



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 11, 2023 – 07:04 AM EDT

PDB ID : 4LT6
Title : Crystal Structure of human poly(A) polymerase gamma
Authors : Yang, Q.; Nausch, L.; Martin, G.; Keller, W.; Doubleie, S.
Deposited on : 2013-07-23
Resolution : 2.79 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 : 2.35.1
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) : 2.35.1

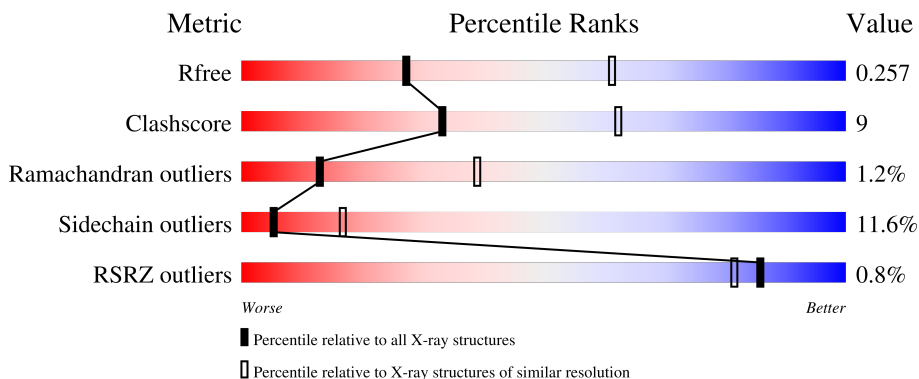
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	514	
1	B	514	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7644 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.

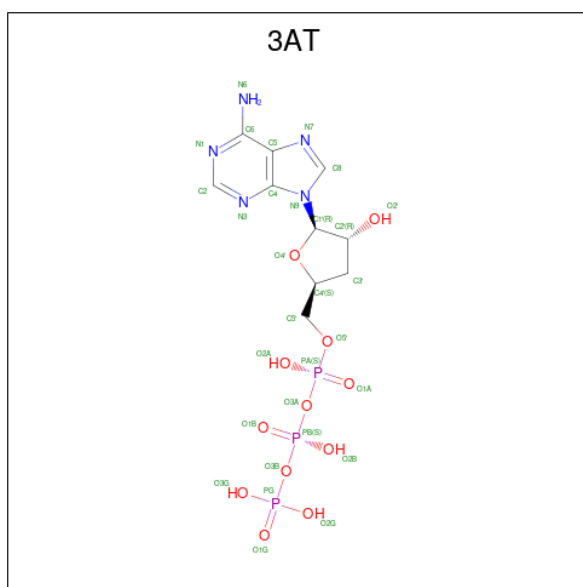
- Molecule 1 is a protein called Poly(A) polymerase gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	467	3784	2436	652	684	12	0	0	0
1	B	462	3745	2410	646	677	12	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP Q9BWT3
A	-4	HIS	-	expression tag	UNP Q9BWT3
A	-3	HIS	-	expression tag	UNP Q9BWT3
A	-2	HIS	-	expression tag	UNP Q9BWT3
A	-1	HIS	-	expression tag	UNP Q9BWT3
A	0	HIS	-	expression tag	UNP Q9BWT3
B	-5	HIS	-	expression tag	UNP Q9BWT3
B	-4	HIS	-	expression tag	UNP Q9BWT3
B	-3	HIS	-	expression tag	UNP Q9BWT3
B	-2	HIS	-	expression tag	UNP Q9BWT3
B	-1	HIS	-	expression tag	UNP Q9BWT3
B	0	HIS	-	expression tag	UNP Q9BWT3

- Molecule 2 is 3'-DEOXYADENOSINE-5'-TRIPHOSPHATE (three-letter code: 3AT) (formula: C₁₀H₁₆N₅O₁₂P₃).



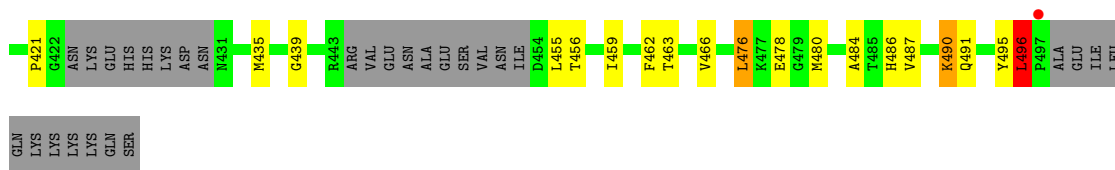
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
2	B	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	27	Total	O	0	0
			27	27		
4	B	26	Total	O	0	0
			26	26		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.87Å 89.92Å 201.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.88 – 2.79 19.84 – 2.79	Depositor EDS
% Data completeness (in resolution range)	95.7 (19.88-2.79) 89.9 (19.84-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 2.79Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.6_289)	Depositor
R, R_{free}	0.193 , 0.257 0.195 , 0.257	Depositor DCC
R_{free} test set	1488 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	38.8	Xtrriage
Anisotropy	0.470	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 30.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7644	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% 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: 3AT, CA

