



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:07 PM UTC

PDB ID : 4EZJ / pdb_00004ezj
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 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

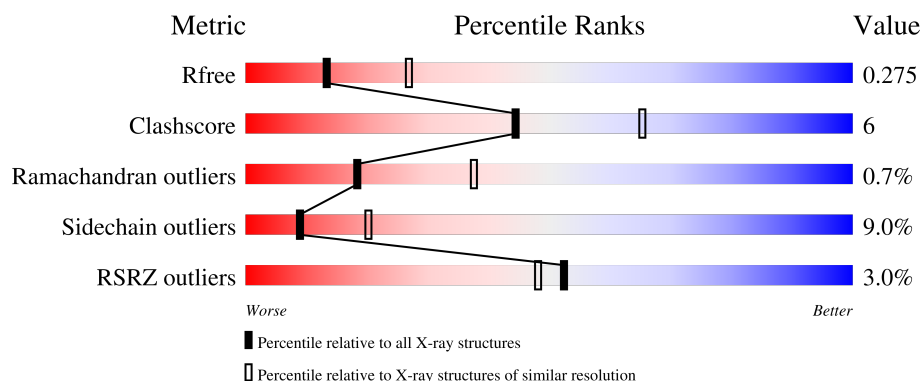
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.67 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}	180053	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (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 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	966	

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.

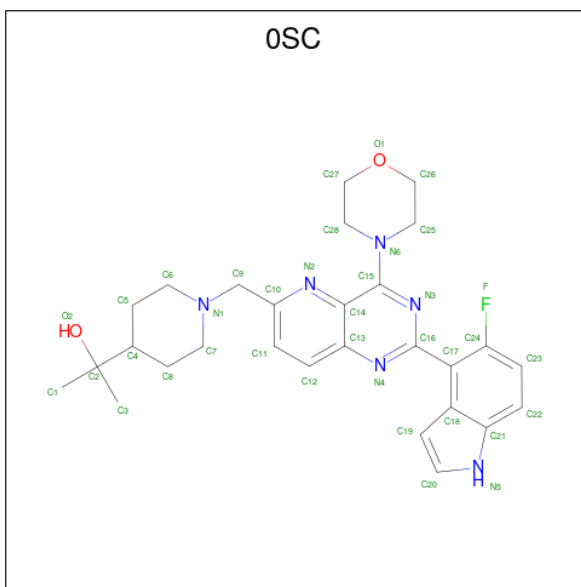
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit gamma isoform.

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 (CCD ID: 0SC) (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		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	141.20Å 67.12Å 104.77Å 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) 98.9 (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 2.68Å)	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 , 52.3	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	0.87	4/6846 (0.1%)	1.44	41/9271 (0.4%)

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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	809	LYS	C-O	11.68	1.29	1.23
1	A	842	MET	SD-CE	-5.62	1.65	1.79
1	A	810	PRO	N-CD	5.57	1.55	1.47
1	A	809	LYS	CA-C	-5.15	1.50	1.53

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	216	ALA	N-CA-C	12.51	124.65	111.14
1	A	1045	LYS	N-CA-C	11.56	135.42	110.80
1	A	1045	LYS	CB-CA-C	-10.02	90.48	110.42
1	A	805	ALA	N-CA-C	9.93	122.18	111.36
1	A	300	GLY	N-CA-C	9.12	128.29	115.43
1	A	809	LYS	N-CA-C	8.73	130.48	112.40
1	A	906	VAL	N-CA-C	8.28	120.06	110.62
1	A	753	SER	CB-CA-C	-7.18	97.59	109.80
1	A	804	MET	CA-C-N	6.51	129.53	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	804	MET	C-N-CA	6.51	129.53	120.29
1	A	498	ASN	CA-CB-CG	6.13	118.73	112.60
1	A	757	TYR	CB-CA-C	-5.99	100.31	109.89
1	A	470	ASP	CA-CB-CG	5.89	118.49	112.60
1	A	1046	GLU	N-CA-C	5.75	120.32	112.04
1	A	761	SER	N-CA-C	-5.68	105.23	111.82
1	A	809	LYS	O-C-N	5.66	127.83	121.32
1	A	676	ALA	CA-C-N	5.61	127.74	120.44
1	A	676	ALA	C-N-CA	5.61	127.74	120.44
1	A	308	ASP	N-CA-C	5.58	116.73	108.86
1	A	227	SER	CB-CA-C	-5.55	110.16	116.54
1	A	1041	GLN	N-CA-C	5.50	117.19	108.67
1	A	964	ASP	N-CA-C	5.49	118.96	111.39
1	A	1008	LYS	CA-C-N	5.38	128.27	120.79
1	A	1008	LYS	C-N-CA	5.38	128.27	120.79
1	A	376	ASN	CA-CB-CG	5.37	117.97	112.60
1	A	1033	MET	CA-C-N	5.30	127.33	120.44
1	A	1033	MET	C-N-CA	5.30	127.33	120.44
1	A	1092	LEU	N-CA-C	5.29	116.05	107.32
1	A	1007	GLN	CA-C-N	5.26	127.28	120.44
1	A	1007	GLN	C-N-CA	5.26	127.28	120.44
1	A	653	ASP	CA-C-N	5.26	127.64	120.54
1	A	653	ASP	C-N-CA	5.26	127.64	120.54
1	A	277	ARG	N-CA-C	5.15	116.91	109.07
1	A	557	ALA	CA-C-N	5.15	127.05	120.56
1	A	557	ALA	C-N-CA	5.15	127.05	120.56
1	A	569	ALA	CA-C-N	5.14	127.16	120.28
1	A	569	ALA	C-N-CA	5.14	127.16	120.28
1	A	797	ALA	N-CA-C	-5.10	102.52	109.71
1	A	503	THR	N-CA-C	5.07	117.69	110.24
1	A	637	ASP	CA-C-N	5.00	126.98	120.28
1	A	637	ASP	C-N-CA	5.00	126.98	120.28

