



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 11:55 pm BST

PDB ID : 4XE0
Title : Idelalisib bound to the p110 subunit of PI3K delta
Authors : Somoza, J.R.; Villasenor, A.
Deposited on : 2014-12-20
Resolution : 2.43 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

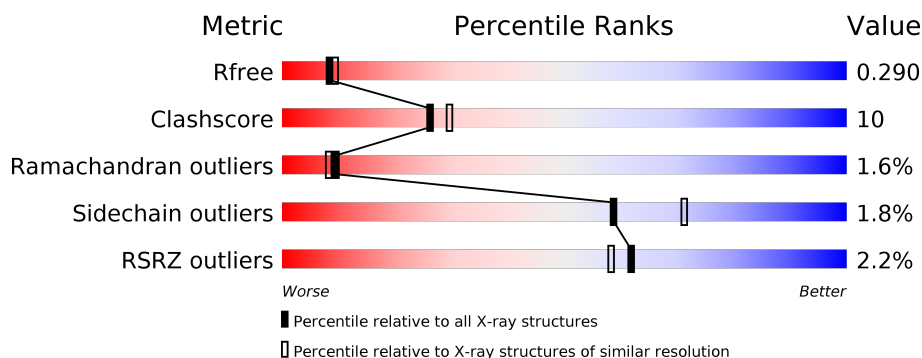
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.43 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	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

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>2%</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 6821 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.

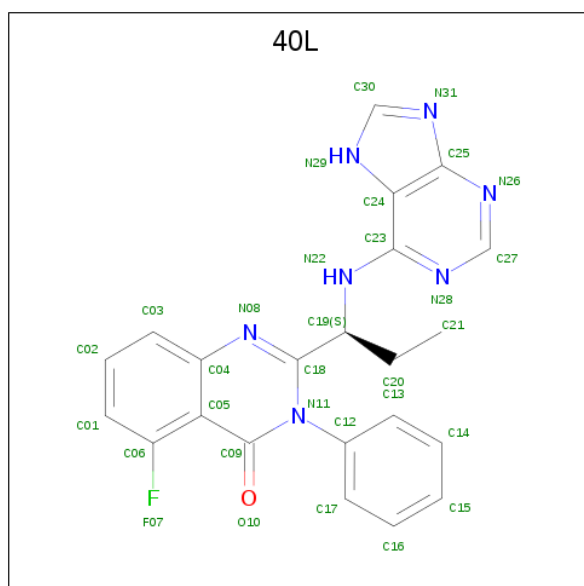
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic sub-unit delta isoform.

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 5-fluoro-3-phenyl-2-[(1S)-1-(7H-purin-6-ylamino)propyl]quinazolin-4(3H)-one (three-letter code: 40L) (formula: C₂₂H₁₈FN₇O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			31	22	1	7	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	224	Total 224	O 224	0	0

- Molecule 1: Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit delta isoform



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	142.05Å 64.59Å 115.96Å 90.00° 103.09° 90.00°	Depositor
Resolution (Å)	69.18 – 2.43 69.18 – 2.43	Depositor EDS
% Data completeness (in resolution range)	99.4 (69.18-2.43) 96.5 (69.18-2.43)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 2.42Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.213 , 0.289 0.215 , 0.290	Depositor DCC
R_{free} test set	2000 reflections (5.20%)	wwPDB-VP
Wilson B-factor (Å ²)	33.8	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6821	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.21% 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: 40L

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	0/6706	0.59	1/9047 (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	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	907	LEU	CA-CB-CG	5.10	127.03	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	528	LYS	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	137	0
2	A	31	0	18	1	0
3	A	224	0	0	18	0
All	All	6821	0	6575	137	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 10.

