



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 03:14 am BST

PDB ID : 4EZJ
Title : Potent and Selective Inhibitors of PI3K-delta: Obtaining Isoform Selectivity from the Affinity Pocket and Tryptophan Shelf
Authors : Murray, J.M.
Deposited on : 2012-05-02
Resolution : 2.67 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

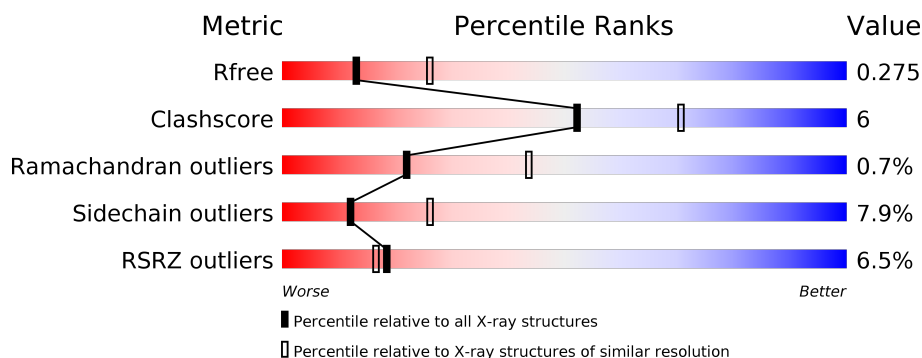
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.67 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	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)

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	966	<div> <div>6%</div> <div> <div></div> <div>70%</div> <div>14%</div> <div>•</div> <div>14%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6831 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.

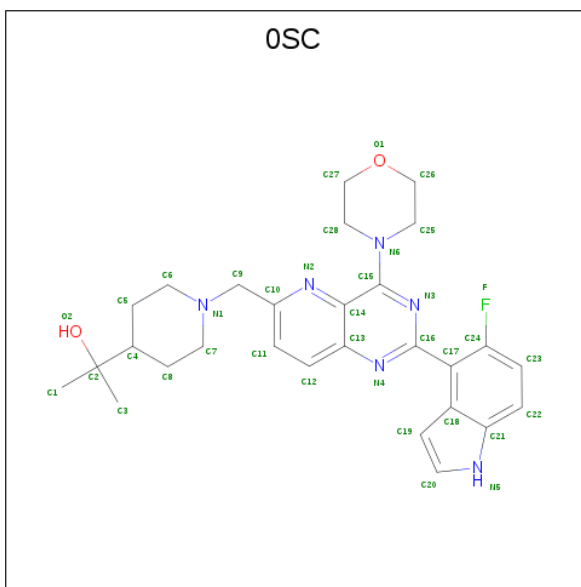
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic sub-unit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	834	Total	C	N	O	S	0	0	0
			6703	4298	1143	1228	34			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	MET	-	EXPRESSION TAG	UNP P48736
A	802	THR	LYS	ENGINEERED MUTATION	UNP P48736
A	1103	HIS	-	EXPRESSION TAG	UNP P48736
A	1104	HIS	-	EXPRESSION TAG	UNP P48736
A	1105	HIS	-	EXPRESSION TAG	UNP P48736
A	1106	HIS	-	EXPRESSION TAG	UNP P48736
A	1107	HIS	-	EXPRESSION TAG	UNP P48736
A	1108	HIS	-	EXPRESSION TAG	UNP P48736

- Molecule 2 is 2-(1-{[2-(5-fluoro-1H-indol-4-yl)-4-(morpholin-4-yl)pyrido[3,2-d]pyrimidin-6-yl]methyl}piperidin-4-yl)propan-2-ol (three-letter code: OSC) (formula: C₂₈H₃₃FN₆O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			37	28	1	6	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	91	Total	O	0	0
			91	91		

