



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 09:51 PM UTC

PDB ID : 4KPY / pdb_00004kpy
Title : DNA binding protein and DNA complex structure
Authors : Sheng, G.; Zhao, H.; Wang, J.; Rao, Y.; Wang, Y.
Deposited on : 2013-05-14
Resolution : 2.41 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

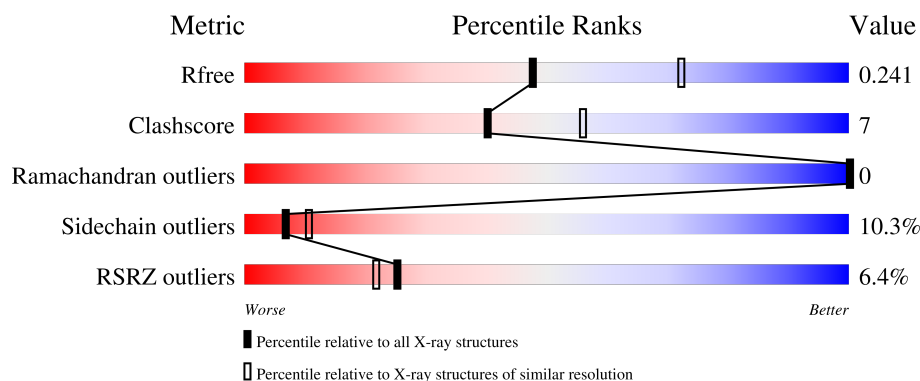
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 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.



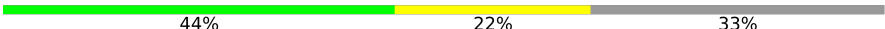
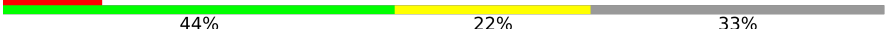
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	6% 78% 18% ..
1	B	685	8% 75% 21% ..
2	C	21	52% 24% 24%
2	E	21	52% 24% 24%
3	D	10	90% 10%

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Mol	Chain	Length	Quality of chain
3	F	10	 90% 10%
4	M	9	 44% 22% 33%
4	N	9	 11% 44% 22% 33%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12268 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	676	Total	C	N	O	S	0	0	0
			5278	3372	992	907	7			
1	B	675	Total	C	N	O	S	0	1	0
			5272	3371	991	904	6			

- Molecule 2 is a DNA chain called DNA (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
2	C	16	Total	C	N	O	P	0	0	0
			338	160	62	100	16			
2	E	16	Total	C	N	O	P	0	0	0
			338	160	62	100	16			

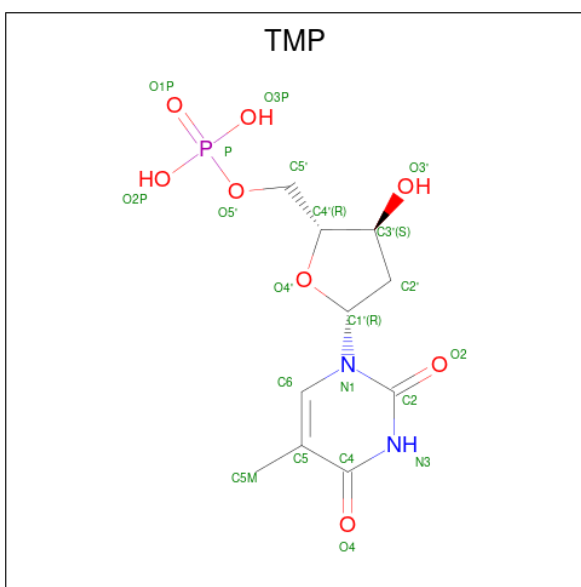
- Molecule 3 is a DNA chain called DNA (5'-D(P*TP*AP*CP*TP*AP*CP*CP*TP*CP*G)-3').

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	6	Total	C	N	O	P	0	0	0
			120	57	24	33	6			
4	N	6	Total	C	N	O	P	0	0	0
			116	57	24	30	5			

- Molecule 5 is THYMIDINE-5'-PHOSPHATE (CCD ID: TMP) (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 MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	138	Total	O	0	0
			138	138		
7	B	161	Total	O	0	0
			161	161		
7	C	17	Total	O	0	0
			17	17		