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	0.45	0/3876	0.61	0/5258
1	B	0.43	0/3837	0.62	2/5206 (0.0%)
All	All	0.44	0/7713	0.62	2/10464 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	415	VAL	CB-CA-C	-5.37	101.19	111.40
1	B	476	LEU	CA-CB-CG	5.13	127.11	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts i

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3784	0	3791	52	0
1	B	3745	0	3745	78	0
2	A	30	0	11	1	0
2	B	30	0	11	5	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	27	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	26	0	0	5	0
All	All	7644	0	7558	130	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (130) 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:461:SER:O	1:A:465:THR:OG1	2.07	0.71
1:B:180:ASN:ND2	4:B:713:HOH:O	2.17	0.71
1:B:177:ILE:HG23	1:B:181:LEU:HD12	1.74	0.69
1:A:94:GLY:H	1:A:177:ILE:HB	1.58	0.68
1:B:74:TRP:O	1:B:77:ASP:N	2.25	0.68
1:A:497:PRO:O	1:A:499:GLU:N	2.24	0.68
1:B:145:LEU:HD23	1:B:158:PHE:HB3	1.77	0.66
2:B:601:3AT:O2'	4:B:724:HOH:O	2.15	0.65
1:A:120:PRO:HG3	1:A:177:ILE:HG12	1.80	0.64
1:A:233:ARG:NH1	1:A:339:GLU:OE1	2.31	0.63
1:A:74:TRP:CE2	1:A:132:PHE:HB2	2.34	0.62
1:B:79:SER:HB3	1:B:89:VAL:HG13	1.82	0.62
1:B:487:VAL:HG13	1:B:491:GLN:HB2	1.82	0.62
1:A:376:LEU:HD21	1:A:462:PHE:HE2	1.65	0.61
1:B:220:ARG:O	1:B:224:ARG:HG3	2.01	0.61
1:B:232:ARG:NH1	1:B:361:LEU:O	2.36	0.58
1:B:200:LEU:O	1:B:204:ARG:HG3	2.04	0.58
1:B:53:ASP:HB2	1:B:56:GLU:H	1.69	0.57
1:B:101:SER:OG	2:B:601:3AT:O3G	2.10	0.57
1:A:103:ARG:HG2	1:A:206:THR:HG21	1.88	0.56
1:A:262:ALA:HB1	1:A:266:THR:HB	1.88	0.55
1:B:71:VAL:HG21	1:B:96:ILE:HD11	1.88	0.55
1:B:459:ILE:O	1:B:463:THR:HG23	2.06	0.55
1:A:121:ARG:HG3	1:A:174:ILE:O	2.07	0.55
1:B:189:LEU:HD22	1:B:197:ILE:HG12	1.88	0.54
1:B:120:PRO:HG3	1:B:177:ILE:HG12	1.90	0.54
1:B:374:ILE:HD11	1:B:455:LEU:HD13	1.90	0.54
1:A:129:PHE:CE2	1:A:149:GLU:HB3	2.43	0.54
1:B:207:ASP:O	1:B:211:HIS:ND1	2.40	0.54
1:A:232:ARG:NH1	1:A:361:LEU:O	2.41	0.53
1:A:21:ILE:HG13	1:A:22:THR:HG23	1.90	0.53
1:B:94:GLY:H	1:B:177:ILE:HB	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:462:PHE:O	1:B:466:VAL:HG23	2.09	0.53
1:A:205:VAL:HG21	2:A:601:3AT:H2	1.90	0.53
