



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 02:23 pm BST

PDB ID : 5I4U
Title : The crystal structure of PI3Kdelta with compound 34
Authors : Somoza, J.R.; Villasenor, A.G.
Deposited on : 2016-02-12
Resolution : 2.37 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 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 : 2.11
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) : 2.11

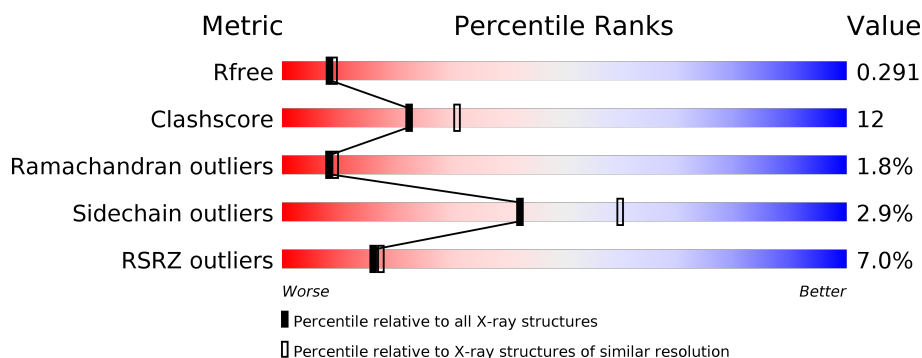
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.37 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	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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 on 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	939	<div> <div>6%</div> <div>65%</div> <div>20%</div> <div>••</div> <div>13%</div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6681 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.

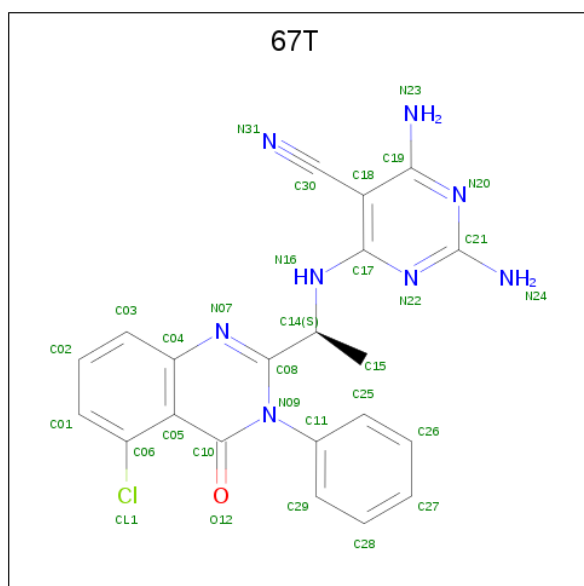
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic sub-unit delta isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	815	Total	C	N	O	S	0	0	0
			6566	4210	1115	1187	54			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	508	GLN	-	insertion	UNP O35904

- Molecule 2 is 2,4-diamino-6-[[[(1S)-1-(5-chloro-4-oxo-3-phenyl-3,4-dihydroquinazolin-2-yl)ethyl]amino]pyrimidine-5-carbonitrile (three-letter code: 67T) (formula: C₂₁H₁₇ClN₈O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			31	21	1	8	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	84	Total	O	0	0
			84	84		

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	64.27Å 143.48Å 221.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.89 – 2.37 45.89 – 2.37	Depositor EDS
% Data completeness (in resolution range)	93.4 (45.89-2.37) 89.1 (45.89-2.37)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.37Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.222 , 0.290 0.226 , 0.291	Depositor DCC
R_{free} test set	1999 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	43.8	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6681	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% 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: 67T

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	0.48	0/6706	0.63	4/9047 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	1012	LEU	CA-CB-CG	8.47	134.79	115.30
1	A	1023	LEU	CA-CB-CG	6.13	129.40	115.30
1	A	1009	GLU	N-CA-C	-5.16	97.08	111.00
1	A	1014	HIS	N-CA-CB	5.03	119.65	110.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1008	GLU	Peptide
1	A	1010	GLU	Peptide
1	A	1012	LEU	Peptide
1	A	333	VAL	Peptide

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	6566	0	6557	153	0
2	A	31	0	0	0	0
3	A	84	0	0	4	0
All	All	6681	0	6557	153	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 12.

