



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:08 AM UTC

PDB ID : 4XE0 / pdb_00004xe0
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 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

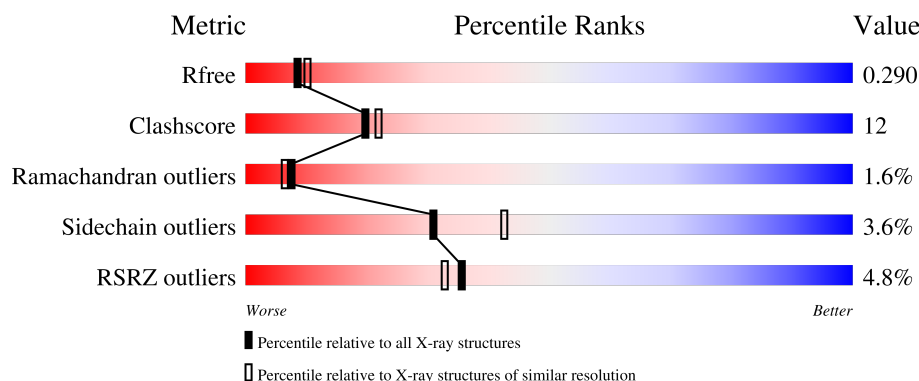
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.43 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}	180053	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (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 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	939	

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.

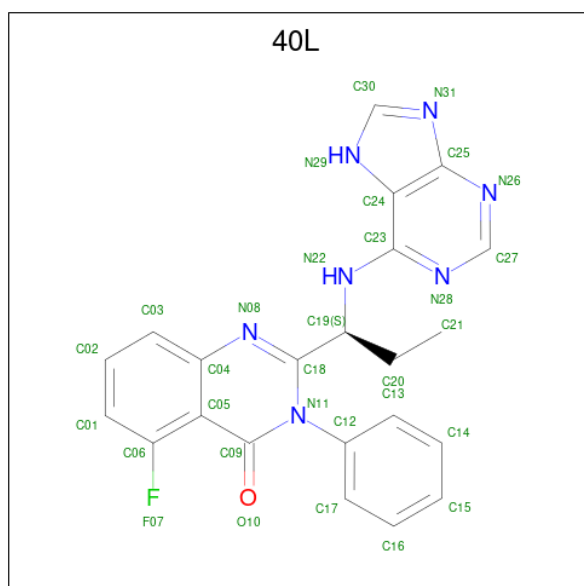
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic sub-unit delta isoform.

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 (CCD ID: 40L) (formula: C₂₂H₁₈FN₇O).