1:B:92:VAL:HG13	1:B:120:PRO:HG2	1.90	0.53
1:B:50:VAL:HG21	1:B:228:LEU:HG	1.89	0.53
1:A:103:ARG:HG2	1:A:206:THR:CG2	2.39	0.53
1:A:207:ASP:O	1:A:211:HIS:ND1	2.43	0.52
1:B:360:LEU:HB3	1:B:361:LEU:HD13	1.92	0.52
1:B:91:THR:HG23	1:B:176:THR:HG21	1.91	0.52
1:B:208:GLU:HG3	1:B:318:ALA:HB2	1.90	0.52
1:A:181:LEU:HD22	1:A:182:ASP:H	1.75	0.52
1:B:229:TRP:CD1	1:B:360:LEU:HD22	2.45	0.51
1:B:486:HIS:HD2	1:B:487:VAL:N	2.09	0.51
1:B:178:SER:OG	1:B:179:ASP:N	2.44	0.51
1:B:186:ASP:OD1	1:B:204:ARG:NH2	2.43	0.51
1:A:186:ASP:OD1	1:A:204:ARG:NH2	2.38	0.50
1:B:134:GLU:O	1:B:138:HIS:ND1	2.41	0.50
1:A:462:PHE:O	1:A:466:VAL:HG23	2.12	0.50
1:B:205:VAL:HG21	2:B:601:3AT:H2	1.92	0.50
1:B:476:LEU:HA	1:B:480:MET:CE	2.42	0.50
1:B:400:LEU:O	1:B:400:LEU:HD22	2.11	0.50
1:B:25:ILE:HD12	1:B:258:LEU:HB3	1.95	0.49
1:B:397:ILE:HG21	1:B:415:VAL:HG11	1.94	0.49
1:A:370:TYR:CD2	1:A:439:GLY:HA3	2.48	0.49
1:B:370:TYR:CD2	1:B:439:GLY:HA3	2.47	0.49
2:B:601:3AT:O2A	4:B:726:HOH:O	2.20	0.49
1:A:205:VAL:HG22	1:A:316:THR:HG23	1.95	0.49
1:B:350:ILE:HD13	1:B:357:TRP:HA	1.96	0.48
1:A:45:MET:HG2	1:A:228:LEU:HD12	1.93	0.48
1:A:496:LEU:HA	1:A:497:PRO:HD3	1.73	0.48
1:A:396:LYS:HE3	1:A:469:GLN:OE1	2.14	0.48
1:A:477:LYS:H	1:A:480:MET:HE2	1.78	0.48
1:B:130:GLN:HG3	1:B:131:SER:H	1.79	0.48
1:A:229:TRP:O	1:A:233:ARG:HB2	2.14	0.48
1:B:121:ARG:HG3	1:B:122:HIS:CD2	2.50	0.47
1:B:476:LEU:HA	1:B:480:MET:HE1	1.96	0.47
1:B:205:VAL:O	1:B:209:ILE:HG13	2.15	0.47
1:B:435:MET:HE1	1:B:495:TYR:HD2	1.80	0.47
1:B:57:LEU:O	1:B:61:LEU:HD23	2.15	0.46
1:A:185:ASP:OD2	1:A:187:SER:OG	2.21	0.46
1:A:79:SER:HB2	1:A:122:HIS:CE1	2.51	0.46
1:A:204:ARG:NH1	1:A:319:TYR:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:GLN:O	1:A:346:VAL:HG23	2.17	0.45
1:A:371:ARG:HA	1:A:371:ARG:HD2	1.67	0.45
1:B:234:GLY:O	4:B:725:HOH:O	2.21	0.45
1:A:243:LEU:N	1:A:336:MET:HE1	2.32	0.45
1:A:499:GLU:O	1:A:501:LEU:N	2.49	0.45
1:B:106:VAL:HG21	1:B:223:LEU:CD1	2.47	0.45
1:B:232:ARG:HA	1:B:232:ARG:HD2	1.57	0.45
1:A:145:LEU:HD23	1:A:145:LEU:HA	1.79	0.44
1:A:258:LEU:HA	1:A:258:LEU:HD23	1.79	0.44
1:B:123:VAL:O	1:B:171:ARG:HG3	2.17	0.44
1:B:105:GLY:HA2	4:B:717:HOH:O	2.16	0.44