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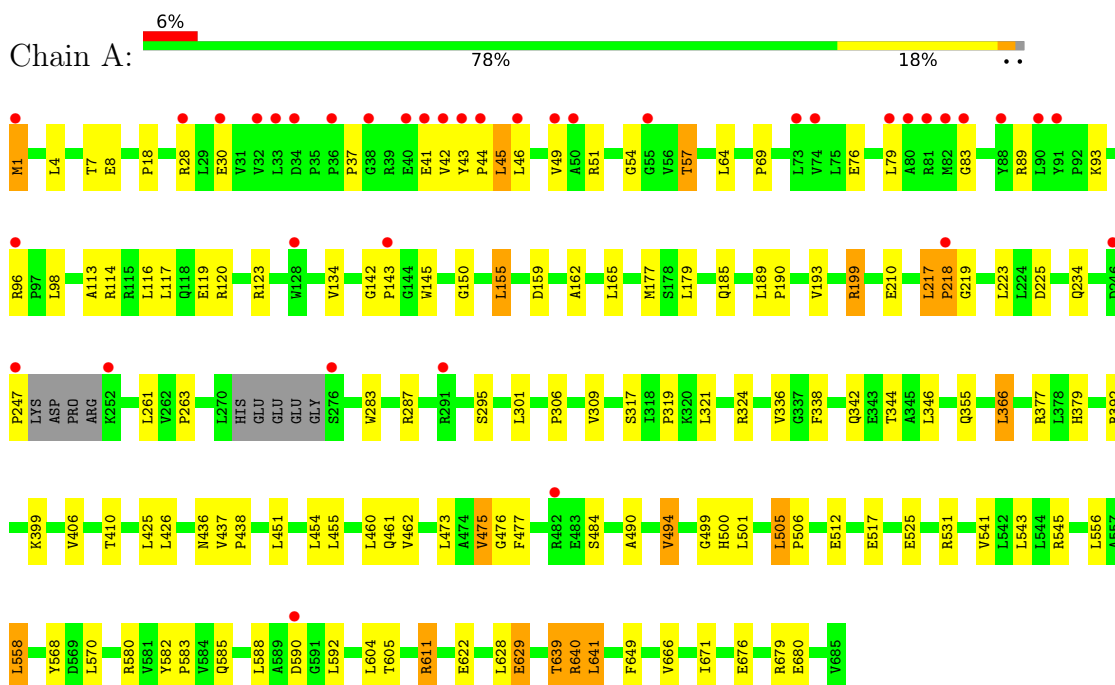
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	9	Total 9	O 9	0	0
7	E	20	Total 20	O 20	0	0
7	F	8	Total 8	O 8	0	0
7	M	3	Total 3	O 3	0	0

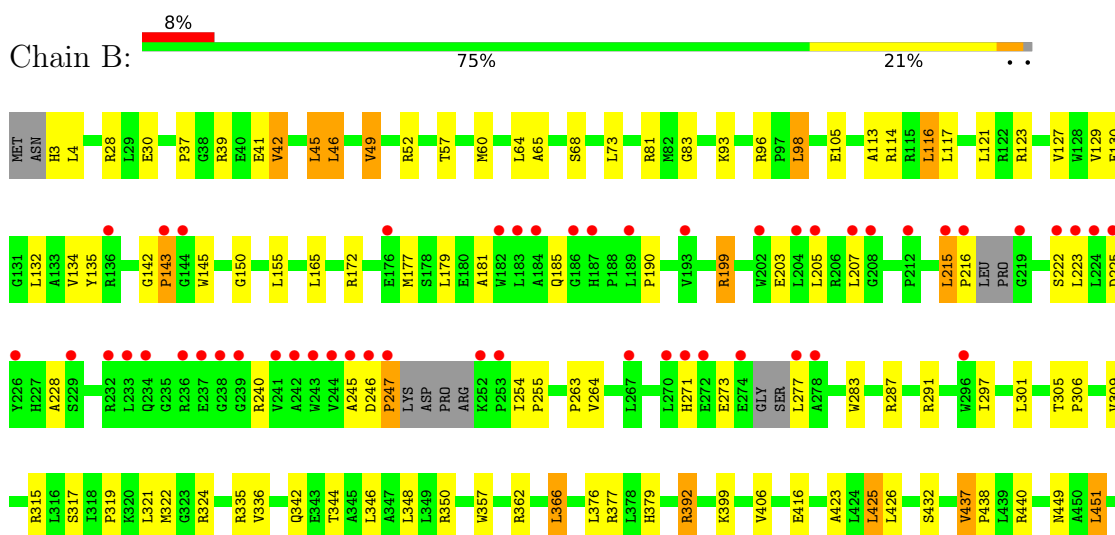
3 Residue-property plots

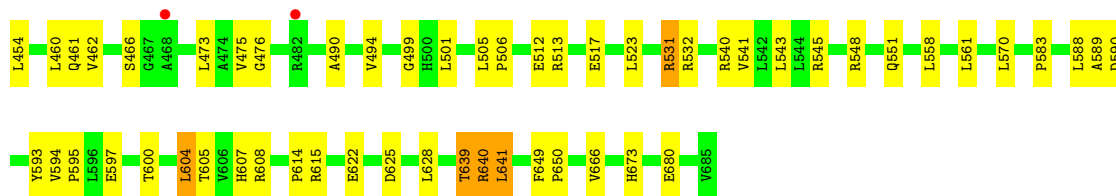
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: Uncharacterized protein

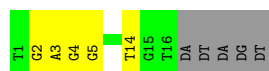




- Molecule 2: DNA (5'-D(P*TP*GP*AP*GP*GP*TP*AP*GP*TP*AP*GP*GP*TP*TP*GP*T
P*AP*TP*AP*GP*T)-3')



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



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



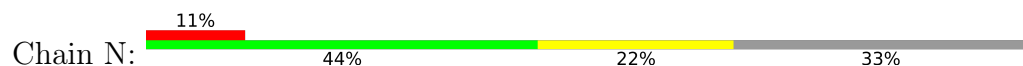
- Molecule 3: DNA (5'-D(P*TP*AP*CP*TP*AP*CP*CP*TP*CP*G)-3')

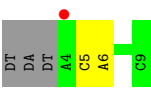


- Molecule 4: DNA (5'-D(*TP*AP*TP*AP*CP*AP*AP*CP*C)-3')



- Molecule 4: DNA (5'-D(*TP*AP*TP*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	111.33Å 118.36Å 160.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.31 – 2.41 48.31 – 2.41	Depositor EDS
% Data completeness (in resolution range)	97.1 (48.31-2.41) 97.0 (48.31-2.41)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.13 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.190 , 0.235 0.198 , 0.241	Depositor DCC
R_{free} test set	4036 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	44.7	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.2	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	12268	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TMP, MN

