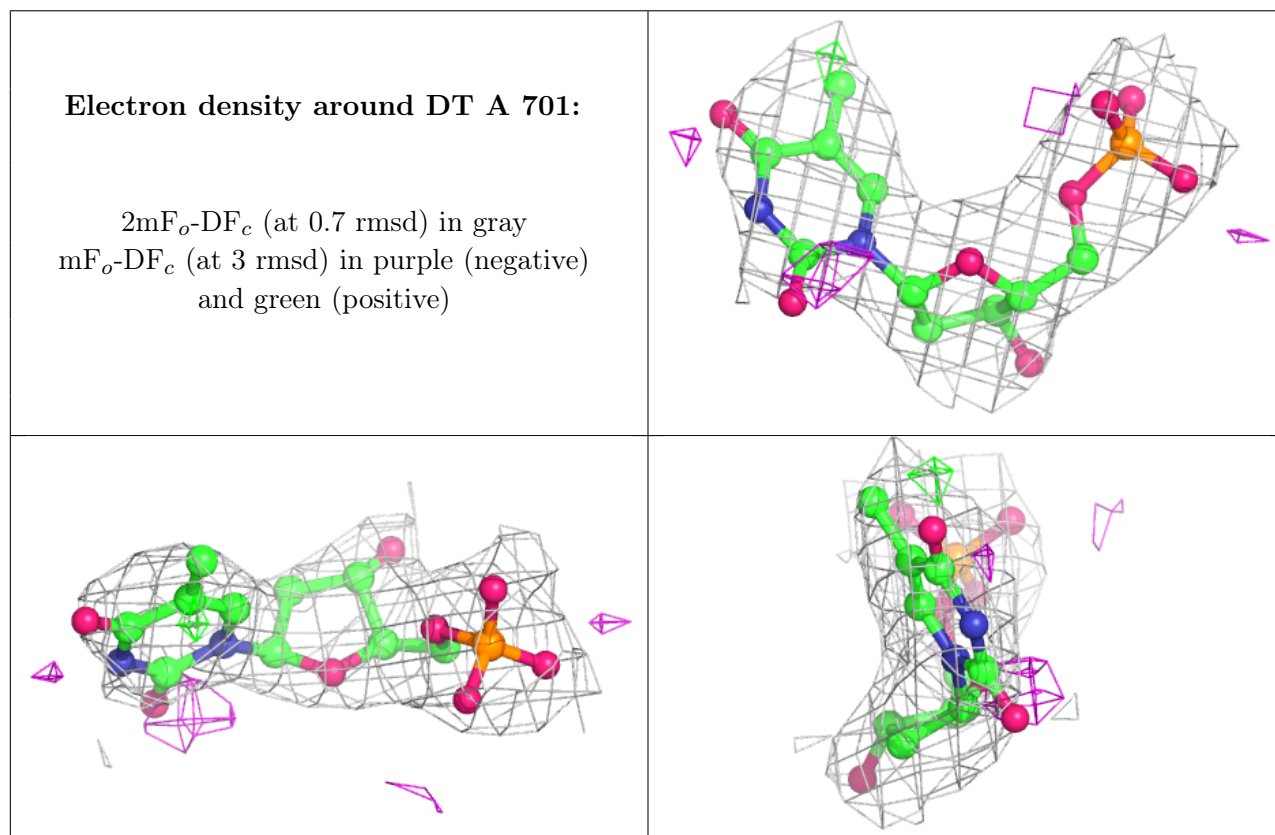
6.4 Ligands [i](#)

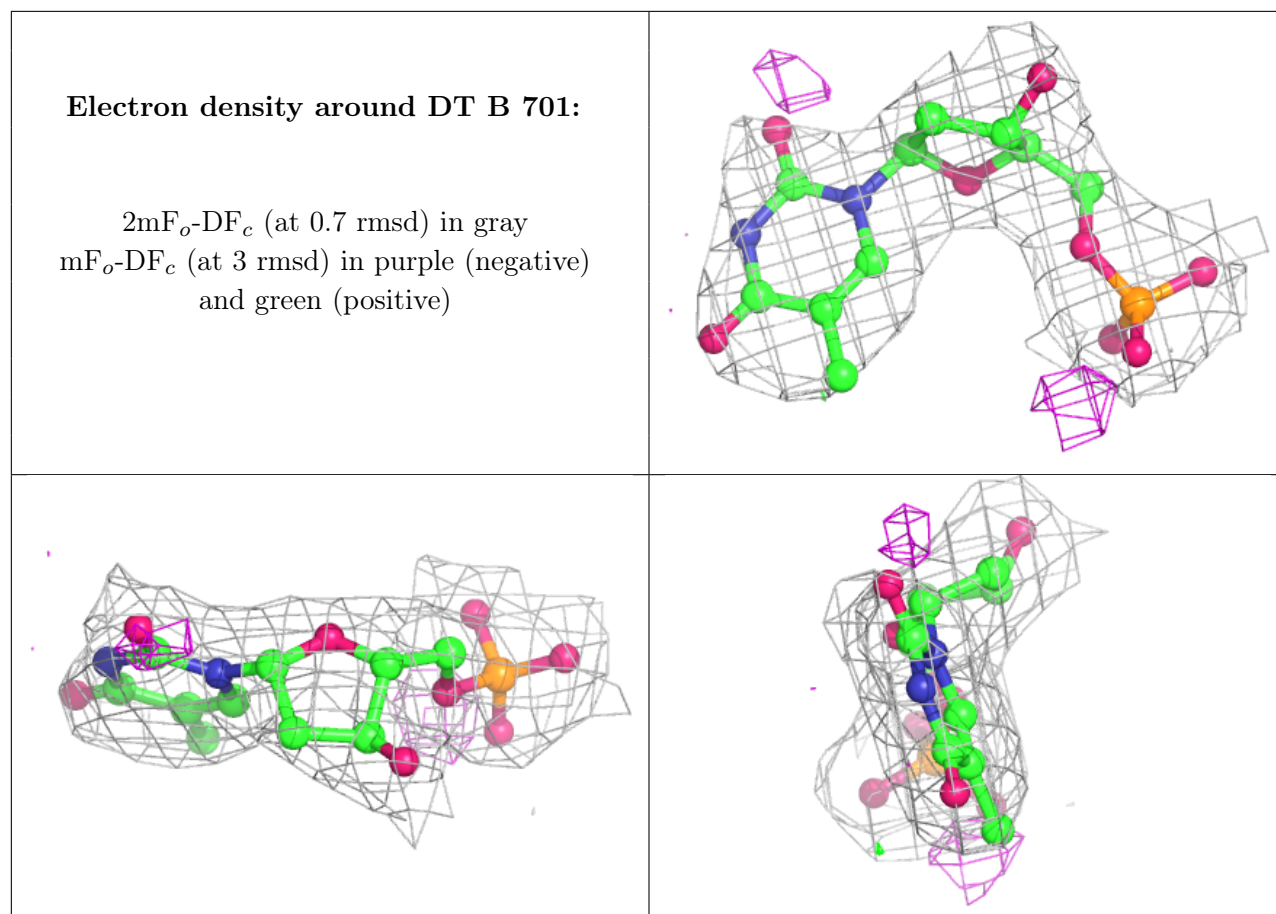
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MG	D	101	1/1	0.87	0.11	67,67,67,67	0
5	DT	A	701	21/21	0.90	0.28	74,84,92,94	0
6	MG	C	101	1/1	0.95	0.08	50,50,50,50	0
5	DT	B	701	21/21	0.96	0.21	56,67,73,79	0
6	MG	A	702	1/1	0.97	0.14	43,43,43,43	0
6	MG	B	702	1/1	0.97	0.12	44,44,44,44	0
6	MG	B	703	1/1	0.98	0.13	51,51,51,51	0
6	MG	E	101	1/1	0.98	0.10	48,48,48,48	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.