1:B:243:LEU:HD13	1:B:336:MET:HE1	1.99	0.44
1:B:288:GLN:HA	1:B:289:PRO:HD3	1.77	0.44
1:A:29:SER:O	1:B:406:ARG:HG2	2.17	0.44
1:A:475:MET:O	1:A:477:LYS:HG3	2.18	0.44
1:B:92:VAL:HA	1:B:176:THR:HG22	2.00	0.44
1:A:74:TRP:CE3	1:A:75:ILE:HG13	2.53	0.44
1:A:121:ARG:NH1	1:A:175:GLN:OE1	2.48	0.44
1:A:496:LEU:HA	1:A:496:LEU:HD12	1.71	0.44
1:B:30:PRO:HD3	1:B:261:ASN:O	2.18	0.44
1:B:181:LEU:HD22	1:B:183:LEU:HD23	2.00	0.44
1:B:120:PRO:HB3	1:B:175:GLN:O	2.18	0.43
1:B:496:LEU:HD12	1:B:496:LEU:HA	1.85	0.43
1:B:19:TYR:CE2	1:B:214:PRO:HA	2.53	0.43
1:B:235:ILE:HB	1:B:336:MET:HE3	2.00	0.43
1:A:128:PHE:CE2	1:A:156:ILE:HG13	2.54	0.43
1:B:92:VAL:HG11	1:B:122:HIS:HE1	1.83	0.43
1:B:181:LEU:HD21	1:B:188:ARG:HH11	1.83	0.43
1:B:125:ARG:O	1:B:129:PHE:HD2	2.02	0.42
1:A:185:ASP:O	1:A:188:ARG:HG3	2.19	0.42
1:A:61:LEU:HD13	4:A:704:HOH:O	2.20	0.42
1:A:67:LEU:HD13	1:A:96:ILE:CD1	2.49	0.42
1:A:145:LEU:HD23	1:A:158:PHE:HB3	2.01	0.42
1:B:246:VAL:HG22	2:B:601:3AT:H2'1	2.02	0.42
1:B:233:ARG:HA	1:B:364:PRO:HD3	2.01	0.42
1:B:268:VAL:O	1:B:271:PHE:HB3	2.19	0.42
1:B:396:LYS:O	1:B:399:VAL:HB	2.20	0.42
1:B:259:TYR:CZ	1:B:270:LYS:HD2	2.54	0.42
1:A:103:ARG:O	1:A:103:ARG:HG3	2.18	0.41
1:B:366:PHE:O	1:B:373:TYR:OH	2.33	0.41
1:B:486:HIS:CD2	1:B:487:VAL:N	2.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:459:ILE:HD13	1:B:484:ALA:O	2.20	0.41
1:A:193:ASP:O	1:A:196:CYS:N	2.54	0.41
1:B:154:PRO:O	1:B:168:VAL:HG22	2.19	0.41
1:B:316:THR:HA	1:B:317:PRO:HD3	1.96	0.41
1:B:243:LEU:N	1:B:336:MET:HE1	2.35	0.41
1:A:487:VAL:HG12	1:A:488:LYS:O	2.21	0.41
1:B:99:PHE:CZ	1:B:114:ASP:HB3	2.56	0.41
1:B:382:THR:OG1	1:B:383:GLU:N	2.53	0.41
1:A:335:VAL:HG21	1:A:414:HIS:CD2	2.56	0.41
1:A:74:TRP:CG	1:A:132:PHE:HD1	2.39	0.40
1:B:184:ARG:HD3	1:B:208:GLU:OE2	2.21	0.40
1:A:28:ALA:HB1	1:B:406:ARG:HB3	2.03	0.40
1:B:112:ASP:HB3	1:B:164:GLU:HB3	2.04	0.40
1:B:213:VAL:HA	1:B:214:PRO:HD2	1.96	0.40
1:A:312:MET:N	1:A:313:PRO:HD3	2.37	0.40
1:B:133:PHE:CZ	1:B:145:LEU:HD13	2.56	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	461/514 (90%)	425 (92%)	31 (7%)	5 (1%)	14	41
1	B	456/514 (89%)	427 (94%)	23 (5%)	6 (1%)	12	36
All	All	917/1028 (89%)	852 (93%)	54 (6%)	11 (1%)	13	39