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



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	141.20 Å 67.12 Å 104.77 Å 90.00° 97.03° 90.00°	Depositor
Resolution (Å)	32.04 – 2.67 32.04 – 2.67	Depositor EDS
% Data completeness (in resolution range)	98.5 (32.04-2.67) 99.0 (32.04-2.67)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 2.68 Å)	Xtriage
Refinement program	BUSTER-TNT, BUSTER 2.11.2	Depositor
R, R_{free}	0.207 , 0.268 0.226 , 0.275	Depositor DCC
R_{free} test set	1406 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	61.9	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 60.1	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	6831	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.75% 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: 0SC

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	0.51	1/6846 (0.0%)	0.75	8/9271 (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	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	810	PRO	N-CD	5.50	1.55	1.47

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1045	LYS	CB-CA-C	-9.96	90.48	110.40
1	A	1045	LYS	N-CA-C	9.04	135.42	111.00
1	A	809	LYS	N-CA-C	7.21	130.48	111.00
1	A	753	SER	CB-CA-C	-6.58	97.59	110.10
1	A	300	GLY	N-CA-C	6.08	128.29	113.10
1	A	809	LYS	C-N-CD	5.40	139.75	128.40
1	A	216	ALA	N-CA-C	5.06	124.65	111.00
1	A	757	TYR	CB-CA-C	-5.05	100.31	110.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	753	SER	Peptide
1	A	806	SER	Peptide
1	A	808	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	6703	0	6676	73	0
2	A	37	0	33	2	0
3	A	91	0	0	0	0
All	All	6831	0	6709	74	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 6.

