



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:06 AM UTC

PDB ID : 6EYZ / pdb_00006eyz
Title : PI3 kinase delta in complex with 4-Fluorophenyl 5-(4-(5-((4-isopropylpiperazin-1-yl)methyl)oxazol-2-yl)-1H-indazol-6-yl)-2-methoxynicotinate
Authors : Convery, M.A.; Campos, S.; Dalton, S.E.
Deposited on : 2017-11-13
Resolution : 2.20 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

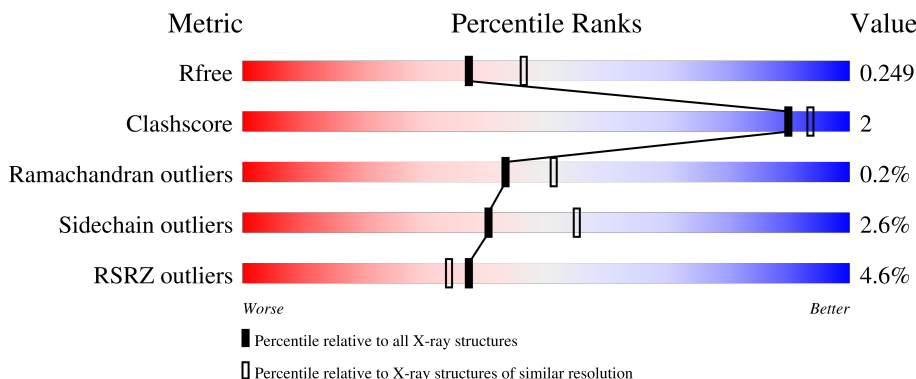
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	1051	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7281 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.

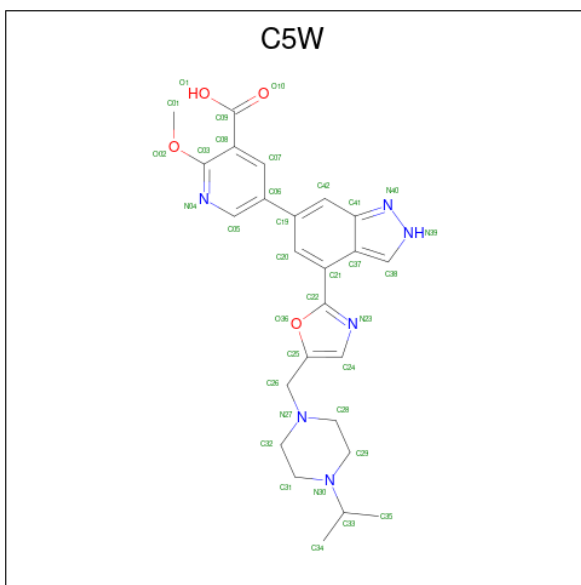
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic sub-unit delta isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	862	Total	C	N	O	S	0	0	0
			6940	4434	1190	1262	54			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	99	GLU	-	insertion	UNP Q3UDT3
A	100	ASN	-	insertion	UNP Q3UDT3
A	101	LEU	-	insertion	UNP Q3UDT3
A	102	TYR	-	insertion	UNP Q3UDT3
A	103	PHE	-	insertion	UNP Q3UDT3
A	104	GLN	-	insertion	UNP Q3UDT3
A	105	GLY	-	insertion	UNP Q3UDT3

- Molecule 2 is 2-methoxy-5-[4-[5-[(4-propan-2-ylpiperazin-1-yl)methyl]-1,3-oxazol-2-yl]-2 {H}-indazol-6-yl]pyridine-3-carboxylic acid (CCD ID: C5W) (formula: C₂₅H₂₈N₆O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			34	25	6	3		