All (153) 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:331:ARG:HD3	1:A:368:GLU:HG3	1.48	0.93
1:A:745:CYS:HB3	1:A:748:GLN:HE21	1.34	0.91
1:A:367:SER:OG	1:A:368:GLU:OE2	1.90	0.88
1:A:512:ARG:HH21	1:A:538:VAL:HG22	1.39	0.86
1:A:331:ARG:HA	1:A:368:GLU:HA	1.57	0.86
1:A:888:VAL:HA	1:A:1001:SER:HB2	1.59	0.83
1:A:1007:THR:HG22	1:A:1010:GLU:HB3	1.62	0.81
1:A:1009:GLU:HG2	1:A:1011:ALA:C	2.03	0.79
1:A:1010:GLU:C	1:A:1012:LEU:H	1.85	0.79
1:A:246:ARG:NH1	1:A:248:GLU:OE1	2.17	0.78
1:A:996:GLN:O	1:A:999:LYS:N	2.15	0.76
1:A:999:LYS:HG3	1:A:1000:ASP:N	2.03	0.74
1:A:786:GLN:NE2	1:A:914:HIS:O	2.23	0.72
1:A:512:ARG:HH22	1:A:531:VAL:HG13	1.55	0.72
1:A:779:LYS:NZ	1:A:782:ASP:OD2	2.23	0.67
1:A:364:ASN:O	1:A:366:CYS:N	2.25	0.67
1:A:1010:GLU:HA	1:A:1012:LEU:HB2	1.77	0.67
1:A:333:VAL:HG11	1:A:367:SER:HA	1.76	0.66
1:A:512:ARG:HH12	1:A:531:VAL:HG22	1.59	0.66
1:A:955:ARG:NH2	3:A:1204:HOH:O	2.29	0.65
1:A:427:ASP:OD1	1:A:431:GLN:N	2.29	0.65
1:A:745:CYS:HB3	1:A:748:GLN:NE2	2.08	0.65
1:A:979:ALA:HA	1:A:995:ILE:HD11	1.79	0.64
1:A:245:GLY:HA3	1:A:768:ALA:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:TRP:C	1:A:373:GLN:H	2.02	0.63
1:A:512:ARG:HG3	1:A:512:ARG:NH1	2.14	0.62
1:A:549:LEU:HG	1:A:564:MET:HE3	1.81	0.62
1:A:331:ARG:HG3	1:A:332:LYS:HD3	1.80	0.62
1:A:512:ARG:NH2	1:A:538:VAL:HG22	2.13	0.62
1:A:333:VAL:O	1:A:334:ASN:ND2	2.33	0.61
1:A:999:LYS:CG	1:A:1000:ASP:N	2.63	0.61
1:A:138:ASP:OD2	1:A:428:TYR:OH	2.16	0.61
1:A:933:ILE:HG12	3:A:1237:HOH:O	2.02	0.60
1:A:895:HIS:CE1	1:A:897:ASP:HB2	2.35	0.60
1:A:1013:LYS:HA	1:A:1016:ARG:CG	2.32	0.60
1:A:331:ARG:NH1	1:A:368:GLU:OE2	2.35	0.59
1:A:745:CYS:CB	1:A:748:GLN:HE21	2.12	0.59
1:A:1010:GLU:O	1:A:1010:GLU:HG3	2.01	0.59
1:A:193:ASN:OD1	1:A:202:SER:OG	2.21	0.59
1:A:271:THR:O	1:A:273:HIS:HD2	1.85	0.58
1:A:325:ILE:HD13	1:A:377:PHE:HE1	1.68	0.58
1:A:1010:GLU:C	1:A:1012:LEU:N	2.56	0.58
1:A:679:MET:O	1:A:683:MET:HG3	2.04	0.57
1:A:331:ARG:HG3	1:A:332:LYS:CD	2.35	0.57
1:A:340:LYS:HG2	1:A:362:GLU:HB3	1.87	0.56
1:A:957:ARG:HG3	1:A:1019:PHE:CE1	2.41	0.55
1:A:333:VAL:CG1	1:A:367:SER:HA	2.36	0.55
1:A:731:LEU:HD11	1:A:741:LEU:HD12	1.88	0.54
1:A:996:GLN:O	1:A:999:LYS:HB3	2.07	0.54
1:A:489:GLU:O	1:A:493:GLU:HG3	2.08	0.54
1:A:581:GLU:HB2	1:A:976:HIS:CD2	2.44	0.53