All (74) 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:755:GLU:O	1:A:756:LYS:CB	2.16	0.94
1:A:753:SER:OG	1:A:754:ALA:HB3	1.71	0.89
1:A:896:VAL:HG12	1:A:897:GLY:H	1.45	0.82
1:A:948:HIS:CD2	1:A:950:ASP:HB2	2.21	0.76
1:A:757:TYR:O	1:A:758:ASP:CB	2.35	0.73
1:A:893:GLN:O	1:A:896:VAL:O	2.07	0.71
1:A:753:SER:HA	1:A:754:ALA:HB2	1.73	0.69
1:A:732:PHE:O	1:A:736:VAL:HG23	1.93	0.68
1:A:428:LEU:HD22	1:A:465:ASN:HB3	1.79	0.63
1:A:273:ARG:HG2	1:A:273:ARG:HH11	1.62	0.63
1:A:753:SER:CA	1:A:754:ALA:CB	2.76	0.63
1:A:899:THR:HB	1:A:901:ALA:H	1.66	0.61
1:A:753:SER:HA	1:A:754:ALA:CB	2.32	0.59
1:A:753:SER:CB	1:A:754:ALA:HB3	2.32	0.59
1:A:374:PRO:O	1:A:376:ASN:HA	2.03	0.58
1:A:500:ASP:O	1:A:503:THR:HG22	2.02	0.58
1:A:163:THR:HG22	1:A:177:ARG:HH12	1.68	0.57
1:A:1035:LEU:HD12	1:A:1048:ILE:HD13	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:622:LEU:HD21	1:A:651:LEU:HD23	1.85	0.56
1:A:775:GLN:OE1	1:A:779:LEU:HD11	2.05	0.56
1:A:753:SER:HG	1:A:754:ALA:HB3	1.70	0.56
1:A:893:GLN:C	1:A:896:VAL:O	2.44	0.56
1:A:908:ASN:HD22	1:A:994:VAL:HA	1.71	0.56
1:A:207:LEU:HD13	1:A:288:LYS:HB2	1.91	0.53
1:A:477:ARG:HA	1:A:520:LEU:HB3	1.89	0.53
1:A:583:LEU:HD22	1:A:610:LEU:HD22	1.91	0.53
1:A:370:ILE:HD12	1:A:514:MET:HB2	1.90	0.52
1:A:948:HIS:CD2	1:A:950:ASP:H	2.27	0.52
1:A:992:LEU:HB3	1:A:997:THR:HG23	1.91	0.51
1:A:374:PRO:C	1:A:376:ASN:HA	2.31	0.49
1:A:583:LEU:HD13	1:A:610:LEU:HD13	1.94	0.49
1:A:564:LEU:HD11	1:A:1048:ILE:HG22	1.94	0.49
1:A:1039:MET:HB2	1:A:1042:LEU:HD11	1.95	0.49
1:A:564:LEU:HD12	1:A:1052:ARG:HD3	1.95	0.48
1:A:407:GLU:OE2	1:A:409:LEU:HD11	2.12	0.48
1:A:896:VAL:HG12	1:A:897:GLY:N	2.20	0.48
1:A:753:SER:CA	1:A:754:ALA:HB3	2.44	0.47
1:A:1043:THR:HG23	1:A:1047:ASP:H	1.78	0.47
1:A:840:GLN:CD	1:A:840:GLN:H	2.17	0.47
1:A:983:VAL:HG13	1:A:1082:VAL:HG21	1.96	0.47
1:A:772:GLU:HG3	1:A:798:ILE:HG21	1.96	0.47
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.97	0.47
1:A:410:TRP:HB3	1:A:412:VAL:HG12	1.96	0.47
1:A:843:LEU:HG	1:A:1034:MET:HG3	1.96	0.47
1:A:1048:ILE:O	1:A:1051:ILE:HG22	2.15	0.46
1:A:948:HIS:HD2	1:A:950:ASP:CB	2.28	0.46
1:A:899:THR:HB	1:A:900:GLY:HA3	1.97	0.45
1:A:948:HIS:CD2	1:A:950:ASP:CB	2.95	0.45
1:A:914:LYS:HB3	1:A:956:GLU:HG2	1.98	0.45
1:A:812:TRP:CZ3	2:A:1201:OSC:H25	2.52	0.45
1:A:296:CYS:HB3	1:A:301:GLU:O	2.17	0.44
1:A:150:PHE:O	1:A:154:LEU:HG	2.17	0.44
1:A:377:THR:OG1	1:A:378:ASP:N	2.51	0.44
1:A:395:CYS:HB3	1:A:416:PHE:HD2	1.83	0.44
1:A:597:LYS:H	1:A:603:ILE:HG21	1.82	0.44
1:A:792:LYS:HB3	1:A:818:ALA:HB3	1.99	0.43
1:A:750:LYS:HA	1:A:753:SER:O	2.18	0.43
1:A:738:VAL:HG21	1:A:783:PHE:CD2	2.53	0.43
1:A:552:ARG:HH21	1:A:581:GLU:CD	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:ILE:HG23	1:A:703:ILE:HD13	1.99	0.43
1:A:273:ARG:HG2	1:A:273:ARG:NH1	2.29	0.42
1:A:149:ALA:HA	1:A:152:ARG:HE	1.84	0.42
1:A:227:SER:OG	1:A:228:THR:N	2.53	0.42
1:A:208:PRO:HD2	1:A:211:LEU:HD12	2.02	0.41
1:A:701:SER:O	1:A:705:GLN:HG2	2.21	0.41
1:A:948:HIS:NE2	1:A:950:ASP:HB2	2.36	0.41
2:A:1201:OSC:N2	2:A:1201:OSC:H9	2.36	0.40
1:A:198:MET:C	1:A:199:HIS:CG	2.94	0.40
1:A:181:VAL:O	1:A:185:MET:HG3	2.21	0.40
1:A:231:GLN:HB3	1:A:248:PHE:HE1	1.86	0.40
1:A:656:VAL:O	1:A:660:LEU:HB2	2.21	0.40
1:A:777:SER:OG	1:A:778:GLN:HB2	2.22	0.40
1:A:163:THR:HG22	1:A:177:ARG:NH1	2.36	0.40
1:A:470:ASP:HB2	1:A:476:ARG:HH21	1.86	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	818/966 (85%)	768 (94%)	44 (5%)	6 (1%)	22	44

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	756	LYS
1	A	758	ASP
1	A	1040	PRO
1	A	1045	LYS
1	A	754	ALA
1	A	1079	GLY

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	736/864 (85%)	678 (92%)	58 (8%)	12	26