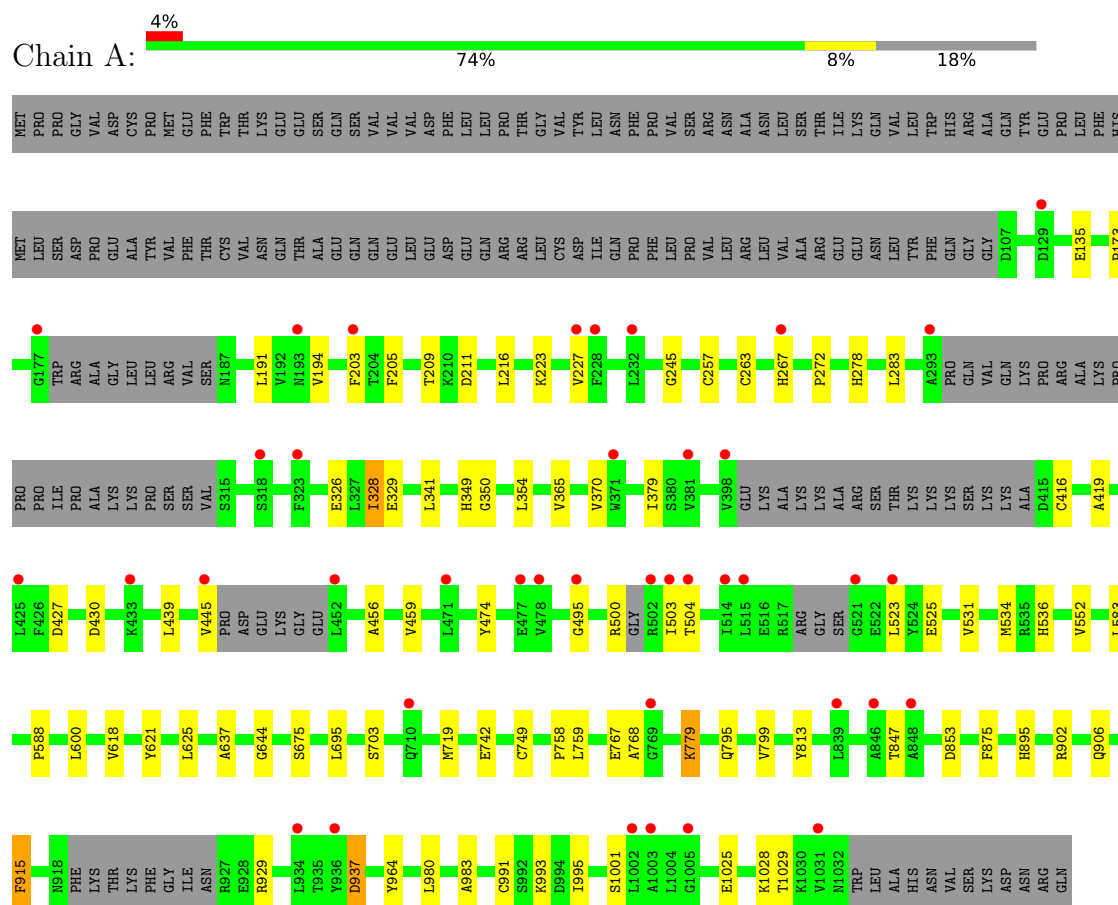
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	307	Total O 307 307	0	0

3 Residue-property plots [i](#)

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	141.83Å 64.58Å 116.41Å 90.00° 102.29° 90.00°	Depositor
Resolution (Å)	54.06 – 2.20 54.06 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.5 (54.06-2.20) 98.5 (54.06-2.20)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 2.20Å)	Xtriage
Refinement program	BUSTER 2.11.6	Depositor
R, R_{free}	0.190 , 0.237 0.203 , 0.249	Depositor DCC
R_{free} test set	2577 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	47.9	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 61.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7281	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.35% 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: C5W

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	0.88	0/7090	1.35	35/9571 (0.4%)