All (137) 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:511:LEU:HB2	1:A:514:ILE:HD11	1.44	0.97
1:A:245:GLY:HA3	1:A:768:ALA:HB2	1.54	0.89
1:A:942:ILE:O	1:A:955:ARG:NH2	2.06	0.88
1:A:918:ASN:O	3:A:1413:HOH:O	1.96	0.82
1:A:328:ILE:HG22	1:A:329:GLU:HG3	1.61	0.82
1:A:333:VAL:O	1:A:334:ASN:ND2	2.16	0.79
1:A:389:ARG:NH2	1:A:623:SER:OG	2.17	0.77
1:A:1018:LYS:NZ	3:A:1340:HOH:O	2.17	0.74
1:A:452:LEU:N	3:A:1360:HOH:O	2.20	0.74
1:A:383:ASP:OD1	1:A:558:HIS:ND1	2.20	0.74
1:A:929:ARG:N	3:A:1297:HOH:O	2.22	0.73
1:A:235:GLN:N	3:A:1346:HOH:O	2.21	0.72
1:A:344:GLN:HB3	1:A:453:LEU:HD11	1.70	0.72
1:A:955:ARG:HG3	1:A:956:PHE:N	2.06	0.70
1:A:246:ARG:NH1	1:A:248:GLU:OE1	2.24	0.70
1:A:1007:THR:HG23	1:A:1010:GLU:H	1.58	0.69
1:A:255:PRO:HG2	1:A:258:HIS:CD2	2.28	0.69
1:A:389:ARG:NH1	3:A:1400:HOH:O	2.03	0.69
1:A:1014:HIS:NE2	3:A:1340:HOH:O	2.25	0.68
1:A:386:ARG:HG3	1:A:387:MET:HE2	1.76	0.68
1:A:329:GLU:HG2	1:A:370:VAL:HG22	1.75	0.67
1:A:512:ARG:NH1	1:A:534:MET:SD	2.67	0.67
1:A:255:PRO:HG2	1:A:258:HIS:HD2	1.58	0.66
1:A:806:LEU:HD22	1:A:962:ARG:HG2	1.77	0.66
1:A:383:ASP:OD2	3:A:1420:HOH:O	2.13	0.66
1:A:530:LEU:O	1:A:534:MET:HB2	1.95	0.66
1:A:876:THR:HG21	1:A:955:ARG:HD2	1.79	0.65
1:A:455:PRO:O	3:A:1400:HOH:O	2.14	0.65
1:A:332:LYS:HB2	1:A:469:ALA:HA	1.79	0.64
1:A:435:GLY:N	1:A:475:LEU:O	2.30	0.64
1:A:421:ALA:HB2	1:A:441:MET:HG2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:754:SER:HB3	1:A:755:LYS:HE3	1.82	0.61
1:A:324:SER:HB3	1:A:376:GLU:HG3	1.83	0.61
1:A:916:LEU:HD22	1:A:997:TYR:HB3	1.83	0.60
1:A:843:ASN:ND2	3:A:1203:HOH:O	2.32	0.59
1:A:834:ILE:HG23	1:A:855:LEU:HD11	1.83	0.59
1:A:561:VAL:HG23	3:A:1410:HOH:O	2.02	0.59
1:A:988:GLU:OE1	1:A:988:GLU:N	2.35	0.58
1:A:554:LYS:O	3:A:1410:HOH:O	2.17	0.58
1:A:707:THR:OG1	1:A:709:PRO:HD2	2.03	0.57
1:A:952:LYS:HD2	1:A:955:ARG:NE	2.20	0.57
1:A:114:ASN:OD1	1:A:673:ARG:NH2	2.32	0.56
1:A:982:ARG:HH11	1:A:995:ILE:HD12	1.70	0.56
1:A:242:GLN:HB2	1:A:249:TYR:CE2	2.42	0.55
1:A:427:ASP:OD2	1:A:429:LYS:HB2	2.07	0.55
1:A:549:LEU:HG	1:A:564:MET:HE3	1.89	0.54
1:A:955:ARG:HG3	1:A:956:PHE:H	1.73	0.53
1:A:152:ALA:HB3	3:A:1260:HOH:O	2.07	0.53
1:A:621:TYR:CZ	1:A:983:ALA:HB2	2.43	0.53
1:A:193:ASN:ND2	1:A:202:SER:OG	2.37	0.53
1:A:673:ARG:NH1	3:A:1259:HOH:O	2.41	0.53
1:A:536:HIS:O	1:A:540:GLU:HG2	2.09	0.53
1:A:347:LEU:HD12	1:A:379:ILE:HG21	1.90	0.53
1:A:528:LYS:O	1:A:531:VAL:N	2.43	0.52
1:A:348:PHE:HE2	1:A:453:LEU:HD23	1.74	0.52
1:A:109:VAL:HG12	1:A:110:LYS:H	1.74	0.52
1:A:452:LEU:N	3:A:1421:HOH:O	2.43	0.52
1:A:876:THR:OG1	1:A:955:ARG:NH1	2.43	0.52
1:A:1017:VAL:O	1:A:1021:GLU:HG3	2.11	0.51
1:A:526:HIS:O	3:A:1399:HOH:O	2.19	0.51
1:A:583:LEU:HD11	1:A:600:LEU:HD11	1.93	0.51
1:A:982:ARG:HD2	1:A:995:ILE:HD11	1.92	0.51
1:A:558:HIS:CD2	1:A:559:GLU:HG3	2.46	0.51
1:A:808:LEU:HA	1:A:877:LEU:HB3	1.93	0.51
1:A:952:LYS:HD2	1:A:955:ARG:CZ	2.41	0.51
1:A:702:SER:OG	1:A:711:THR:HG22	2.11	0.50
1:A:227:VAL:HG12	1:A:228:PHE:CD2	2.47	0.50
1:A:419:ALA:HB1	1:A:441:MET:HB3	1.94	0.50
1:A:1008:GLU:H	1:A:1008:GLU:CD	2.16	0.49