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	0.41	0/5402	0.81	8/7333 (0.1%)
1	B	0.43	0/5399	0.80	4/7329 (0.1%)
2	C	0.24	0/379	0.81	0/584
2	E	0.22	0/379	0.83	0/584
3	D	0.22	0/223	0.81	0/339
3	F	0.22	0/223	0.83	0/339
4	M	0.28	0/134	0.90	1/203 (0.5%)
4	N	0.18	0/130	0.65	0/198
All	All	0.40	0/12269	0.81	13/16909 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	5	DC	C4'-C3'-O3'	7.15	120.72	110.00
1	B	247	PRO	N-CA-CB	6.92	110.62	103.00
1	B	143	PRO	N-CA-CB	6.69	110.27	103.25
1	A	247	PRO	N-CA-CB	6.67	110.34	103.00
1	A	143	PRO	N-CA-CB	6.62	110.20	103.25
1	A	218	PRO	CB-CA-C	6.19	119.50	111.64
1	A	218	PRO	N-CA-C	-5.99	101.50	111.26
1	A	219	GLY	N-CA-C	5.65	122.27	114.92
1	A	611	ARG	N-CA-C	5.26	119.41	113.15
1	A	69	PRO	CA-C-N	5.11	124.77	119.56
1	A	69	PRO	C-N-CA	5.11	124.77	119.56
1	B	143	PRO	N-CA-C	-5.10	101.96	112.47
1	B	594	VAL	N-CA-C	5.03	113.13	108.15