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

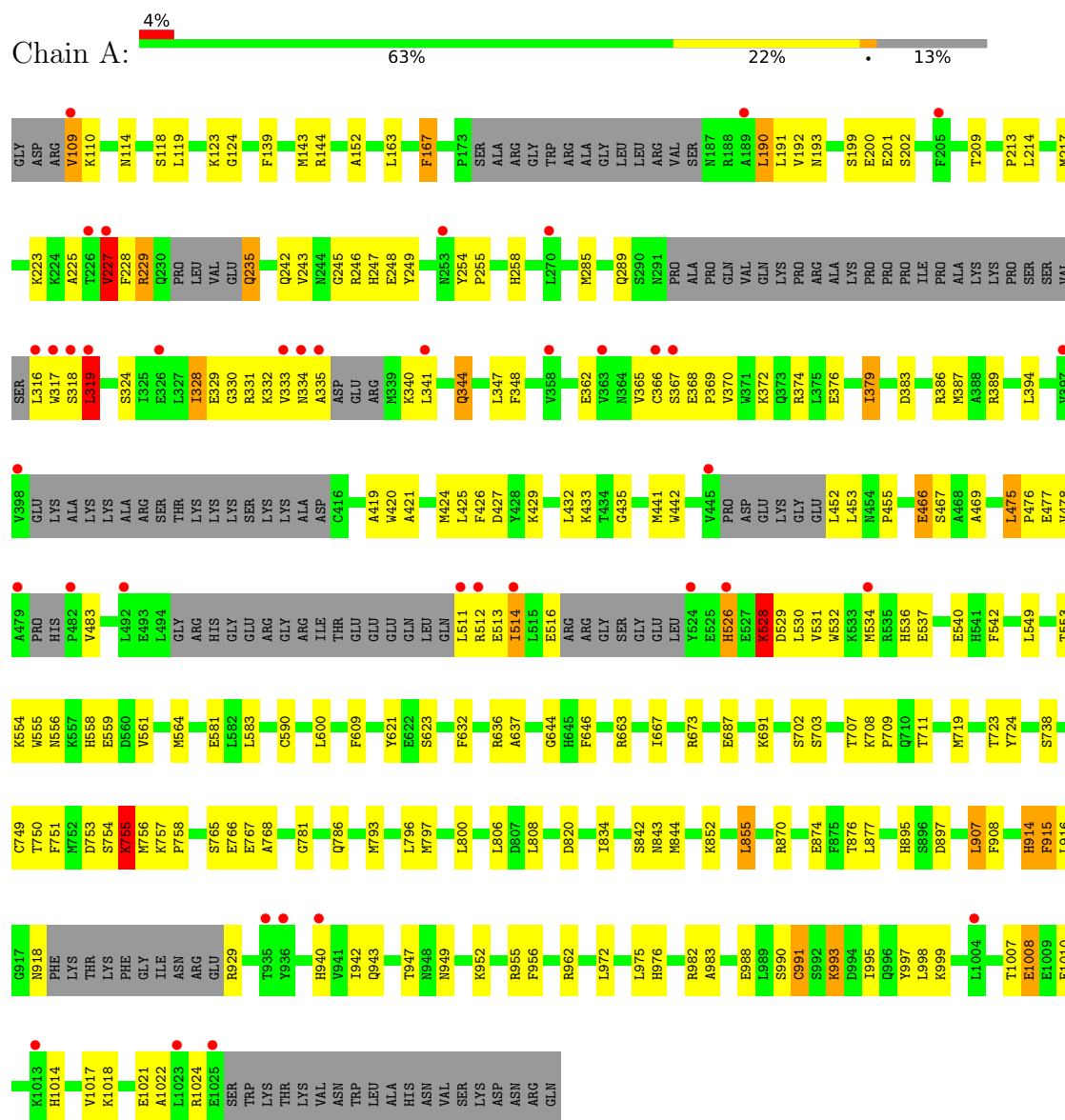
- Molecule 3 is water.

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

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: 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)	0.35 , 47.9	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	0.90	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	0.56	0/6706	0.87	9/9047 (0.1%)

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 (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	235	GLN	CA-C-N	6.65	126.91	119.32
1	A	235	GLN	C-N-CA	6.65	126.91	119.32
1	A	200	GLU	N-CA-C	-5.55	107.15	114.31
1	A	526	HIS	N-CA-C	-5.42	105.89	112.88
1	A	167	PHE	CA-C-N	-5.41	114.20	119.78
1	A	167	PHE	C-N-CA	-5.41	114.20	119.78
1	A	475	LEU	CA-C-N	5.15	125.06	119.76
1	A	475	LEU	C-N-CA	5.15	125.06	119.76
1	A	914	HIS	N-CA-C	5.10	121.65	110.80