1:A:512:ARG:HH11	1:A:512:ARG:HG3	1.73	0.53
1:A:999:LYS:O	1:A:1003:ALA:N	2.42	0.53
1:A:610:GLN:O	1:A:792:GLN:NE2	2.40	0.52
1:A:532:TRP:HZ3	1:A:564:MET:HE2	1.73	0.52
1:A:1012:LEU:HD22	1:A:1013:LYS:HB3	1.91	0.52
1:A:321:GLN:N	1:A:321:GLN:OE1	2.34	0.52
1:A:947:THR:O	1:A:948:ASN:ND2	2.43	0.52
1:A:188:ARG:HD3	1:A:189:ALA:O	2.10	0.51
1:A:594:SER:HB3	1:A:598:LYS:NZ	2.25	0.51
1:A:155:GLN:OE1	1:A:290:SER:HB3	2.10	0.51
1:A:713:GLU:O	1:A:717:MET:HG3	2.10	0.51
1:A:209:THR:HB	1:A:257:CYS:HB3	1.92	0.50
1:A:332:LYS:HB2	1:A:469:ALA:HA	1.92	0.50
1:A:1007:THR:HG22	1:A:1010:GLU:CB	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:856:LEU:O	1:A:860:LYS:HG3	2.11	0.50
1:A:848:ALA:HB1	1:A:853:ASP:HB2	1.94	0.49
1:A:349:HIS:O	1:A:352:GLU:HG3	2.12	0.49
1:A:594:SER:HB3	1:A:598:LYS:HZ3	1.78	0.49
1:A:929:ARG:NH2	1:A:1000:ASP:HB2	2.28	0.49
1:A:162:TRP:CD1	1:A:286:ARG:HG3	2.48	0.49
1:A:189:ALA:HA	1:A:208:SER:HA	1.94	0.49
1:A:339:MET:O	1:A:365:VAL:HG23	2.12	0.49
1:A:1013:LYS:HA	1:A:1016:ARG:HG2	1.95	0.49
1:A:331:ARG:HA	1:A:368:GLU:CA	2.37	0.49
1:A:157:LEU:HB3	1:A:161:GLU:HB2	1.95	0.49
1:A:270:LEU:HD22	1:A:770:SER:HB3	1.95	0.49
1:A:1007:THR:OG1	1:A:1008:GLU:N	2.47	0.48
1:A:1009:GLU:O	1:A:1012:LEU:HB2	2.13	0.48
1:A:915:PHE:HD1	1:A:916:LEU:HG	1.79	0.48
1:A:516:GLU:OE1	1:A:516:GLU:N	2.46	0.48
1:A:386:ARG:NH2	1:A:430:ASP:OD1	2.34	0.48
1:A:335:ALA:C	1:A:365:VAL:HG11	2.34	0.47
1:A:890:GLY:O	1:A:915:PHE:HA	2.14	0.47
1:A:329:GLU:HB2	1:A:369:PRO:O	2.14	0.47
1:A:536:HIS:O	1:A:540:GLU:HG2	2.14	0.47
1:A:999:LYS:CG	1:A:1000:ASP:H	2.27	0.47
1:A:194:VAL:HG21	1:A:216:LEU:HD21	1.96	0.47
1:A:383:ASP:HB3	1:A:556:ASN:O	2.15	0.47
1:A:1007:THR:HG23	1:A:1008:GLU:HB2	1.97	0.47
1:A:663:ARG:O	1:A:667:ILE:HG13	2.15	0.47
1:A:549:LEU:HG	1:A:564:MET:CE	2.44	0.47
1:A:349:HIS:O	1:A:352:GLU:CG	2.63	0.47
1:A:325:ILE:HD13	1:A:377:PHE:CE1	2.49	0.47
1:A:996:GLN:HG3	1:A:999:LYS:HB3	1.95	0.47
1:A:350:GLY:N	1:A:588:PRO:HG3	2.30	0.46
1:A:731:LEU:HD12	1:A:732:GLN:O	2.16	0.46
1:A:340:LYS:HG3	1:A:363:VAL:O	2.15	0.46
1:A:1009:GLU:HG2	1:A:1012:LEU:N	2.32	0.45
1:A:512:ARG:NH2	1:A:531:VAL:HG13	2.28	0.45
1:A:991:CYS:HB2	1:A:993:LYS:H	1.81	0.45
1:A:131:LEU:HD23	3:A:1209:HOH:O	2.16	0.45
1:A:915:PHE:CD1	1:A:916:LEU:HG	2.52	0.45