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	5278	0	5338	66	0
1	B	5272	0	5330	85	0
2	C	338	0	183	5	0
2	E	338	0	183	4	0
3	D	201	0	114	1	0
3	F	201	0	114	1	0
4	M	120	0	66	2	0
4	N	116	0	64	2	0
5	A	21	0	13	1	0
5	B	21	0	13	0	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
6	C	1	0	0	0	0
6	E	1	0	0	0	0
7	A	138	0	0	2	0
7	B	161	0	0	6	0
7	C	17	0	0	0	0
7	D	9	0	0	0	0
7	E	20	0	0	1	0
7	F	8	0	0	0	0
7	M	3	0	0	0	0
All	All	12268	0	11418	154	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 (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:A:319:PRO:HG2	1:A:640:ARG:HD2	1.63	0.81
1:B:344:THR:HG21	1:B:460:LEU:HD11	1.66	0.76
1:B:513:ARG:NH2	1:B:551:GLN:O	2.17	0.75
1:B:597:GLU:O	7:B:900:HOH:O	2.05	0.73
1:B:322:MET:HE2	1:B:466:SER:HB2	1.72	0.72
1:A:512:GLU:OE2	1:A:545:ARG:NH2	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:14:DT:H3	4:M:6:DA:H2	1.37	0.71
1:A:679:ARG:NH1	7:A:852:HOH:O	2.23	0.71
1:A:28:ARG:NH1	1:A:93:LYS:O	2.25	0.69
1:A:49:VAL:HG22	1:A:79:LEU:HD11	1.76	0.67
1:A:344:THR:HG21	1:A:460:LEU:HD11	1.76	0.67
1:A:28:ARG:NH2	1:A:96:ARG:HB2	2.10	0.67
1:B:319:PRO:HG3	1:B:640:ARG:HD2	1.77	0.67
1:B:512:GLU:OE2	1:B:545:ARG:NH2	2.27	0.66
1:A:583:PRO:HD3	1:A:588:LEU:HD13	1.78	0.66
2:C:3:DA:H2'	2:C:4:DG:C8	2.32	0.65
1:A:30:GLU:OE2	1:A:93:LYS:NZ	2.30	0.64
1:B:190:PRO:HG3	1:B:263:PRO:HB3	1.79	0.64
5:A:701:TMP:O2	1:B:39:ARG:NH1	2.30	0.63
1:B:121:LEU:HD22	1:B:134:VAL:HG21	1.82	0.62
2:E:3:DA:H2'	2:E:4:DG:C8	2.37	0.60
1:A:4:LEU:HD22	1:A:317:SER:HA	1.82	0.60
1:A:37:PRO:HB3	1:A:45:LEU:HD23	1.85	0.59
1:B:377:ARG:HD2	1:B:379:HIS:NE2	2.19	0.58
1:B:593:TYR:CZ	1:B:595:PRO:HG3	2.38	0.58
1:A:525:GLU:OE1	1:B:392:ARG:NH1	2.37	0.57
1:A:41:GLU:O	1:A:45:LEU:HB2	2.04	0.57
1:A:114:ARG:HH12	4:N:6:DA:H3'	1.70	0.56
1:B:461:GLN:HG3	1:B:499:GLY:O	2.04	0.56
1:A:190:PRO:HG3	1:A:263:PRO:HB3	1.88	0.56
1:B:590:ASP:OD2	3:F:19:DG:N1	2.28	0.56
1:B:37:PRO:HB3	1:B:45:LEU:HD23	1.88	0.55
1:B:423:ALA:HB1	1:B:673:HIS:CE1	2.41	0.55
1:B:607:HIS:O	1:B:608:ARG:HD2	2.07	0.55
1:B:130:GLU:OE1	1:B:172:ARG:NH1	2.40	0.55
1:B:41:GLU:O	1:B:45:LEU:HB2	2.07	0.54
1:B:362:ARG:NH2	7:B:904:HOH:O	2.40	0.54
1:A:120:ARG:NH1	1:A:301:LEU:O	2.41	0.54
1:B:135:TYR:HA	1:B:150:GLY:HA3	1.90	0.53
1:A:639:THR:HG21	1:A:640:ARG:HH21	1.72	0.53
1:B:283:TRP:HZ3	1:B:287:ARG:HH21	1.56	0.53
1:B:319:PRO:CG	1:B:640:ARG:HD2	2.38	0.53
1:A:45:LEU:O	1:A:49:VAL:HG23	2.07	0.53
1:B:98:LEU:HG	1:B:105:GLU:HB3	1.90	0.53
1:B:425:LEU:HD12	1:B:432:SER:HB3	1.91	0.53
1:B:350:ARG:NH1	7:B:825:HOH:O	2.42	0.52
1:B:639:THR:HG22	1:B:640:ARG:HE	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:615:ARG:HD3	7:E:207:HOH:O	2.10	0.51
1:B:583:PRO:HD3	1:B:588:LEU:HD13	1.92	0.51
1:B:639:THR:HG21	1:B:640:ARG:HH21	1.76	0.51
1:B:506:PRO:HG2	1:B:666:VAL:HG21	1.92	0.51
1:A:461:GLN:HG3	1:A:499:GLY:O	2.10	0.51
1:A:611:ARG:HD3	2:C:5:DG:H1'	1.93	0.50
1:B:114:ARG:NH1	4:M:6:DA:OP2	2.43	0.50
1:B:437:VAL:HG22	1:B:438:PRO:HA	1.94	0.50
1:A:119:GLU:O	1:A:123:ARG:HG3	2.12	0.50
1:A:177:MET:HE1	1:A:185:GLN:HG3	1.95	0.49
1:A:134:VAL:O	1:A:150:GLY:HA3	2.12	0.49
1:B:246:ASP:OD1	1:B:247:PRO:N	2.45	0.49
1:A:142:GLY:HA3	1:A:145:TRP:CE2	2.48	0.49
1:A:113:ALA:HB1	1:A:155:LEU:HD13	1.96	0.48
1:B:30:GLU:OE1	1:B:93:LYS:NZ	2.47	0.48
1:A:475:VAL:HG22	1:A:477:PHE:CE1	2.49	0.47
1:B:199:ARG:N	1:B:199:ARG:HD2	2.27	0.47
1:A:640:ARG:HG3	1:A:649:PHE:CE1	2.50	0.47
1:B:203:GLU:HB3	1:B:245:ALA:HB3	1.96	0.47
1:B:532:ARG:NH1	7:B:934:HOH:O	2.47	0.47
1:B:177:MET:HE1	1:B:185:GLN:HG3	1.96	0.47
1:B:532:ARG:NH2	7:B:905:HOH:O	2.46	0.47
1:A:295:SER:HA	1:A:306:PRO:HG3	1.96	0.47
1:B:605:THR:O	1:B:640:ARG:NH2	2.46	0.47
1:A:640:ARG:HG3	1:A:649:PHE:CD1	2.50	0.46
1:A:83:GLY:HA3	1:B:83:GLY:HA3	1.97	0.46
1:A:199:ARG:NH1	7:A:855:HOH:O	2.49	0.46
1:A:611:ARG:HD3	2:C:5:DG:C1'	2.45	0.46
1:A:193:VAL:HG21	1:A:261:LEU:HB3	1.97	0.46
1:A:338:PHE:CZ	1:A:455:LEU:HD13	2.51	0.46
1:A:287:ARG:HG3	1:A:582:TYR:CG	2.51	0.46
1:A:377:ARG:HD2	1:A:379:HIS:NE2	2.31	0.46
1:B:4:LEU:HD13	1:B:317:SER:HA	1.98	0.46
1:A:225:ASP:OD1	1:A:225:ASP:N	2.49	0.45
1:B:540:ARG:NH2	1:B:625:ASP:OD1	2.48	0.45
1:A:217:LEU:O	1:A:218:PRO:C	2.59	0.45
1:A:410:THR:O	1:A:436:ASN:HA	2.16	0.45
1:B:461:GLN:HE21	1:B:499:GLY:HA2	1.82	0.45
1:B:523:LEU:HD21	1:B:561:LEU:HD11	1.99	0.45
1:A:159:ASP:OD1	1:A:159:ASP:N	2.49	0.45
1:B:207:LEU:HD13	1:B:240:ARG:HE	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:639:THR:CG2	1:A:640:ARG:HH21	2.30	0.44
1:B:68:SER:HB2	1:B:73:LEU:HD21	1.99	0.44
1:A:18:PRO:HA	1:A:162:ALA:HA	1.99	0.44
1:B:39:ARG:O	1:B:42:VAL:HG12	2.18	0.44
1:B:315:ARG:HH12	1:B:589:ALA:HB3	1.83	0.44
1:B:476:GLY:O	1:B:490:ALA:HA	2.17	0.44
1:A:76:GLU:HG2	1:A:89:ARG:HG3	1.99	0.44
1:A:605:THR:O	1:A:640:ARG:NH2	2.50	0.44
1:B:473:LEU:HB3	1:B:541:VAL:HG12	2.00	0.44
1:B:113:ALA:O	1:B:116:LEU:HB3	2.17	0.44
1:B:215:LEU:HD13	1:B:216:PRO:HD2	1.98	0.44
1:B:215:LEU:O	1:B:222:SER:HA	2.18	0.44
1:B:225:ASP:HA	1:B:228:ALA:HB3	2.00	0.44
1:A:45:LEU:HA	1:A:45:LEU:HD12	1.69	0.43
1:A:366:LEU:HD12	1:A:366:LEU:HA	1.87	0.43
1:A:501:LEU:HD21	1:A:641:LEU:HD13	1.99	0.43
1:A:505:LEU:HD22	1:A:671:ILE:HD11	2.00	0.43
1:B:60:MET:HE2	1:B:65:ALA:HB2	1.99	0.43
1:B:342:GLN:O	1:B:344:THR:HG23	2.18	0.43
1:B:366:LEU:HD13	1:B:376:LEU:HD23	2.00	0.43
1:B:449:ASN:ND2	2:E:2:DG:H21	2.17	0.43
1:B:640:ARG:HG3	1:B:649:PHE:CE1	2.54	0.43
1:B:639:THR:CG2	1:B:640:ARG:HH21	2.31	0.43
1:B:177:MET:HB3	1:B:181:ALA:HB3	2.00	0.43
1:B:287:ARG:HH11	1:B:291:ARG:HH22	1.66	0.43
1:B:531:ARG:C	1:B:531:ARG:HE	2.27	0.43
1:B:501:LEU:HD21	1:B:641:LEU:HD13	2.01	0.43
2:C:4:DG:H2'	2:C:5:DG:C8	2.54	0.43
1:B:305:THR:HA	1:B:306:PRO:HD3	1.87	0.42
1:B:28:ARG:NH2	1:B:96:ARG:HB2	2.34	0.42
1:B:46:LEU:O	1:B:49:VAL:HG12	2.19	0.42
2:C:12:DG:H2'	2:C:13:DT:H72	2.00	0.42
1:A:28:ARG:HH21	1:A:96:ARG:HB2	1.81	0.42
1:B:143:PRO:O	1:B:145:TRP:CD1	2.72	0.42
1:A:1:MET:HG2	1:A:629:GLU:HG2	2.02	0.42
1:A:558:LEU:HG	1:A:568:TYR:CE1	2.55	0.42
1:B:416:GLU:H	1:B:416:GLU:CD	2.27	0.42
1:B:127:VAL:HG23	1:B:129:VAL:HG23	2.02	0.42
1:A:506:PRO:HG2	1:A:666:VAL:HG21	2.02	0.41
1:A:437:VAL:HA	1:A:438:PRO:C	2.46	0.41
1:A:476:GLY:O	1:A:490:ALA:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:GLY:HA3	1:B:145:TRP:CE2	2.55	0.41
1:A:117:LEU:HD22	1:A:155:LEU:HB2	2.02	0.41
1:A:342:GLN:H	1:A:342:GLN:HG2	1.65	0.41
1:A:473:LEU:HB3	1:A:541:VAL:HG12	2.01	0.41
1:B:451:LEU:HD12	1:B:451:LEU:HA	1.87	0.41
1:A:83:GLY:CA	1:B:83:GLY:HA3	2.51	0.41
1:B:205:LEU:HD11	1:B:245:ALA:HB2	2.02	0.41
1:A:7:THR:OG1	1:A:8:GLU:N	2.54	0.41
1:A:590:ASP:OD2	3:D:19:DG:N1	2.33	0.41
1:A:189:LEU:HA	1:A:190:PRO:HD2	1.93	0.41
1:B:348:LEU:HB2	1:B:357:TRP:CE2	2.56	0.41
1:B:649:PHE:HA	1:B:650:PRO:HD3	1.91	0.41
1:A:43:TYR:N	1:A:44:PRO:HD2	2.36	0.41
1:B:45:LEU:HD13	1:B:81:ARG:HD3	2.03	0.41
1:B:640:ARG:HG3	1:B:649:PHE:CD1	2.56	0.40
1:A:54:GLY:O	1:A:57:THR:HG23	2.22	0.40
1:B:297:ILE:HG23	1:B:301:LEU:HD22	2.02	0.40
1:A:51:ARG:NE	4:N:5:DC:OP1	2.50	0.40
1:B:254:ILE:HA	1:B:255:PRO:HD3	1.94	0.40
1:B:604:LEU:HD21	1:B:614:PRO:HB2	2.04	0.40
1:A:283:TRP:HZ3	1:A:287:ARG:HH21	1.69	0.40
1:B:117:LEU:HD23	1:B:132:LEU:HD22	2.01	0.40
1:B:123:ARG:NH2	7:B:949:HOH:O	2.53	0.40
1:A:494:VAL:HG22	1:A:500:HIS:HB2	2.04	0.40
2:E:4:DG:H2'	2:E:5:DG:C8	2.57	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	670/685 (98%)	657 (98%)	13 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	668/685 (98%)	656 (98%)	12 (2%)	0	100	100
All	All	1338/1370 (98%)	1313 (98%)	25 (2%)	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	521/549 (95%)	468 (90%)	53 (10%)	7	11
1	B	520/549 (95%)	466 (90%)	54 (10%)	7	10
All	All	1041/1098 (95%)	934 (90%)	107 (10%)	7	11