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	152	0
2	A	31	0	18	1	0
3	A	224	0	0	21	0
All	All	6821	0	6575	152	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 (152) 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:756:MET:HE2	1:A:781:GLY:HA3	1.55	0.85
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: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:386:ARG:HG3	1:A:387:MET:HE2	1.69	0.73
1:A:929:ARG:N	3:A:1297:HOH:O	2.22	0.73
1:A:1018:LYS:NZ	3:A:1340:HOH:O	2.17	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:246:ARG:NH1	1:A:248:GLU:OE1	2.24	0.70
1:A:955:ARG:HG3	1:A:956:PHE:N	2.06	0.70
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:1007:THR:HG23	1:A:1010:GLU:H	1.58	0.69
1:A:1014:HIS:NE2	3:A:1340:HOH:O	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:167:PHE:HZ	1:A:285:MET:HE1	1.66	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:N	1:A:988:GLU:OE1	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:143:MET:HA	1:A:143:MET:HE2	1.87	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:553:THR:OG1	1:A:564:MET:HE3	2.05	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:HE1	1.88	0.55
1:A:755:LYS:NZ	3:A:1329:HOH:O	2.19	0.54
1:A:1008:GLU:H	1:A:1008:GLU:CD	2.16	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:214:LEU:HA	1:A:217:MET:HE3	1.89	0.53
1:A:193:ASN:ND2	1:A:202:SER:OG	2.37	0.53
1:A:387:MET:HE3	1:A:590:CYS:SG	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:876:THR:OG1	1:A:955:ARG:NH1	2.43	0.52
1:A:427:ASP:CG	1:A:429:LYS:H	2.18	0.51
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:1022:ALA:C	1:A:1024:ARG:H	2.19	0.50
1:A:419:ALA:HB1	1:A:441:MET:HB3	1.94	0.50
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
1:A:335:ALA:C	1:A:365:VAL:HG11	2.37	0.49
1:A:118:SER:HB3	1:A:124:GLY:HA2	1.95	0.49
1:A:367:SER:HB2	1:A:368:GLU:C	2.37	0.49
1:A:511:LEU:O	1:A:511:LEU:HD12	2.12	0.48
1:A:433:LYS:NZ	3:A:1292:HOH:O	2.29	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:394:LEU:HD22	1:A:441:MET:HE1	1.94	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:549:LEU:CG	1:A:564:MET:HE1	2.46	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: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:719:MET:HE1	1:A:749:CYS:SG	2.58	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: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: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
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:110:LYS:HZ1	1:A:144:ARG:HH12	1.66	0.42
1:A:895:HIS:CE1	1:A:897:ASP:HB2	2.55	0.41
1:A:532:TRP:HZ3	1:A:564:MET:HE2	1.85	0.41
1:A:952:LYS:O	1:A:955:ARG:HG2	2.19	0.41
1:A:765:SER:C	1:A:767:GLU:H	2.27	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:225:ALA:C	1:A:227:VAL:H	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:MET:HE3	3:A:1358:HOH:O	2.21	0.40
1:A:842:SER:O	1:A:844:MET:HG2	2.21	0.40
1:A:330:GLY:C	1:A:369:PRO:HD2	2.46	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%)	7 6

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%)	695 (96%)	26 (4%)	31	42

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	VAL
1	A	119	LEU
1	A	163	LEU
1	A	190	LEU
1	A	192	VAL
1	A	209	THR
1	A	223	LYS
1	A	227	VAL
1	A	319	LEU
1	A	344	GLN
1	A	379	ILE
1	A	466	GLU
1	A	477	GLU
1	A	514	ILE
1	A	537	GLU
1	A	723	THR
1	A	755	LYS
1	A	766	GLU
1	A	855	LEU
1	A	907	LEU
1	A	947	THR
1	A	990	SER
1	A	991	CYS
1	A	993	LYS
1	A	998	LEU
1	A	1008	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	155	GLN
1	A	258	HIS
1	A	334	ASN
1	A	344	GLN
1	A	526	HIS
1	A	721	GLN
1	A	780	ASN
1	A	795	GLN
1	A	918	ASN

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 oligosaccharides 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	-	35,35,35	1.02	1 (2%)	42,50,50	2.42	12 (28%)

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	-	-	0/10/14/14	0/5/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	40L	C19-C18	2.65	1.54	1.51

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	40L	C25-C24-N29	8.54	111.02	105.28
2	A	1101	40L	C24-C25-N31	-6.90	104.97	110.46
2	A	1101	40L	C25-N31-C30	5.13	107.11	103.84
2	A	1101	40L	C24-C25-N26	4.20	127.86	124.21
2	A	1101	40L	N22-C23-N28	2.79	121.96	118.00
2	A	1101	40L	C23-C24-N29	-2.72	131.26	135.17
2	A	1101	40L	C17-C12-N11	2.68	122.86	119.65
2	A	1101	40L	C24-N29-C30	-2.64	104.05	106.27
2	A	1101	40L	O10-C09-N11	2.57	123.80	120.38
2	A	1101	40L	C23-N22-C19	-2.54	117.47	122.92
2	A	1101	40L	C04-N08-C18	2.44	120.83	117.46
2	A	1101	40L	O10-C09-C05	-2.13	119.78	124.19

There are no chirality outliers.

There are no torsion outliers.