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	500	ILE
1	B	496	LEU

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Mol	Chain	Res	Type
1	B	237	SER
1	B	490	LYS
1	A	237	SER
1	A	497	PRO
1	A	498	ALA
1	B	75	ILE
1	B	421	PRO
1	A	303	VAL
1	B	148	VAL

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	420/465 (90%)	368 (88%)	52 (12%)	4	14
1	B	416/465 (90%)	371 (89%)	45 (11%)	6	19
All	All	836/930 (90%)	739 (88%)	97 (12%)	5	17

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LEU
1	A	61	LEU
1	A	67	LEU
1	A	73	GLU
1	A	96	ILE
1	A	103	ARG
1	A	130	GLN
1	A	144	ASN
1	A	145	LEU
1	A	146	ARG
1	A	160	PHE
1	A	168	VAL
1	A	181	LEU
1	A	184	ARG

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Mol	Chain	Res	Type
1	A	207	ASP
1	A	213	VAL
1	A	223	LEU
1	A	228	LEU
1	A	232	ARG
1	A	233	ARG
1	A	239	MET
1	A	254	ARG
1	A	273	LEU
1	A	288	GLN
1	A	306	SER
1	A	316	THR
1	A	321	GLN
1	A	330	THR
1	A	342	GLN
1	A	360	LEU
1	A	361	LEU
1	A	369	LYS
1	A	371	ARG
1	A	376	LEU
1	A	379	SER
1	A	381	SER
1	A	383	GLU
1	A	384	GLU
1	A	400	LEU
1	A	411	THR
1	A	433	VAL
1	A	435	MET
1	A	443	ARG
1	A	455	LEU
1	A	461	SER
1	A	468	ARG
1	A	473	ILE
1	A	478	GLU
1	A	491	GLN
1	A	492	LEU
1	A	499	GLU
1	A	500	ILE
1	B	29	SER
1	B	41	LEU
1	B	67	LEU
1	B	68	ASN

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Mol	Chain	Res	Type
1	B	69	ASN
1	B	79	SER
1	B	84	LEU
1	B	103	ARG
1	B	121	ARG
1	B	124	GLU
1	B	145	LEU
1	B	146	ARG
1	B	160	PHE
1	B	181	LEU
1	B	182	ASP
1	B	184	ARG
1	B	217	GLU
1	B	223	LEU
1	B	228	LEU
1	B	232	ARG
1	B	239	MET
1	B	246	VAL
1	B	254	ARG
1	B	273	LEU
1	B	290	GLU
1	B	316	THR
1	B	321	GLN
1	B	342	GLN
1	B	355	SER
1	B	360	LEU
1	B	361	LEU
1	B	376	LEU
1	B	382	THR
1	B	383	GLU
1	B	384	GLU
1	B	387	LEU
1	B	390	VAL
1	B	392	LEU
1	B	400	LEU
1	B	415	VAL
1	B	418	GLN
1	B	456	THR
1	B	478	GLU
1	B	490	LYS
1	B	496	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	493	HIS
1	A	494	HIS
1	B	122	HIS
1	B	486	HIS

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 4 ligands modelled in this entry, 2 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
2	3AT	B	601	3	25,32,32	1.82	6 (24%)	28,50,50	1.56	6 (21%)
2	3AT	A	601	3	25,32,32	1.67	5 (20%)	28,50,50	1.47	4 (14%)

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
2	3AT	B	601	3	-	2/18/34/34	0/3/3/3
2	3AT	A	601	3	-	1/18/34/34	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	3AT	O2'-C2'	-4.82	1.33	1.43
2	B	601	3AT	C2'-C1'	-4.55	1.49	1.54
2	A	601	3AT	O2'-C2'	-4.41	1.34	1.43
2	A	601	3AT	C2'-C1'	-3.71	1.50	1.54
2	B	601	3AT	C6-N6	2.64	1.43	1.34
2	A	601	3AT	C6-N6	2.45	1.43	1.34
2	B	601	3AT	O4'-C4'	2.36	1.49	1.44
2	A	601	3AT	C3'-C4'	-2.15	1.48	1.52
2	B	601	3AT	PG-O1G	2.14	1.57	1.50
2	A	601	3AT	PG-O1G	2.13	1.57	1.50
2	B	601	3AT	C3'-C4'	-2.02	1.48	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	3AT	N3-C2-N1	-5.03	120.81	128.68
2	A	601	3AT	N3-C2-N1	-4.79	121.20	128.68
2	B	601	3AT	PB-O3B-PG	-2.88	122.93	132.83
2	A	601	3AT	O2G-PG-O3B	2.43	112.78	104.64
2	A	601	3AT	C2-N1-C6	2.18	122.48	118.75
2	B	601	3AT	PA-O3A-PB	-2.17	125.36	132.83
2	B	601	3AT	C4-C5-N7	-2.13	107.18	109.40
2	B	601	3AT	C2-N1-C6	2.08	122.32	118.75
2	A	601	3AT	N6-C6-N1	2.07	122.88	118.57
2	B	601	3AT	O4'-C4'-C5'	2.01	112.82	109.52

There are no chirality outliers.