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	42	VAL
1	A	45	LEU
1	A	46	LEU
1	A	57	THR
1	A	64	LEU
1	A	98	LEU
1	A	116	LEU
1	A	155	LEU
1	A	165	LEU
1	A	179	LEU
1	A	199	ARG
1	A	210	GLU
1	A	217	LEU
1	A	223	LEU
1	A	234	GLN
1	A	309	VAL
1	A	321	LEU

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Mol	Chain	Res	Type
1	A	324	ARG
1	A	336	VAL
1	A	346	LEU
1	A	355	GLN
1	A	366	LEU
1	A	392	ARG
1	A	399	LYS
1	A	406	VAL
1	A	425	LEU
1	A	426	LEU
1	A	451	LEU
1	A	454	LEU
1	A	462	VAL
1	A	475	VAL
1	A	484	SER
1	A	494	VAL
1	A	505	LEU
1	A	517	GLU
1	A	531	ARG
1	A	543	LEU
1	A	556	LEU
1	A	558	LEU
1	A	570	LEU
1	A	580	ARG
1	A	585	GLN
1	A	592	LEU
1	A	604	LEU
1	A	622	GLU
1	A	628	LEU
1	A	629	GLU
1	A	639	THR
1	A	640	ARG
1	A	641	LEU
1	A	676	GLU
1	A	680	GLU
1	B	3	HIS
1	B	42	VAL
1	B	45	LEU
1	B	46	LEU
1	B	49	VAL
1	B	52	ARG
1	B	57	THR