1:A:364:ASN:C	1:A:366:CYS:H	2.16	0.44
1:A:634:LEU:HD23	1:A:634:LEU:HA	1.80	0.44
1:A:859:LEU:HD21	1:A:901:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:GLN:HG2	1:A:677:HIS:CD2	2.52	0.44
1:A:696:ASN:O	1:A:700:LYS:HG3	2.16	0.44
1:A:535:ARG:HA	1:A:538:VAL:HG23	1.99	0.44
1:A:564:MET:HE2	1:A:564:MET:HB2	1.84	0.44
1:A:187:ASN:HB2	1:A:210:LYS:HG3	1.99	0.44
1:A:191:LEU:O	1:A:272:PRO:HD2	2.18	0.44
1:A:316:LEU:HB3	1:A:318:SER:OG	2.18	0.44
1:A:548:ARG:O	1:A:552:VAL:HG13	2.17	0.44
1:A:597:ILE:HA	1:A:597:ILE:HD13	1.80	0.43
1:A:349:HIS:CE1	1:A:588:PRO:HG2	2.53	0.43
1:A:340:LYS:CD	1:A:362:GLU:HB3	2.48	0.43
1:A:342:VAL:HB	1:A:395:TYR:CZ	2.54	0.43
1:A:671:TYR:OH	1:A:678:HIS:ND1	2.39	0.43
1:A:326:GLU:HB3	1:A:474:TYR:HB3	1.99	0.43
1:A:371:TRP:O	1:A:373:GLN:N	2.49	0.43
1:A:756:MET:CE	1:A:781:GLY:HA3	2.49	0.43
1:A:386:ARG:HG3	1:A:387:MET:HE2	2.01	0.43
1:A:802:LYS:C	1:A:804:GLU:H	2.22	0.43
1:A:474:TYR:O	1:A:476:PRO:HD3	2.18	0.43
1:A:600:LEU:HD23	1:A:600:LEU:HA	1.81	0.42
1:A:754:SER:HB2	1:A:755:LYS:HG3	2.01	0.42
1:A:895:HIS:HE1	1:A:897:ASP:HB2	1.84	0.42
1:A:116:GLN:HB3	1:A:683:MET:SD	2.60	0.42
1:A:999:LYS:HG3	1:A:1000:ASP:OD1	2.20	0.42
1:A:356:LYS:HB2	1:A:356:LYS:HE3	1.78	0.42
1:A:691:LYS:HG3	1:A:724:TYR:CE2	2.54	0.42
1:A:783:ASP:OD1	1:A:785:ARG:HD3	2.20	0.42
1:A:187:ASN:HB3	1:A:209:THR:OG1	2.19	0.42
1:A:347:LEU:HD23	1:A:347:LEU:HA	1.83	0.41
1:A:317:TRP:HA	1:A:382:CYS:HB2	2.03	0.41
1:A:317:TRP:CZ3	1:A:494:LEU:HD22	2.55	0.41
1:A:842:SER:O	1:A:843:ASN:HB3	2.19	0.41
1:A:891:ILE:HD13	1:A:912:PHE:CD1	2.55	0.41
1:A:868:LEU:O	1:A:872:ILE:HG12	2.20	0.41
1:A:188:ARG:HD3	1:A:188:ARG:C	2.41	0.41
1:A:416:CYS:HA	1:A:417:PRO:HD3	1.87	0.41
1:A:594:SER:O	1:A:598:LYS:HG3	2.20	0.41
1:A:598:LYS:O	1:A:601:ARG:HG3	2.21	0.41
1:A:872:ILE:HB	3:A:1228:HOH:O	2.21	0.41
1:A:950:SER:O	1:A:954:GLU:HG2	2.21	0.41
1:A:1013:LYS:HA	1:A:1016:ARG:HG3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:SER:OG	1:A:373:GLN:NE2	2.54	0.40
1:A:394:LEU:HD23	1:A:418:ILE:HB	2.03	0.40
1:A:856:LEU:HG	1:A:860:LYS:CE	2.52	0.40
1:A:800:LEU:HD22	1:A:970:HIS:CG	2.57	0.40
1:A:323:PHE:CE2	1:A:325:ILE:HD11	2.55	0.40
1:A:543:PRO:O	1:A:571:TRP:NE1	2.50	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	793/939 (84%)	734 (93%)	45 (6%)	14 (2%)	8 9