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	915	PHE	CA-CB-CG	8.48	122.28	113.80
1	A	853	ASP	CA-CB-CG	7.92	120.52	112.60
1	A	937	ASP	CA-CB-CG	6.10	118.70	112.60
1	A	427	ASP	CA-CB-CG	5.90	118.50	112.60
1	A	1028	LYS	N-CA-C	-5.86	105.62	112.89
1	A	742	GLU	CB-CG-CD	5.74	122.36	112.60
1	A	263	CYS	CA-C-N	5.62	127.82	120.28
1	A	263	CYS	C-N-CA	5.62	127.82	120.28
1	A	456	ALA	CA-C-N	5.59	125.41	120.10
1	A	456	ALA	C-N-CA	5.59	125.41	120.10
1	A	964	TYR	CA-C-N	5.49	127.58	120.44
1	A	964	TYR	C-N-CA	5.49	127.58	120.44
1	A	223	LYS	CA-C-N	5.46	127.59	120.28
1	A	223	LYS	C-N-CA	5.46	127.59	120.28
1	A	875	PHE	CA-C-N	5.38	127.75	120.44
1	A	875	PHE	C-N-CA	5.38	127.75	120.44
1	A	675	SER	CA-C-N	5.27	127.29	120.44
1	A	675	SER	C-N-CA	5.27	127.29	120.44
1	A	205	PHE	CA-CB-CG	5.25	119.05	113.80
1	A	534	MET	CA-C-N	5.23	127.55	120.38
1	A	534	MET	C-N-CA	5.23	127.55	120.38
1	A	419	ALA	N-CA-C	5.19	115.91	108.74
1	A	329	GLU	CA-C-N	5.17	126.11	122.33
1	A	329	GLU	C-N-CA	5.17	126.11	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	813	TYR	CA-C-N	5.17	124.88	119.92
1	A	813	TYR	C-N-CA	5.17	124.88	119.92
1	A	211	ASP	CA-CB-CG	5.12	117.72	112.60
1	A	278	HIS	CA-C-N	5.11	127.38	120.38
1	A	278	HIS	C-N-CA	5.11	127.38	120.38
1	A	495	GLY	CA-C-N	5.07	127.58	120.28
1	A	495	GLY	C-N-CA	5.07	127.58	120.28
1	A	1025	GLU	CA-C-N	5.05	127.56	120.28
1	A	1025	GLU	C-N-CA	5.05	127.56	120.28
1	A	504	THR	CA-C-N	5.05	127.76	120.38
1	A	504	THR	C-N-CA	5.05	127.76	120.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6940	0	6910	25	0
2	A	34	0	0	0	0
3	A	307	0	0	1	0
All	All	7281	0	6910	25	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 2.

All (25) 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:350:GLY:HA3	1:A:588:PRO:HG3	1.79	0.65
1:A:531:VAL:HG13	1:A:552:VAL:HG21	1.81	0.61
1:A:349:HIS:HB2	1:A:354:LEU:HD21	1.84	0.58
1:A:341:LEU:HG	1:A:365:VAL:HG22	1.85	0.58
1:A:719:MET:HE1	1:A:749:CYS:SG	2.46	0.56
1:A:929:ARG:HH22	1:A:1001:SER:HA	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:583:LEU:HD11	1:A:600:LEU:HD11	1.91	0.53
1:A:695:LEU:HD23	1:A:759:LEU:HD13	1.90	0.53
1:A:328:ILE:HD11	1:A:474:TYR:HB2	1.92	0.52
1:A:703:SER:HA	3:A:1331:HOH:O	2.11	0.50
1:A:902:ARG:HD3	1:A:906:GLN:HB2	1.93	0.50
1:A:209:THR:HB	1:A:257:CYS:HB3	1.96	0.47
1:A:618:VAL:HG11	1:A:980:LEU:HD22	1.98	0.46
1:A:500:ARG:HE	1:A:536:HIS:HB3	1.82	0.45
1:A:621:TYR:CZ	1:A:983:ALA:HB2	2.52	0.44
1:A:991:CYS:SG	1:A:993:LYS:HG2	2.57	0.44
1:A:758:PRO:HB3	1:A:779:LYS:HG2	2.00	0.44
1:A:637:ALA:HB1	1:A:644:GLY:HA2	2.00	0.43
1:A:191:LEU:O	1:A:272:PRO:HD2	2.19	0.42
1:A:135:GLU:HG2	1:A:625:LEU:HD12	2.01	0.41
1:A:326:GLU:HB3	1:A:474:TYR:HB3	2.01	0.41
1:A:245:GLY:HA3	1:A:768:ALA:HB2	2.02	0.41
1:A:194:VAL:HG21	1:A:216:LEU:HD21	2.01	0.41
1:A:203:PHE:HE1	1:A:227:VAL:HG21	1.86	0.40
1:A:173:PRO:HB3	1:A:799:VAL:HG13	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	846/1051 (80%)	823 (97%)	21 (2%)	2 (0%)	43 51

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	328	ILE
1	A	379	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	760/931 (82%)	740 (97%)	20 (3%)	40 55