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Mol	Chain	Res	Type
1	B	64	LEU
1	B	98	LEU
1	B	116	LEU
1	B	155	LEU
1	B	165	LEU
1	B	179	LEU
1	B	199	ARG
1	B	215	LEU
1	B	223	LEU
1	B	264	VAL
1	B	271	HIS
1	B	273	GLU
1	B	277	LEU
1	B	309	VAL
1	B	321	LEU
1	B	324	ARG
1	B	335	ARG
1	B	336	VAL
1	B	346	LEU
1	B	366	LEU
1	B	392	ARG
1	B	399	LYS
1	B	406	VAL
1	B	425	LEU
1	B	426	LEU
1	B	437	VAL
1	B	440	ARG
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	517	GLU
1	B	531	ARG
1	B	543	LEU
1	B	548	ARG
1	B	558	LEU
1	B	570	LEU
1	B	600	THR
1	B	604	LEU
1	B	622	GLU

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Mol	Chain	Res	Type
1	B	628	LEU
1	B	639	THR
1	B	640	ARG
1	B	641	LEU
1	B	680	GLU

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

Mol	Chain	Res	Type
1	B	187	HIS
1	B	500	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 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	TMP	A	701	-	22,22,22	0.68	0	32,33,33	0.94	1 (3%)
5	TMP	B	701	-	22,22,22	0.62	0	32,33,33	0.83	1 (3%)

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	TMP	A	701	-	-	0/10/22/22	0/2/2/2
5	TMP	B	701	-	-	3/10/22/22	0/2/2/2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	701	TMP	O4-C4-C5	-3.18	121.27	124.92
5	B	701	TMP	O4-C4-C5	-2.67	121.86	124.92

There are no chirality outliers.

All (3) torsion outliers are listed below:

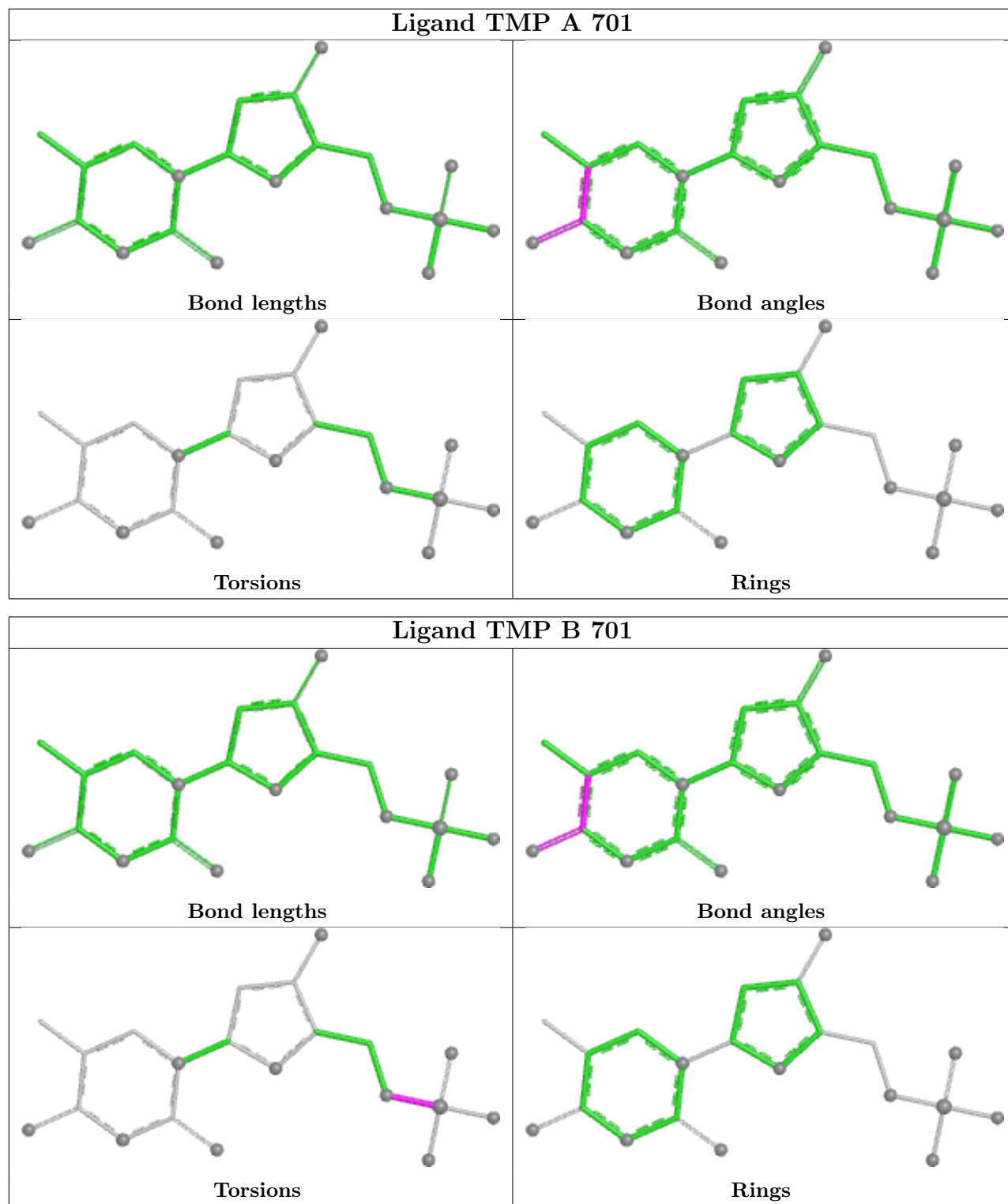
Mol	Chain	Res	Type	Atoms
5	B	701	TMP	C5'-O5'-P-O1P
5	B	701	TMP	C5'-O5'-P-O2P
5	B	701	TMP	C5'-O5'-P-O3P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	701	TMP	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.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	676/685 (98%)	0.13	38 (5%) 30 26	19, 45, 95, 141	0
1	B	675/685 (98%)	0.07	52 (7%) 19 16	16, 40, 111, 140	1 (0%)
2	C	16/21 (76%)	-0.60	0 100 100	27, 41, 70, 92	0
2	E	16/21 (76%)	-0.64	0 100 100	32, 38, 60, 62	0
3	D	10/10 (100%)	-0.59	0 100 100	36, 46, 52, 59	0
3	F	10/10 (100%)	-0.32	0 100 100	37, 56, 59, 62	0
4	M	6/9 (66%)	-0.07	0 100 100	39, 53, 76, 79	0
4	N	6/9 (66%)	0.62	1 (16%) 4 3	36, 60, 89, 94	0
All	All	1415/1450 (97%)	0.08	91 (6%) 25 22	16, 42, 101, 141	1 (0%)