All (3) torsion outliers are listed below:

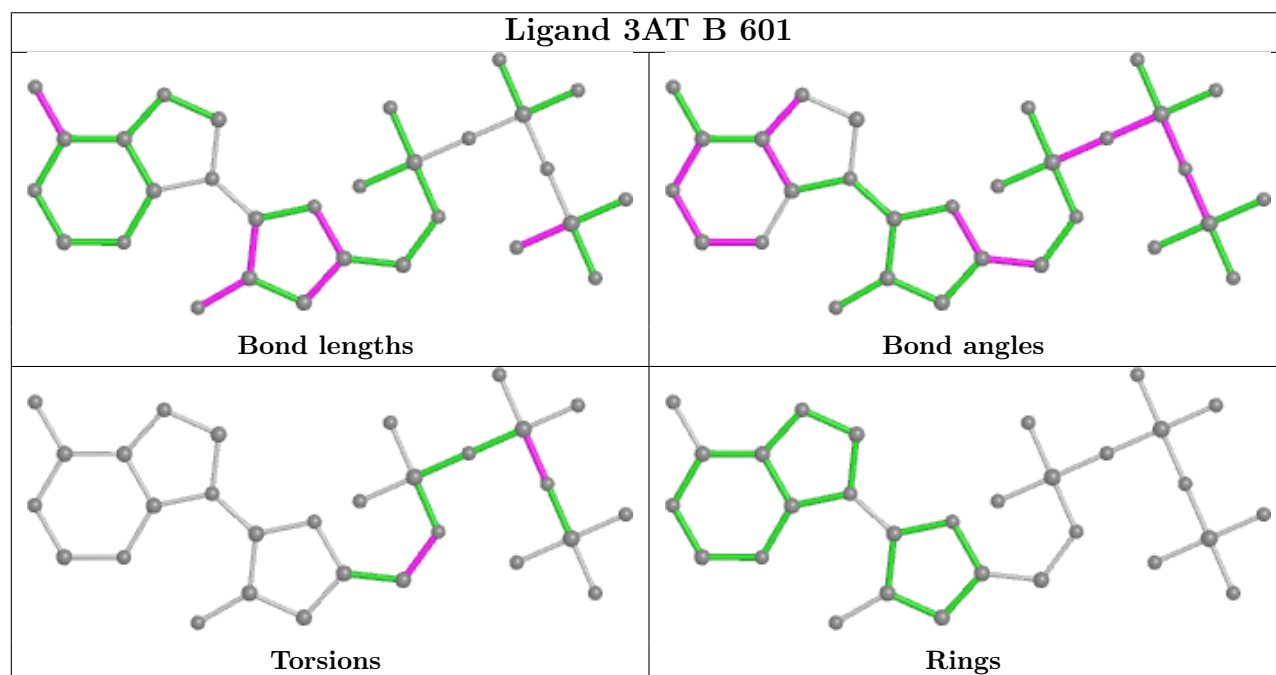
Mol	Chain	Res	Type	Atoms
2	A	601	3AT	PB-O3A-PA-O1A
2	B	601	3AT	C4'-C5'-O5'-PA
2	B	601	3AT	PG-O3B-PB-O1B

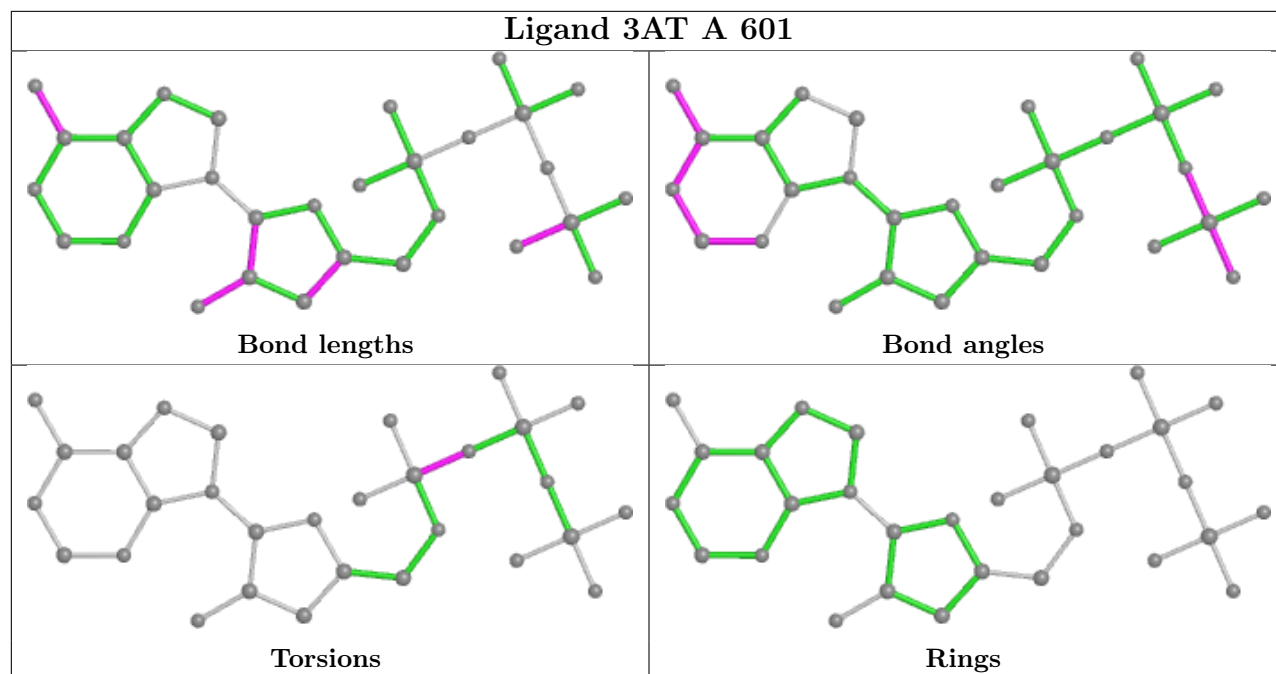
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	3AT	5	0
2	A	601	3AT	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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	467/514 (90%)	-0.31	4 (0%) 84 80	5, 21, 62, 99	2 (0%)
1	B	462/514 (89%)	-0.27	3 (0%) 89 86	6, 23, 59, 92	2 (0%)
All	All	929/1028 (90%)	-0.29	7 (0%) 86 81	5, 22, 62, 99	4 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	152	PHE	3.0
1	B	497	PRO	2.9
1	A	86	PRO	2.8
1	A	457	TYR	2.5
1	A	431	ASN	2.5
1	A	498	ALA	2.3
1	B	191	SER	2.1