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	267	HIS
1	A	283	LEU
1	A	370	VAL
1	A	416	CYS
1	A	430	ASP
1	A	439	LEU
1	A	445	VAL
1	A	459	VAL
1	A	503	ILE
1	A	523	LEU
1	A	525	GLU
1	A	767	GLU
1	A	779	LYS
1	A	795	GLN
1	A	847	THR
1	A	895	HIS
1	A	915	PHE
1	A	937	ASP
1	A	995	ILE
1	A	1029	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	GLN
1	A	126	HIS
1	A	193	ASN
1	A	230	GLN
1	A	289	GLN

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Mol	Chain	Res	Type
1	A	344	GLN
1	A	364	ASN
1	A	422	ASN
1	A	481	HIS
1	A	610	GLN
1	A	721	GLN
1	A	773	ASN
1	A	780	ASN
1	A	792	GLN
1	A	996	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	C5W	A	1101	1	37,38,39	0.90	2 (5%)	48,54,56	1.31	5 (10%)

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	C5W	A	1101	1	-	4/20/30/32	0/5/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	C5W	C41-N40	3.81	1.38	1.33
2	A	1101	C5W	C21-C37	-2.52	1.40	1.44

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	C5W	C38-N39-N40	-4.02	106.43	112.59
2	A	1101	C5W	C37-C38-N39	3.80	110.90	107.05
2	A	1101	C5W	C19-C42-C41	-3.21	118.36	121.42
2	A	1101	C5W	C41-N40-N39	2.99	111.61	105.24
2	A	1101	C5W	C31-N30-C33	-2.29	109.35	113.01

There are no chirality outliers.

All (4) torsion outliers are listed below:

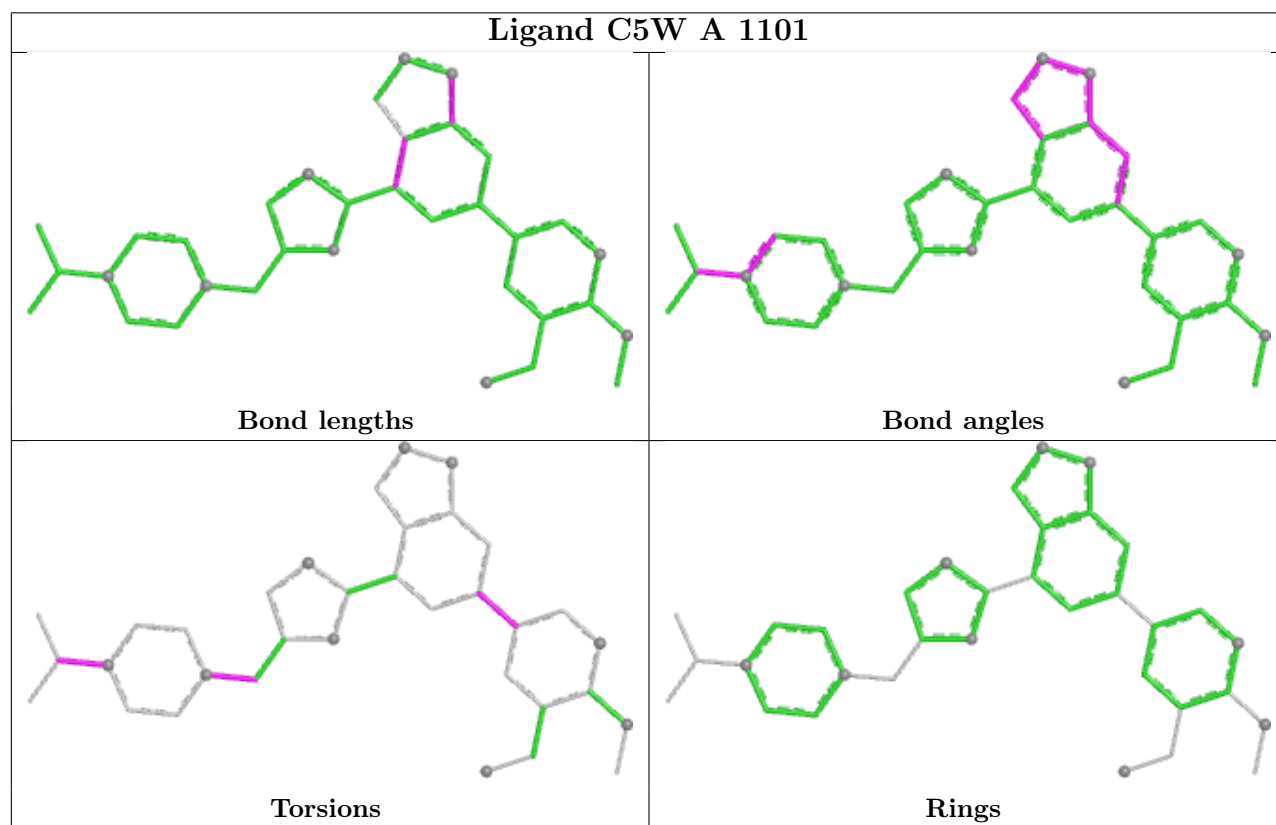
Mol	Chain	Res	Type	Atoms
2	A	1101	C5W	C25-C26-N27-C32
2	A	1101	C5W	C34-C33-N30-C29
2	A	1101	C5W	C07-C06-C19-C20
2	A	1101	C5W	C07-C06-C19-C42