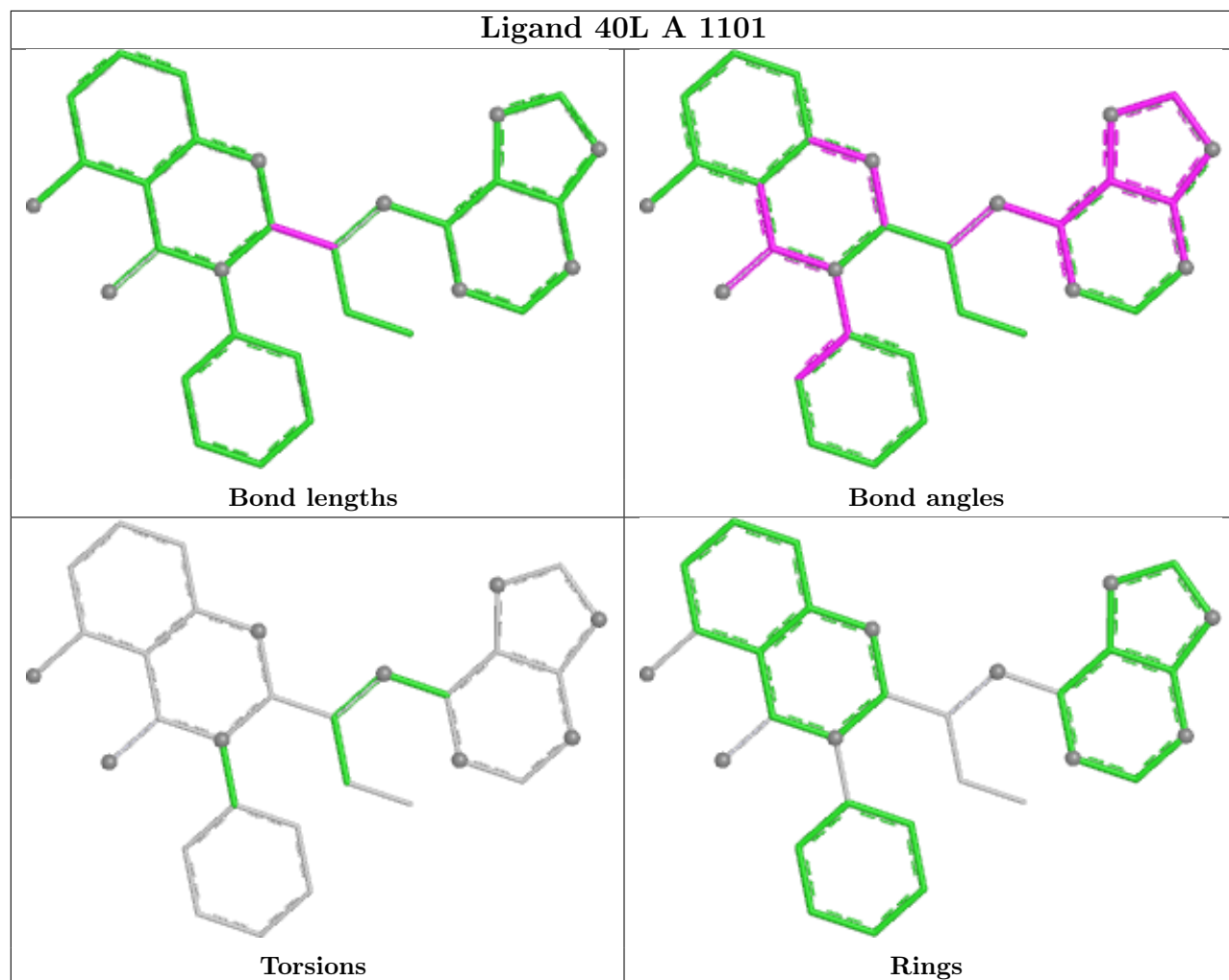
There are no ring outliers.

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%)	0.36	39 (4%) 35 33	20, 39, 63, 84	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	366	CYS	6.0
1	A	511	LEU	5.7
1	A	445	VAL	4.3
1	A	398	VAL	4.2
1	A	335	ALA	4.1
1	A	317	TRP	4.0
1	A	316	LEU	3.6
1	A	333	VAL	3.5
1	A	482	PRO	3.3
1	A	109	VAL	3.2
1	A	479	ALA	3.2
1	A	363	VAL	3.1
1	A	205	PHE	3.1
1	A	334	ASN	3.0
1	A	514	ILE	2.9
1	A	227	VAL	2.8
1	A	253	ASN	2.7
1	A	940	HIS	2.7
1	A	512	ARG	2.7
1	A	936	TYR	2.7
1	A	367	SER	2.5
1	A	341	LEU	2.5
1	A	318	SER	2.5
1	A	358	VAL	2.5
1	A	524	TYR	2.4
1	A	492	LEU	2.4
1	A	1013	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	226	THR	2.4
1	A	1004	LEU	2.3
1	A	1025	GLU	2.3
1	A	319	LEU	2.3
1	A	935	THR	2.3
1	A	189	ALA	2.2
1	A	270	LEU	2.2
1	A	397	VAL	2.1
1	A	526	HIS	2.1
1	A	534	MET	2.1
1	A	326	GLU	2.1
1	A	1023	LEU	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](#)