1:A:852:LYS:HG3	1:A:940:HIS:CE1	2.48	0.49
1:A:753:ASP:OD1	1:A:757:LYS:HE2	2.12	0.49
1:A:319:LEU:HD11	1:A:483:VAL:HG11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:SER:HB3	1:A:124:GLY:HA2	1.95	0.49
1:A:511:LEU:O	1:A:511:LEU:HD12	2.12	0.48
1:A:796:LEU:O	1:A:800:LEU:HG	2.14	0.48
1:A:975:LEU:HD21	1:A:999:LYS:HG3	1.95	0.48
1:A:870:ARG:O	1:A:874:GLU:HG2	2.14	0.48
1:A:516:GLU:N	1:A:516:GLU:OE1	2.47	0.47
1:A:609:PHE:HE1	1:A:646:PHE:CD2	2.31	0.47
1:A:750:THR:OG1	1:A:751:PHE:N	2.45	0.47
1:A:952:LYS:HA	1:A:955:ARG:HG2	1.95	0.47
1:A:341:LEU:HG	1:A:365:VAL:HA	1.97	0.47
1:A:367:SER:HA	1:A:368:GLU:HB2	1.97	0.46
1:A:555:TRP:CE3	1:A:561:VAL:HG22	2.50	0.46
1:A:687:GLU:OE1	3:A:1254:HOH:O	2.20	0.46
1:A:972:LEU:O	1:A:976:HIS:ND1	2.48	0.46
1:A:427:ASP:CG	1:A:429:LYS:H	2.18	0.46
1:A:225:ALA:O	1:A:229:ARG:N	2.48	0.46
1:A:914:HIS:O	1:A:915:PHE:CG	2.69	0.46
1:A:213:PRO:HD3	1:A:254:TYR:O	2.16	0.46
1:A:316:LEU:HD23	1:A:317:TRP:N	2.30	0.46
1:A:703:SER:HA	1:A:711:THR:HG21	1.97	0.46
1:A:793:MET:O	1:A:797:MET:HG3	2.16	0.45
1:A:907:LEU:HD23	1:A:908:PHE:N	2.31	0.45
1:A:316:LEU:HD23	1:A:318:SER:H	1.80	0.45
1:A:426:PHE:CZ	1:A:432:LEU:HD13	2.51	0.45
1:A:255:PRO:CG	1:A:258:HIS:HD2	2.28	0.45
1:A:374:ARG:HH11	1:A:374:ARG:HG3	1.81	0.45
1:A:637:ALA:HB1	1:A:644:GLY:HA2	1.99	0.45
1:A:335:ALA:C	1:A:365:VAL:HG11	2.37	0.44
1:A:952:LYS:HB3	1:A:955:ARG:HH21	1.83	0.44
1:A:139:PHE:CZ	1:A:143:MET:HG3	2.52	0.44
1:A:1022:ALA:C	1:A:1024:ARG:H	2.19	0.44
1:A:245:GLY:HA3	1:A:768:ALA:CB	2.35	0.44
1:A:991:CYS:HB2	1:A:993:LYS:H	1.81	0.44
1:A:367:SER:HB2	1:A:368:GLU:C	2.37	0.44
1:A:786:GLN:HB2	3:A:1232:HOH:O	2.18	0.44
1:A:581:GLU:HB2	1:A:976:HIS:CD2	2.53	0.44
1:A:239:TYR:CG	1:A:276:MET:HE3	2.53	0.43
1:A:758:PRO:HB2	2:A:1101:40L:H10	2.00	0.43
1:A:383:ASP:HB3	1:A:556:ASN:O	2.18	0.43
1:A:285:MET:O	1:A:289:GLN:HG3	2.19	0.43
1:A:331:ARG:O	1:A:332:LYS:HD2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:663:ARG:O	1:A:667:ILE:HG13	2.19	0.43
1:A:123:LYS:HE3	1:A:123:LYS:HB2	1.80	0.43
1:A:190:LEU:HD12	1:A:191:LEU:O	2.19	0.43
1:A:475:LEU:HA	1:A:476:PRO:HD3	1.79	0.43
1:A:426:PHE:CE2	1:A:432:LEU:HD13	2.54	0.43
1:A:982:ARG:HD2	1:A:995:ILE:CD1	2.49	0.43
1:A:632:PHE:O	1:A:636:ARG:HG2	2.19	0.42
1:A:242:GLN:HG2	1:A:243:VAL:O	2.18	0.42
1:A:432:LEU:HB3	1:A:483:VAL:HG23	2.00	0.42
1:A:247:HIS:HB2	1:A:738:SER:HA	2.01	0.42
1:A:366:CYS:O	1:A:367:SER:OG	2.17	0.42
1:A:425:LEU:HD23	1:A:425:LEU:HA	1.84	0.42
1:A:756:MET:HE2	1:A:781:GLY:HA3	2.02	0.42
1:A:895:HIS:CE1	1:A:897:ASP:HB2	2.55	0.41
1:A:952:LYS:O	1:A:955:ARG:HG2	2.19	0.41
1:A:466:GLU:HG2	1:A:467:SER:N	2.35	0.41
1:A:691:LYS:HG3	1:A:724:TYR:CE2	2.56	0.41
1:A:199:SER:OG	1:A:201:GLU:N	2.53	0.41
1:A:708:LYS:HB3	1:A:709:PRO:HD3	2.03	0.41
1:A:420:TRP:CE2	1:A:442:TRP:HB2	2.56	0.41
1:A:513:GLU:HG2	1:A:542:PHE:CZ	2.55	0.41
1:A:842:SER:O	1:A:844:MET:HG2	2.21	0.40
1:A:852:LYS:HG3	1:A:940:HIS:HE1	1.85	0.40
1:A:340:LYS:HD3	1:A:362:GLU:OE1	2.21	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%)	745 (94%)	35 (4%)	13 (2%)	9 8