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	365	VAL
1	A	372	LYS
1	A	770	SER
1	A	913	GLY
1	A	915	PHE
1	A	1008	GLU
1	A	1011	ALA
1	A	1013	LYS
1	A	769	GLY
1	A	229	ARG
1	A	464	ASN
1	A	576	VAL
1	A	328	ILE
1	A	227	VAL

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	721/827 (87%)	700 (97%)	21 (3%)	42 60

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	188	ARG
1	A	333	VAL
1	A	352	GLU
1	A	366	CYS
1	A	367	SER
1	A	372	LYS
1	A	423	LEU
1	A	445	VAL
1	A	512	ARG
1	A	560	ASP
1	A	738	SER
1	A	748	GLN
1	A	841	LYS
1	A	915	PHE
1	A	944	GLN
1	A	991	CYS
1	A	1006	LYS
1	A	1010	GLU
1	A	1013	LYS
1	A	1014	HIS
1	A	1017	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	193	ASN
1	A	247	HIS
1	A	273	HIS
1	A	334	ASN

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Mol	Chain	Res	Type
1	A	748	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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	67T	A	1101	-	34,34,34	1.72	7 (20%)	35,49,49	1.36	3 (8%)

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	67T	A	1101	-	-	0/10/14/14	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	67T	C10-C05	5.48	1.51	1.41
2	A	1101	67T	C18-C17	-3.24	1.38	1.41
2	A	1101	67T	C10-N09	2.69	1.42	1.37
2	A	1101	67T	C18-C19	-2.60	1.39	1.42
2	A	1101	67T	C01-C06	2.37	1.41	1.36
2	A	1101	67T	C08-C14	2.13	1.53	1.50
2	A	1101	67T	C04-N07	2.01	1.40	1.37

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	67T	C25-C11-N09	3.47	122.46	119.24
2	A	1101	67T	C19-C18-C17	-3.14	117.22	119.44
2	A	1101	67T	C14-C08-N07	-2.11	114.13	115.82