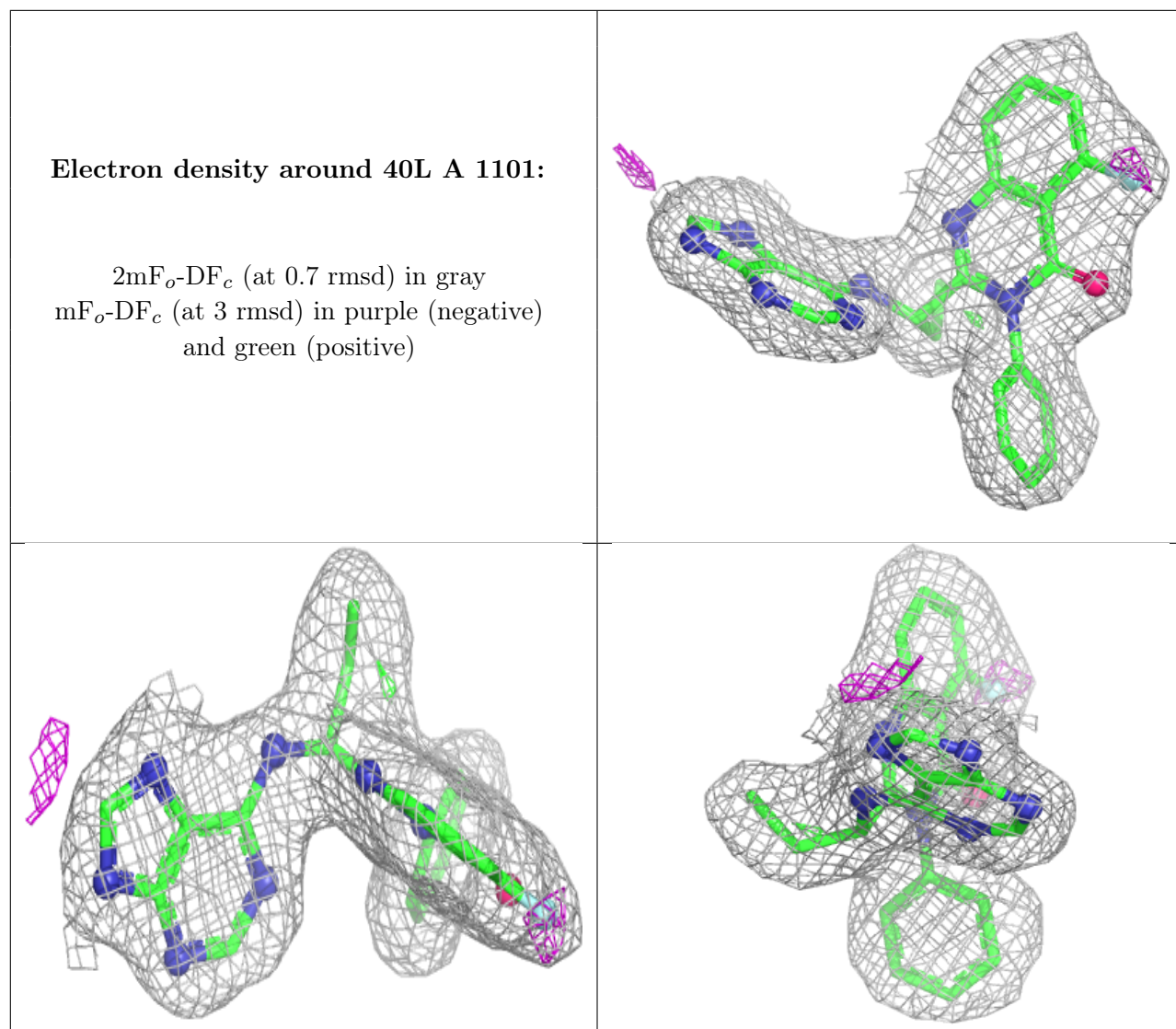
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
2	40L	A	1101	31/31	0.95	0.07	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 ⓘ

There are no such residues in this entry.