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](#)

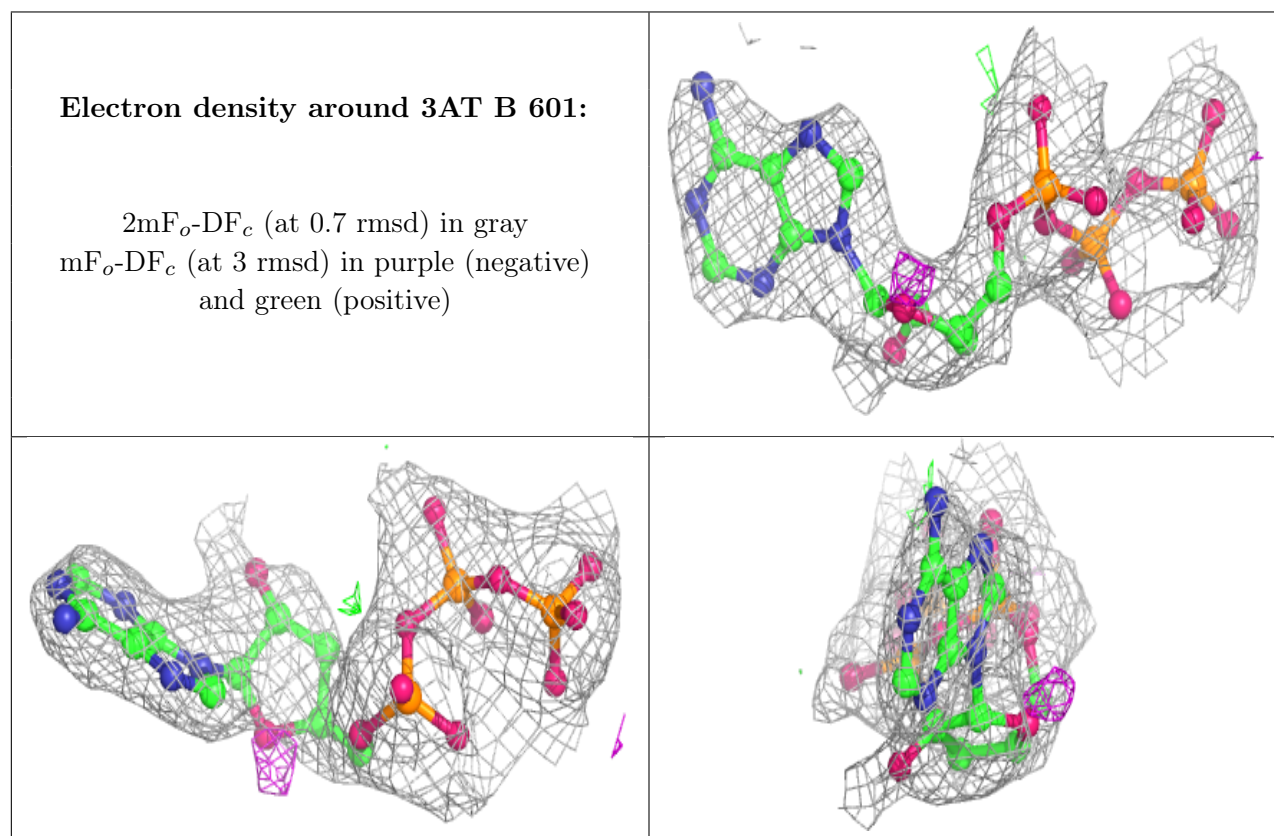
There are no monosaccharides in this entry.