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	372	LYS
1	A	529	ASP
1	A	229	ARG
1	A	755	LYS
1	A	915	PHE
1	A	820	ASP
1	A	943	GLN
1	A	478	VAL
1	A	949	ASN
1	A	319	LEU
1	A	528	LYS
1	A	227	VAL
1	A	328	ILE

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%)	708 (98%)	13 (2%)	59 71

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	SER
1	A	119	LEU
1	A	190	LEU
1	A	209	THR
1	A	344	GLN
1	A	379	ILE
1	A	514	ILE
1	A	537	GLU
1	A	723	THR
1	A	855	LEU
1	A	990	SER
1	A	991	CYS

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Mol	Chain	Res	Type
1	A	998	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	258	HIS
1	A	334	ASN
1	A	344	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	40L	A	1101	-	31,35,35	1.62	7 (22%)	25,50,50	1.70	5 (20%)

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	40L	A	1101	-	-	0/11/14/14	0/5/5/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	40L	C09-C05	4.05	1.48	1.41
2	A	1101	40L	C01-C06	3.19	1.39	1.36
2	A	1101	40L	C23-N28	2.84	1.38	1.34
2	A	1101	40L	C18-C19	2.34	1.54	1.50
2	A	1101	40L	C05-C04	-2.24	1.39	1.42
2	A	1101	40L	C27-N26	2.23	1.35	1.32
2	A	1101	40L	C12-N11	-2.06	1.43	1.45

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	40L	C17-C12-N11	3.90	122.86	119.24
2	A	1101	40L	C01-C06-C05	-3.33	121.48	124.18
2	A	1101	40L	C09-C05-C06	-3.31	122.43	125.89
2	A	1101	40L	N22-C23-N28	2.57	121.96	118.06
2	A	1101	40L	C27-N28-C23	2.39	118.64	116.59

There are no chirality outliers.