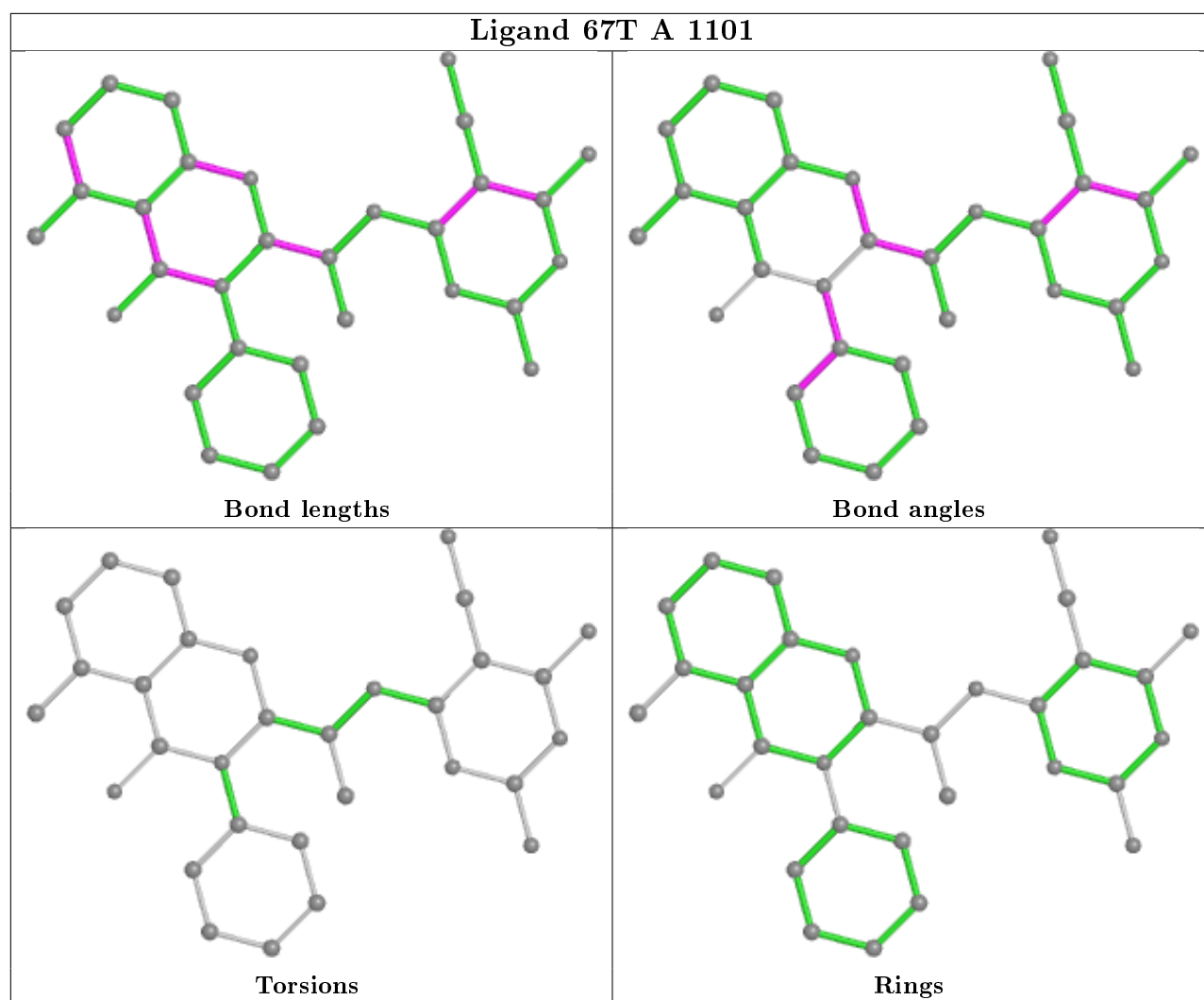
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	815/939 (86%)	0.50	57 (6%) 16 17	32, 54, 82, 254	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	335	ALA	7.6
1	A	934	LEU	5.2
1	A	333	VAL	5.2
1	A	331	ARG	4.6
1	A	1008	GLU	4.6
1	A	1000	ASP	4.5
1	A	932	PHE	4.4
1	A	842	SER	3.8
1	A	488	LEU	3.7
1	A	1014	HIS	3.7
1	A	1012	LEU	3.6
1	A	1023	LEU	3.5
1	A	228	PHE	3.4
1	A	1011	ALA	3.4
1	A	1010	GLU	3.3
1	A	929	ARG	3.1
1	A	468	ALA	3.0
1	A	846	ALA	3.0
1	A	915	PHE	2.9
1	A	1017	VAL	2.9
1	A	944	GLN	2.9
1	A	914	HIS	2.9
1	A	394	LEU	2.9
1	A	330	GLY	2.8
1	A	1006	LYS	2.8
1	A	203	PHE	2.8
1	A	370	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	396	ALA	2.8
1	A	200	GLU	2.8
1	A	371	TRP	2.8
1	A	1007	THR	2.7
1	A	1024	ARG	2.7
1	A	512	ARG	2.7
1	A	334	ASN	2.7
1	A	153	HIS	2.7
1	A	226	THR	2.7
1	A	470	ALA	2.5
1	A	936	TYR	2.5
1	A	1016	ARG	2.4
1	A	933	ILE	2.4
1	A	372	LYS	2.4
1	A	608	LEU	2.4
1	A	214	LEU	2.4
1	A	367	SER	2.3
1	A	365	VAL	2.3
1	A	205	PHE	2.2
1	A	317	TRP	2.2
1	A	513	GLU	2.2
1	A	366	CYS	2.2
1	A	201	GLU	2.2
1	A	341	LEU	2.1
1	A	619	LEU	2.1
1	A	1025	GLU	2.0
1	A	343	VAL	2.0
1	A	358	VAL	2.0
1	A	930	VAL	2.0
1	A	397	VAL	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 ⓘ