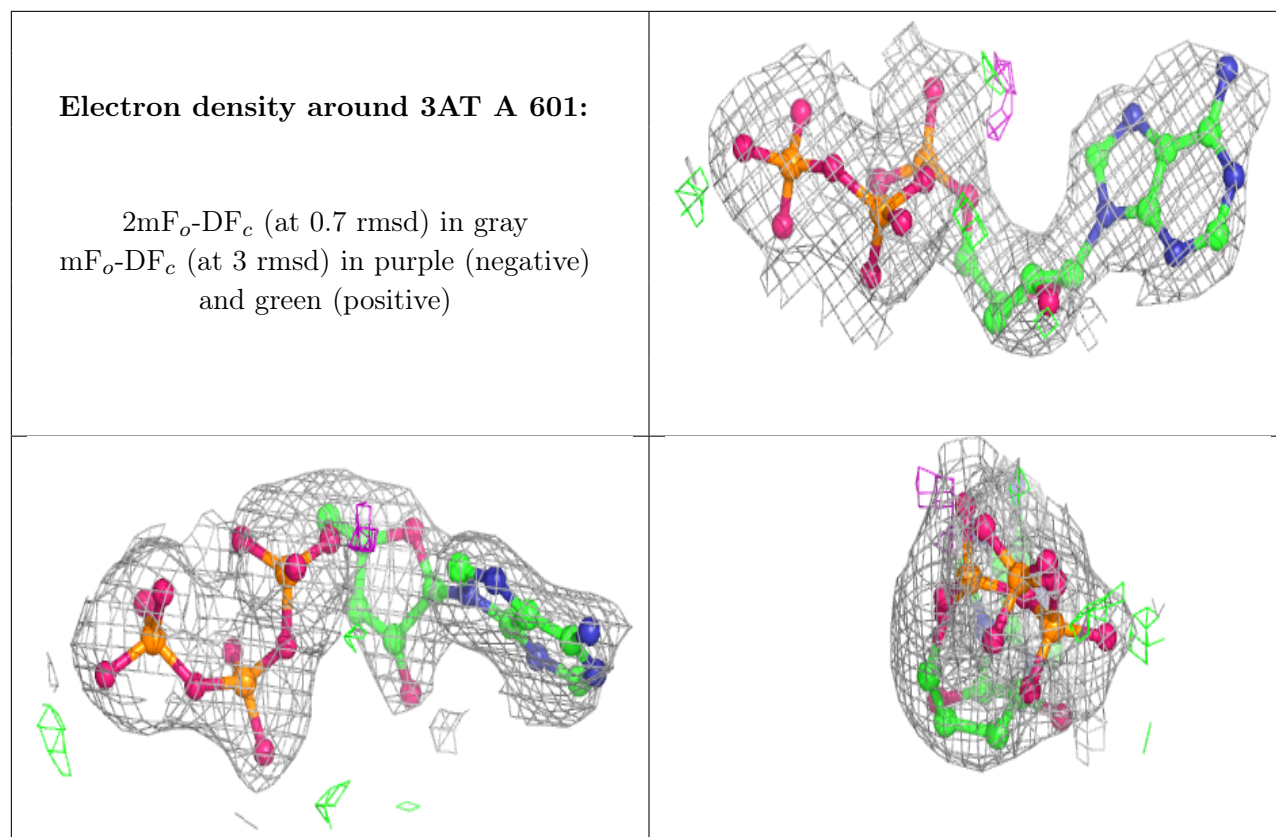
6.4 Ligands [i](#)

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(\AA^2)	Q<0.9
3	CA	A	602	1/1	0.95	0.08	31,31,31,31	0
2	3AT	B	601	30/30	0.96	0.15	16,25,37,48	7
2	3AT	A	601	30/30	0.96	0.17	11,24,29,37	7
3	CA	B	602	1/1	0.98	0.05	34,34,34,34	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.