There are no torsion outliers.

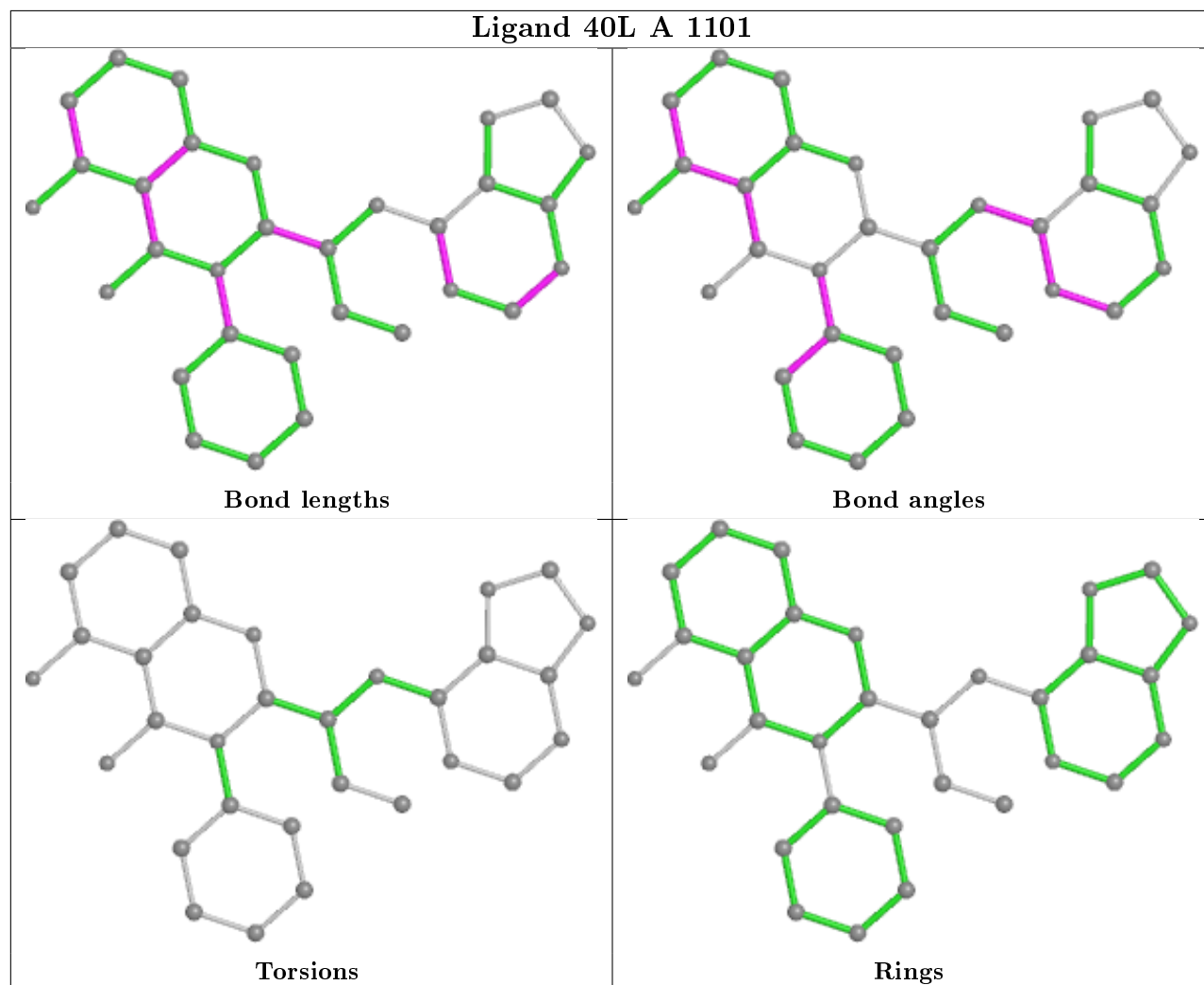
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	40L	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 ⓘ

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%)	0.20	18 (2%) 62 58	20, 39, 63, 84	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	366	CYS	5.3
1	A	317	TRP	4.4
1	A	367	SER	3.6
1	A	363	VAL	3.4
1	A	511	LEU	3.1
1	A	397	VAL	2.7
1	A	936	TYR	2.7
1	A	341	LEU	2.6
1	A	333	VAL	2.5
1	A	205	PHE	2.5
1	A	445	VAL	2.3
1	A	935	THR	2.3
1	A	226	THR	2.3
1	A	492	LEU	2.3
1	A	326	GLU	2.2
1	A	398	VAL	2.2
1	A	334	ASN	2.1
1	A	561	VAL	2.1