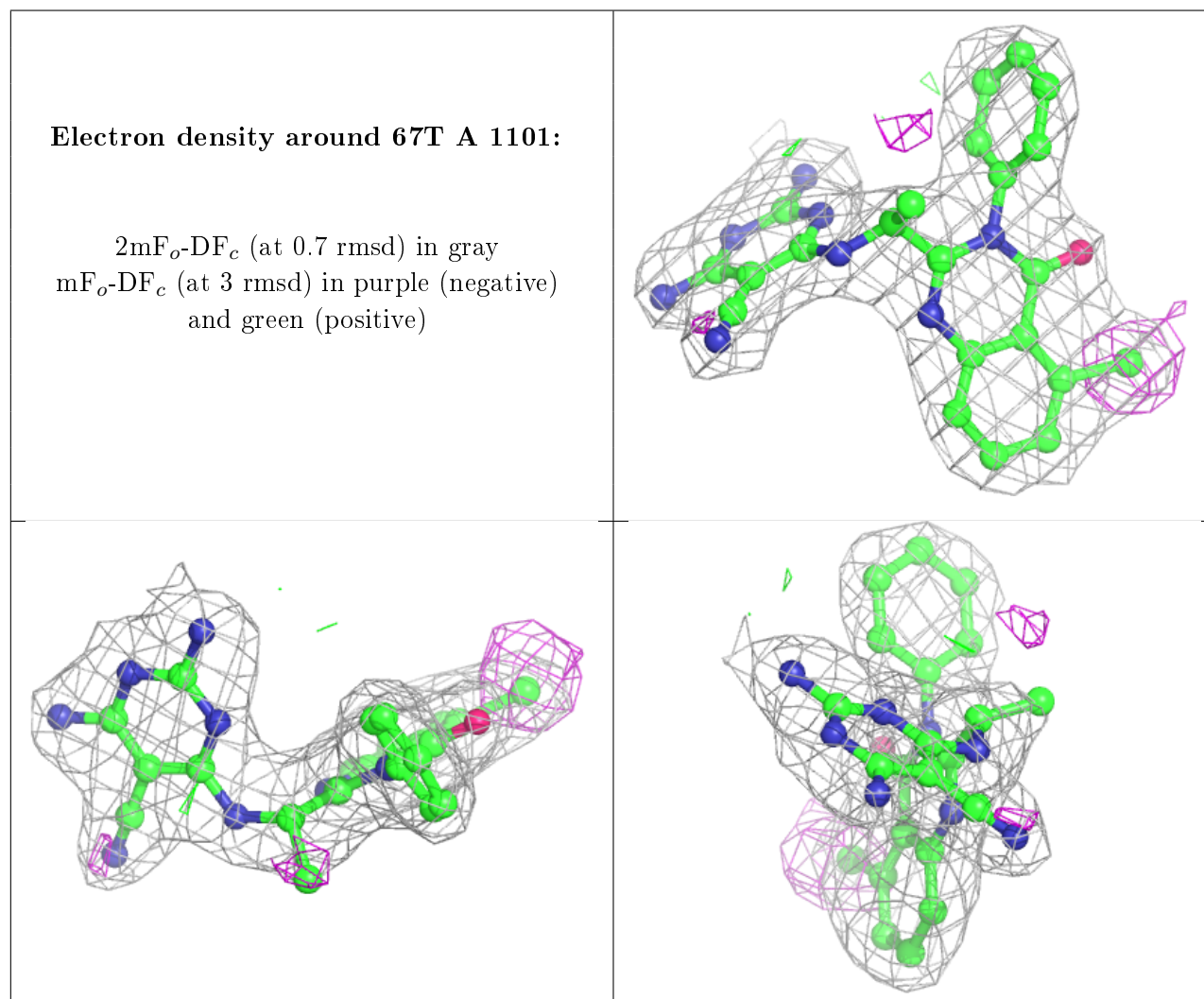
There are no carbohydrates in this entry.

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
2	67T	A	1101	31/31	0.93	0.16	32,40,47,56	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.