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	SER
1	A	146	GLU
1	A	147	SER
1	A	153	GLN
1	A	203	THR
1	A	213	LYS
1	A	238	ASP
1	A	245	LEU
1	A	249	PHE
1	A	285	THR
1	A	358	ASP
1	A	369	ASP
1	A	372	VAL
1	A	376	ASN
1	A	378	ASP
1	A	381	VAL
1	A	391	GLN
1	A	392	GLN
1	A	395	CYS
1	A	411	ASN
1	A	470	ASP
1	A	520	LEU
1	A	525	HIS
1	A	570	GLU
1	A	601	GLN
1	A	610	LEU
1	A	622	LEU
1	A	626	LEU
1	A	647	LYS
1	A	650	SER

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Mol	Chain	Res	Type
1	A	682	LEU
1	A	700	ARG
1	A	717	LEU
1	A	743	GLN
1	A	767	LEU
1	A	777	SER
1	A	779	LEU
1	A	791	LEU
1	A	806	SER
1	A	825	ASN
1	A	826	GLU
1	A	838	LEU
1	A	840	GLN
1	A	841	ASP
1	A	848	LEU
1	A	858	GLU
1	A	859	SER
1	A	876	ILE
1	A	907	LEU
1	A	927	ARG
1	A	959	ASN
1	A	1000	LYS
1	A	1026	LEU
1	A	1039	MET
1	A	1041	GLN
1	A	1048	ILE
1	A	1051	ILE
1	A	1052	ARG

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	304	HIS
1	A	391	GLN
1	A	908	ASN
1	A	948	HIS
1	A	951	ASN

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 carbohydrates 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	OSC	A	1201	-	38,42,42	0.75	2 (5%)	53,62,62	1.50	5 (9%)

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	OSC	A	1201	-	-	4/18/36/36	0/6/6/6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	OSC	C15-N6	2.43	1.44	1.37
2	A	1201	OSC	C15-N3	2.33	1.35	1.32

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	OSC	C15-C14-N2	7.89	127.03	120.44
2	A	1201	OSC	C13-C14-N2	-3.84	117.16	121.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	OSC	C14-C15-N3	-3.20	118.15	120.81
2	A	1201	OSC	C10-N2-C14	2.30	121.76	118.04
2	A	1201	OSC	C15-N3-C16	2.12	121.15	116.17

There are no chirality outliers.

All (4) torsion outliers are listed below:

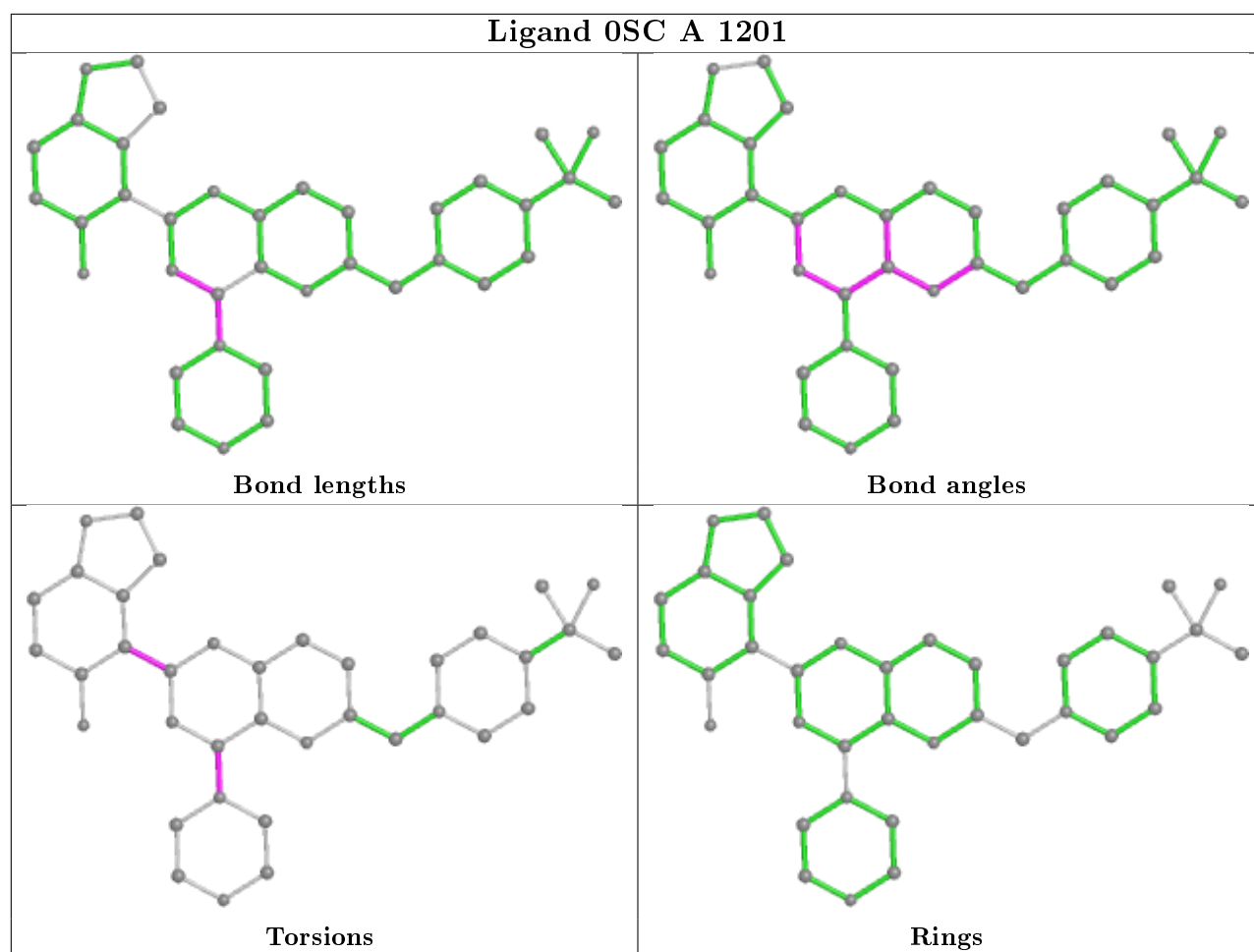
Mol	Chain	Res	Type	Atoms
2	A	1201	OSC	N4-C16-C17-C18
2	A	1201	OSC	C14-C15-N6-C28
2	A	1201	OSC	N4-C16-C17-C24
2	A	1201	OSC	N3-C16-C17-C24

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	OSC	2	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	834/966 (86%)	0.25	54 (6%) 18 16	28, 67, 106, 148	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	143	MET	7.5
1	A	374	PRO	7.3
1	A	377	THR	7.2
1	A	1044	SER	6.0
1	A	757	TYR	5.6
1	A	375	ARG	5.4
1	A	378	ASP	4.5
1	A	754	ALA	4.4
1	A	1046	GLU	4.4
1	A	981	GLU	4.3
1	A	376	ASN	3.7
1	A	823	LEU	3.5
1	A	267	GLU	3.4
1	A	269	ASP	3.4
1	A	807	LYS	3.2
1	A	216	ALA	3.1
1	A	379	LEU	3.1
1	A	146	GLU	3.1
1	A	228	THR	3.1
1	A	1084	PHE	3.0
1	A	776	ASN	2.9
1	A	371	PRO	2.9
1	A	752	LEU	2.8
1	A	148	GLN	2.7
1	A	489	GLY	2.7
1	A	404	PHE	2.7
1	A	526	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	730	HIS	2.6
1	A	227	SER	2.6
1	A	211	LEU	2.6
1	A	778	GLN	2.5
1	A	756	LYS	2.5
1	A	245	LEU	2.4
1	A	806	SER	2.4
1	A	320	LYS	2.3
1	A	896	VAL	2.3
1	A	409	LEU	2.3
1	A	986	VAL	2.3
1	A	758	ASP	2.3
1	A	1045	LYS	2.3
1	A	751	SER	2.2
1	A	461	LEU	2.2
1	A	373	LEU	2.2
1	A	231	GLN	2.2
1	A	1040	PRO	2.2
1	A	1091	VAL	2.1
1	A	306	VAL	2.1
1	A	895	THR	2.1
1	A	915	SER	2.1
1	A	749	ILE	2.0
1	A	234	LYS	2.0
1	A	777	SER	2.0
1	A	212	TRP	2.0
1	A	667	VAL	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 carbohydrates in this entry.