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	247	PRO	4.7
1	A	42	VAL	4.6
1	A	43	TYR	4.3
1	A	247	PRO	4.2
1	B	189	LEU	4.2
1	B	272	GLU	4.1
1	B	143	PRO	4.0
1	A	276	SER	4.0
1	A	82	MET	4.0
1	B	237	GLU	3.9
1	A	28	ARG	3.8
1	A	252	LYS	3.8
1	A	79	LEU	3.8
1	A	88	TYR	3.6
1	B	219	GLY	3.5
1	B	216	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	271	HIS	3.3
1	A	36	PRO	3.3
1	B	223	LEU	3.3
1	A	80	ALA	3.2
1	A	96	ARG	3.1
1	B	207	LEU	3.1
1	B	204	LEU	3.0
1	B	186	GLY	3.0
1	A	128	TRP	2.9
1	B	252	LYS	2.9
1	A	218	PRO	2.9
1	B	253	PRO	2.9
1	A	81	ARG	2.9
1	A	91	TYR	2.9
1	B	183	LEU	2.8
1	B	205	LEU	2.8
1	B	246	ASP	2.8
4	N	4	DA	2.7
1	A	482	ARG	2.7
1	B	274	GLU	2.6
1	B	236	ARG	2.6
1	B	233	LEU	2.6
1	A	32	VAL	2.6
1	B	222	SER	2.6
1	B	277	LEU	2.5
1	A	1	MET	2.5
1	A	83	GLY	2.5
1	B	202	TRP	2.5
1	B	224	LEU	2.5
1	A	41	GLU	2.5
1	B	238	GLY	2.5
1	A	50	ALA	2.5
1	B	239	GLY	2.4
1	B	193	VAL	2.4
1	A	49	VAL	2.4
1	B	241	VAL	2.4
1	B	229	SER	2.4
1	A	44	PRO	2.4
1	B	182	TRP	2.4
1	A	40	GLU	2.3
1	B	234	GLN	2.3
1	A	30	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	291	ARG	2.3
1	B	136	ARG	2.3
1	B	144	GLY	2.3
1	B	212	PRO	2.3
1	B	208	GLY	2.3
1	A	46	LEU	2.3
1	B	267	LEU	2.3
1	B	278	ALA	2.2
1	B	184	ALA	2.2
1	B	187	HIS	2.2
1	A	33	LEU	2.2
1	A	246	ASP	2.2
1	B	225	ASP	2.2
1	B	482	ARG	2.2
1	B	468	ALA	2.2
1	A	55	GLY	2.2
1	B	226	TYR	2.2
1	B	232	ARG	2.2
1	B	243	TRP	2.2
1	A	74	VAL	2.1
1	B	270	LEU	2.1
1	B	176	GLU	2.1
1	B	242	ALA	2.1
1	A	590	ASP	2.1
1	A	143	PRO	2.1
1	B	244	VAL	2.1
1	B	296	TRP	2.1
1	A	34	ASP	2.1
1	B	245	ALA	2.1
1	A	90	LEU	2.1
1	B	215	LEU	2.1
1	A	73	LEU	2.0
1	A	38	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