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 [i](#)

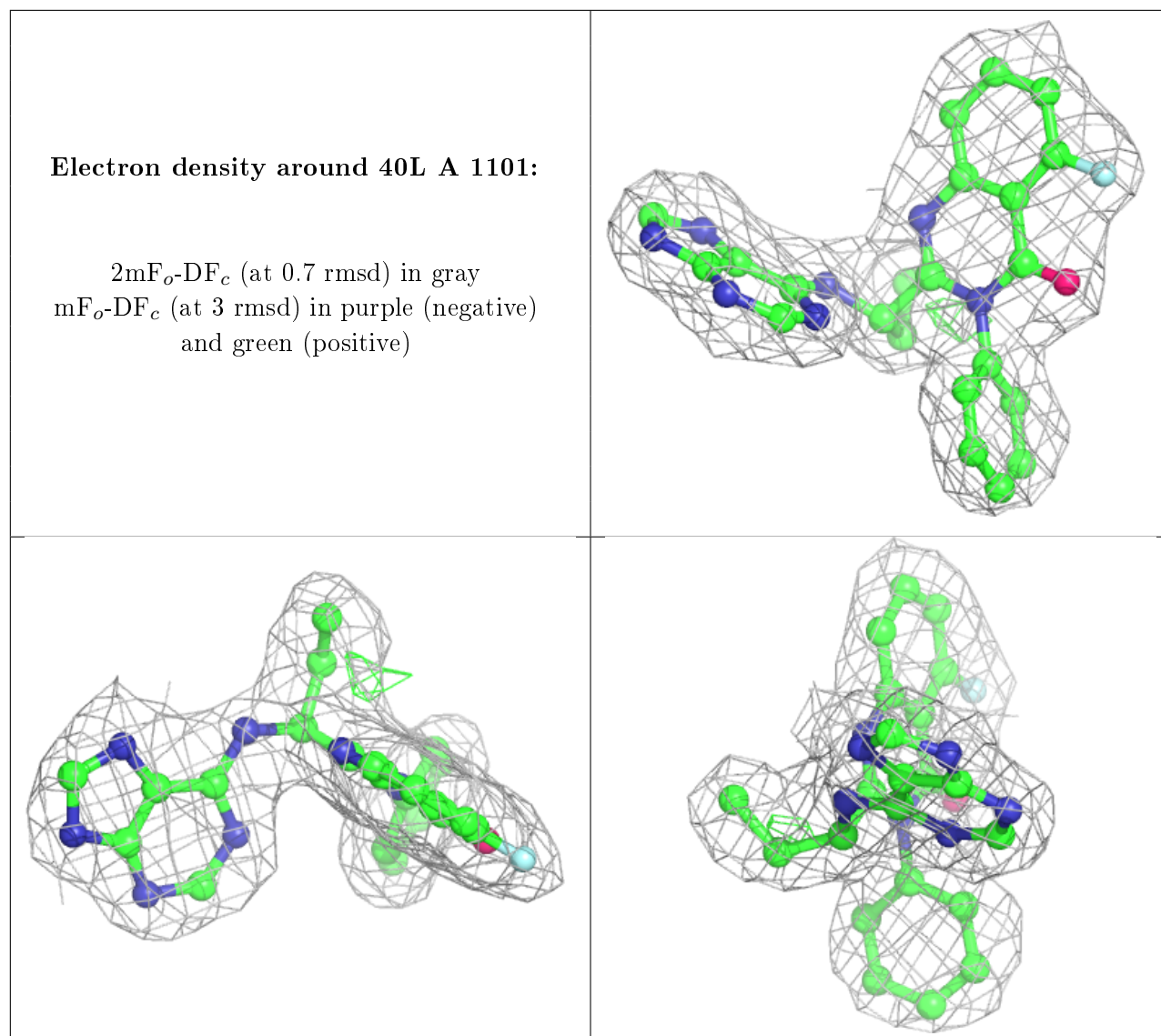
There are no carbohydrates in this entry.

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	40L	A	1101	31/31	0.96	0.16	17,24,29,31	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.