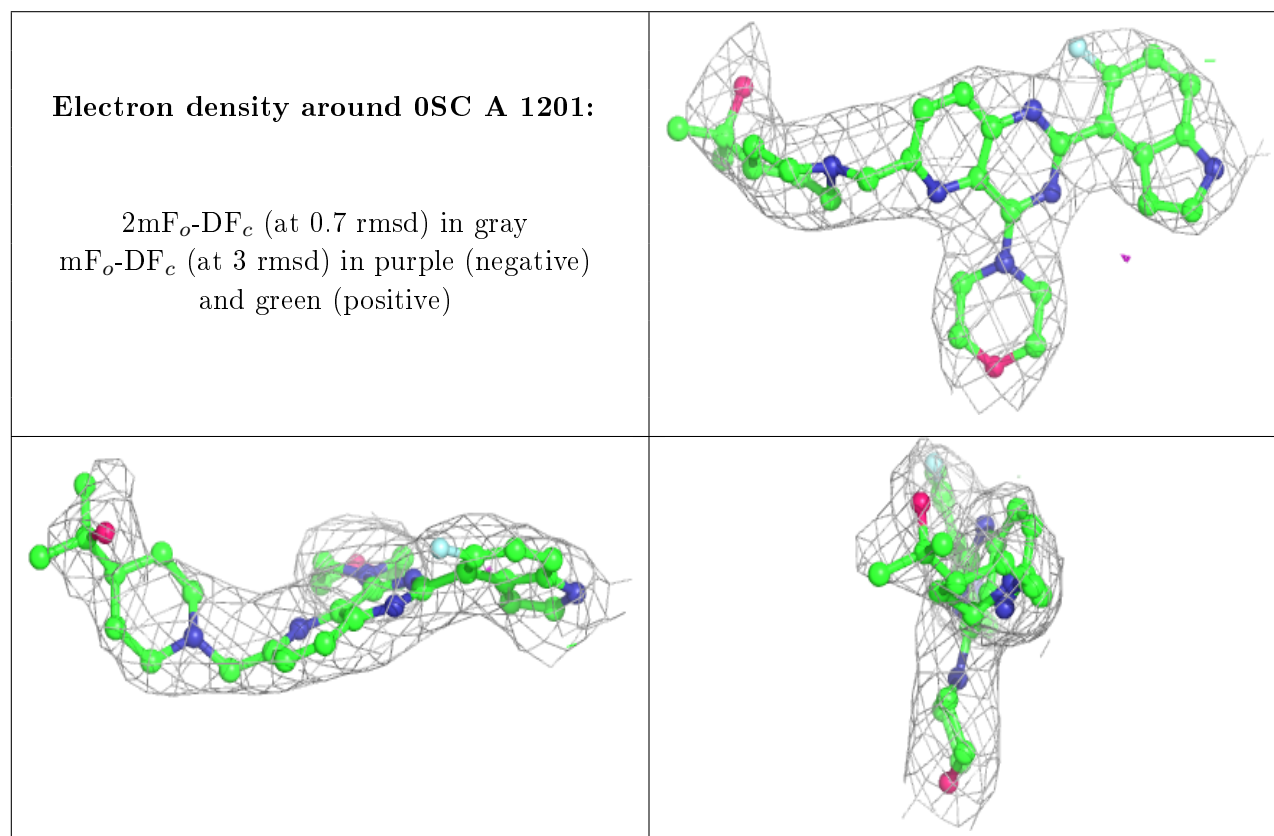
6.4 Ligands [i](#)

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	OSC	A	1201	37/37	0.92	0.19	53,63,82,85	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.