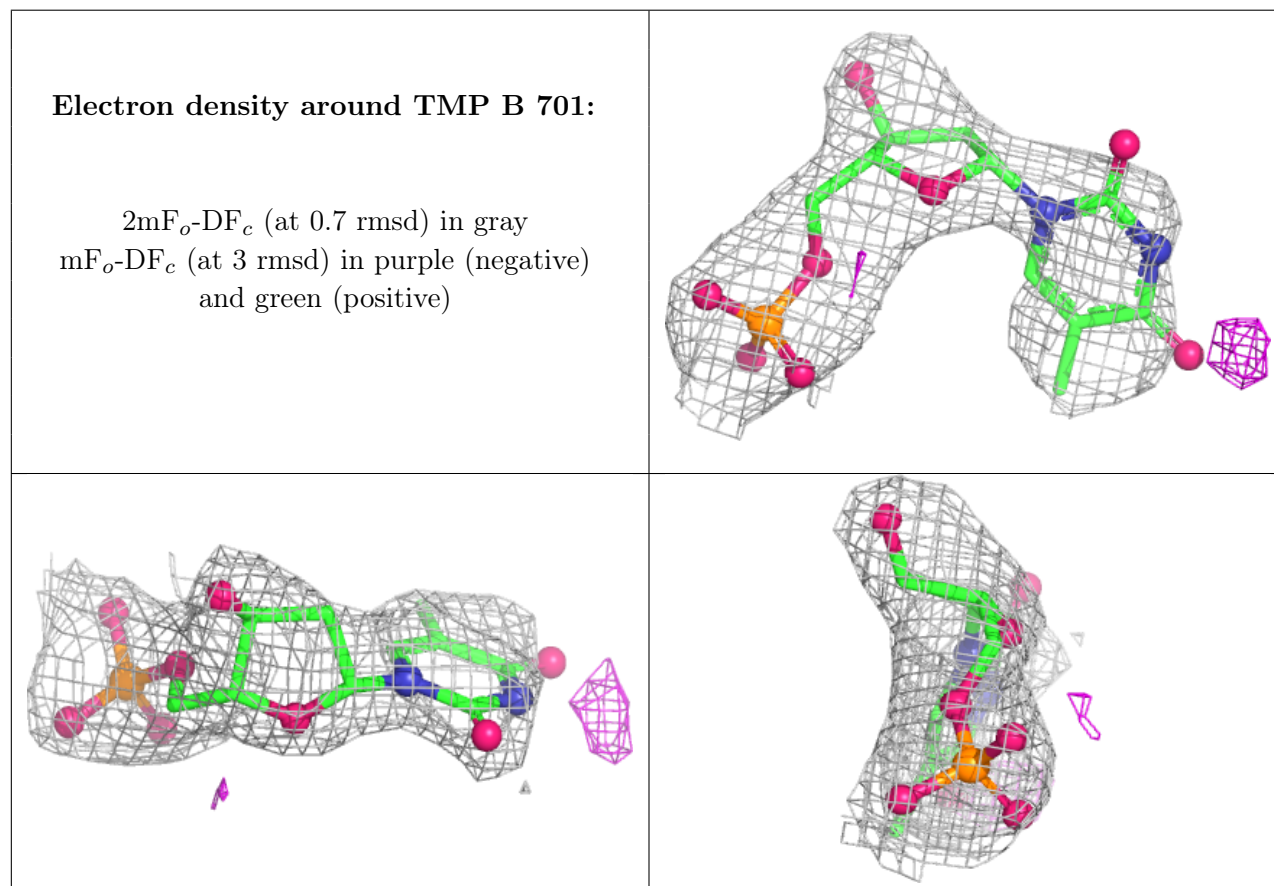
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

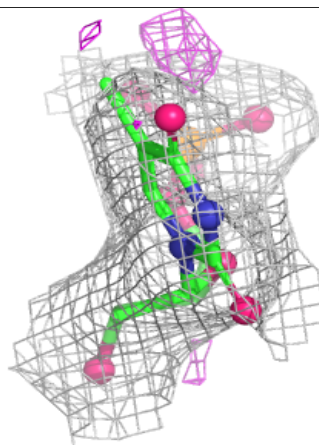
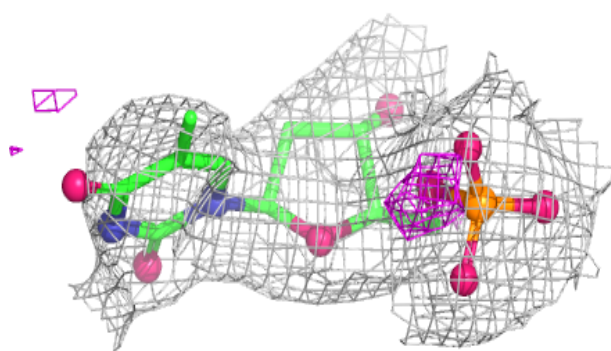
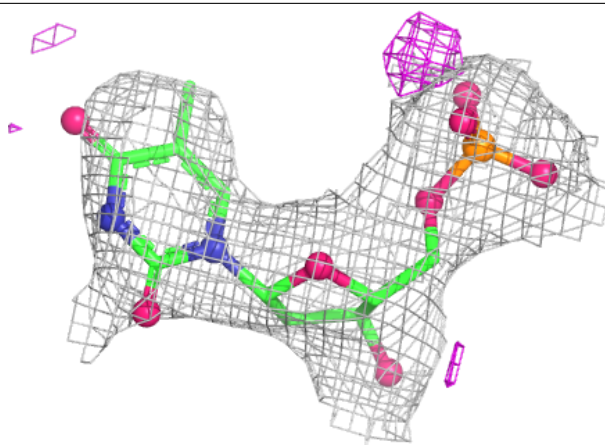
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	TMP	B	701	21/21	0.87	0.13	82,102,118,122	0
5	TMP	A	701	21/21	0.96	0.10	43,53,84,93	0
6	MN	A	703	1/1	0.99	0.03	32,32,32,32	0
6	MN	A	702	1/1	1.00	0.02	32,32,32,32	0
6	MN	B	702	1/1	1.00	0.02	32,32,32,32	0
6	MN	B	703	1/1	1.00	0.03	34,34,34,34	0
6	MN	C	101	1/1	1.00	0.02	28,28,28,28	0
6	MN	E	101	1/1	1.00	0.01	33,33,33,33	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 TMP 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.