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	862/1051 (82%)	0.46	40 (4%)	37 34	35, 64, 111, 177	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	445	VAL	3.8
1	A	502	ARG	3.7
1	A	452	LEU	3.5
1	A	936	TYR	3.2
1	A	381	VAL	3.1
1	A	293	ALA	3.1
1	A	523	LEU	3.1
1	A	398	VAL	3.0
1	A	227	VAL	2.9
1	A	1031	VAL	2.9
1	A	323	PHE	2.9
1	A	846	ALA	2.9
1	A	177	GLY	2.8
1	A	521	GLY	2.7
1	A	371	TRP	2.7
1	A	193	ASN	2.6
1	A	477	GLU	2.6
1	A	471	LEU	2.6
1	A	710	GLN	2.6
1	A	129	ASP	2.6
1	A	839	LEU	2.5
1	A	503	ILE	2.5
1	A	515	LEU	2.5
1	A	203	PHE	2.4
1	A	228	PHE	2.4
1	A	1003	ALA	2.4
1	A	504	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	1002	LEU	2.3
1	A	769	GLY	2.3
1	A	514	ILE	2.3
1	A	934	LEU	2.2
1	A	1005	GLY	2.2
1	A	318	SER	2.2
1	A	478	VAL	2.2
1	A	267	HIS	2.1
1	A	495	GLY	2.1
1	A	232	LEU	2.1
1	A	425	LEU	2.1
1	A	848	ALA	2.1
1	A	433	LYS	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](#)

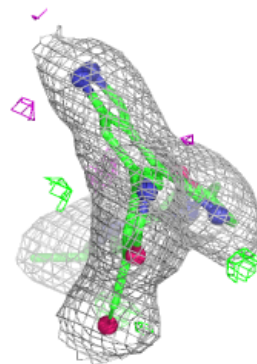
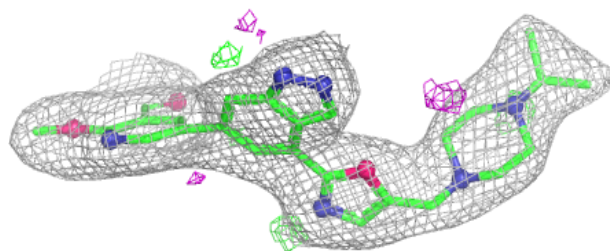
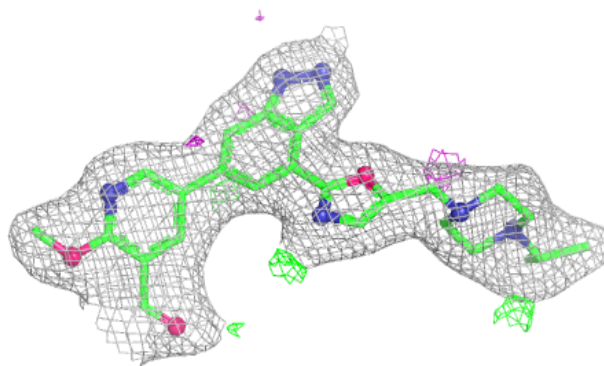
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	C5W	A	1101	34/35	0.95	0.08	30,40,51,52	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around C5W A 1101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.