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	79	0
2	A	37	0	33	2	0
3	A	91	0	0	0	0
All	All	6831	0	6709	80	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 (80) 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:181:VAL:HG12	1:A:185:MET:HE2	1.81	0.63
1:A:628:MET:HE1	1:A:662:GLN:HB3	1.80	0.61
1:A:899:THR:HB	1:A:901:ALA:H	1.66	0.61
1:A:893:GLN:C	1:A:896:VAL:O	2.44	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:908:ASN:HD22	1:A:994:VAL:HA	1.71	0.56
1:A:374:PRO:C	1:A:376:ASN:HA	2.31	0.54
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:840:GLN:H	1:A:840:GLN:CD	2.17	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: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:842:MET:HE3	1:A:870:ILE:HA	1.95	0.48
1:A:552:ARG:HH21	1:A:581:GLU:CD	2.22	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: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:948:HIS:HD2	1:A:950:ASP:CB	2.28	0.46
1:A:1048:ILE:O	1:A:1051:ILE:HG22	2.15	0.46
1:A:899:THR:HB	1:A:900:GLY:HA3	1.97	0.45
1:A:914:LYS:HB3	1:A:956:GLU:HG2	1.98	0.45
1:A:948:HIS:CD2	1:A:950:ASP:CB	2.95	0.45
1:A:198:MET:C	1:A:199:HIS:CG	2.94	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ALA:HA	1:A:152:ARG:HE	1.84	0.42
1:A:199:HIS:O	1:A:200:PRO:C	2.62	0.42
1:A:226:ARG:O	1:A:227:SER:C	2.63	0.42
1:A:227:SER:OG	1:A:228:THR:N	2.53	0.42
1:A:698:PHE:CE1	1:A:842:MET:HE2	2.55	0.41
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: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 [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	818/966 (85%)	768 (94%)	44 (5%)	6 (1%)	18 37

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%)	670 (91%)	66 (9%)	9 20

All (66) 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	190	SER
1	A	202	VAL
1	A	203	THR
1	A	213	LYS
1	A	235	VAL
1	A	238	ASP
1	A	245	LEU
1	A	281	LEU
1	A	285	THR
1	A	299	ASN
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	469	ILE
1	A	470	ASP
1	A	510	LYS
1	A	520	LEU
1	A	525	HIS
1	A	570	GLU
1	A	610	LEU

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Mol	Chain	Res	Type
1	A	622	LEU
1	A	626	LEU
1	A	647	LYS
1	A	650	SER
1	A	682	LEU
1	A	700	ARG
1	A	717	LEU
1	A	743	GLN
1	A	746	THR
1	A	767	LEU
1	A	777	SER
1	A	779	LEU
1	A	791	LEU
1	A	800	LYS
1	A	806	SER
1	A	823	LEU
1	A	825	ASN
1	A	826	GLU
1	A	838	LEU
1	A	841	ASP
1	A	848	LEU
1	A	858	GLU
1	A	859	SER
1	A	865	LEU
1	A	876	ILE
1	A	907	LEU
1	A	927	ARG
1	A	937	VAL
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	218	ASN
1	A	231	GLN

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Mol	Chain	Res	Type
1	A	304	HIS
1	A	391	GLN
1	A	483	HIS
1	A	512	ASN
1	A	601	GLN
1	A	646	GLN
1	A	658	HIS
1	A	710	GLN
1	A	734	GLN
1	A	892	GLN
1	A	908	ASN
1	A	948	HIS
1	A	951	ASN
1	A	1060	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	OSC	A	1201	-	42,42,42	0.83	2 (4%)	57,62,62	1.45	8 (14%)

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	-	-	5/18/36/36	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-N3	3.07	1.35	1.32
2	A	1201	OSC	C18-C21	-2.77	1.38	1.41

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	OSC	C15-C14-N2	6.85	127.03	120.37
2	A	1201	OSC	C13-C14-N2	-3.97	117.16	121.41
2	A	1201	OSC	C18-C17-C24	-3.41	114.76	118.13
2	A	1201	OSC	C10-N2-C14	2.54	121.76	118.17
2	A	1201	OSC	C22-C21-C18	-2.46	120.71	122.66
2	A	1201	OSC	C14-C15-N6	2.42	125.31	120.59
2	A	1201	OSC	C15-N3-C16	2.19	121.15	115.84
2	A	1201	OSC	C28-N6-C15	2.17	124.02	116.86

There are no chirality outliers.

All (5) torsion outliers are listed below:

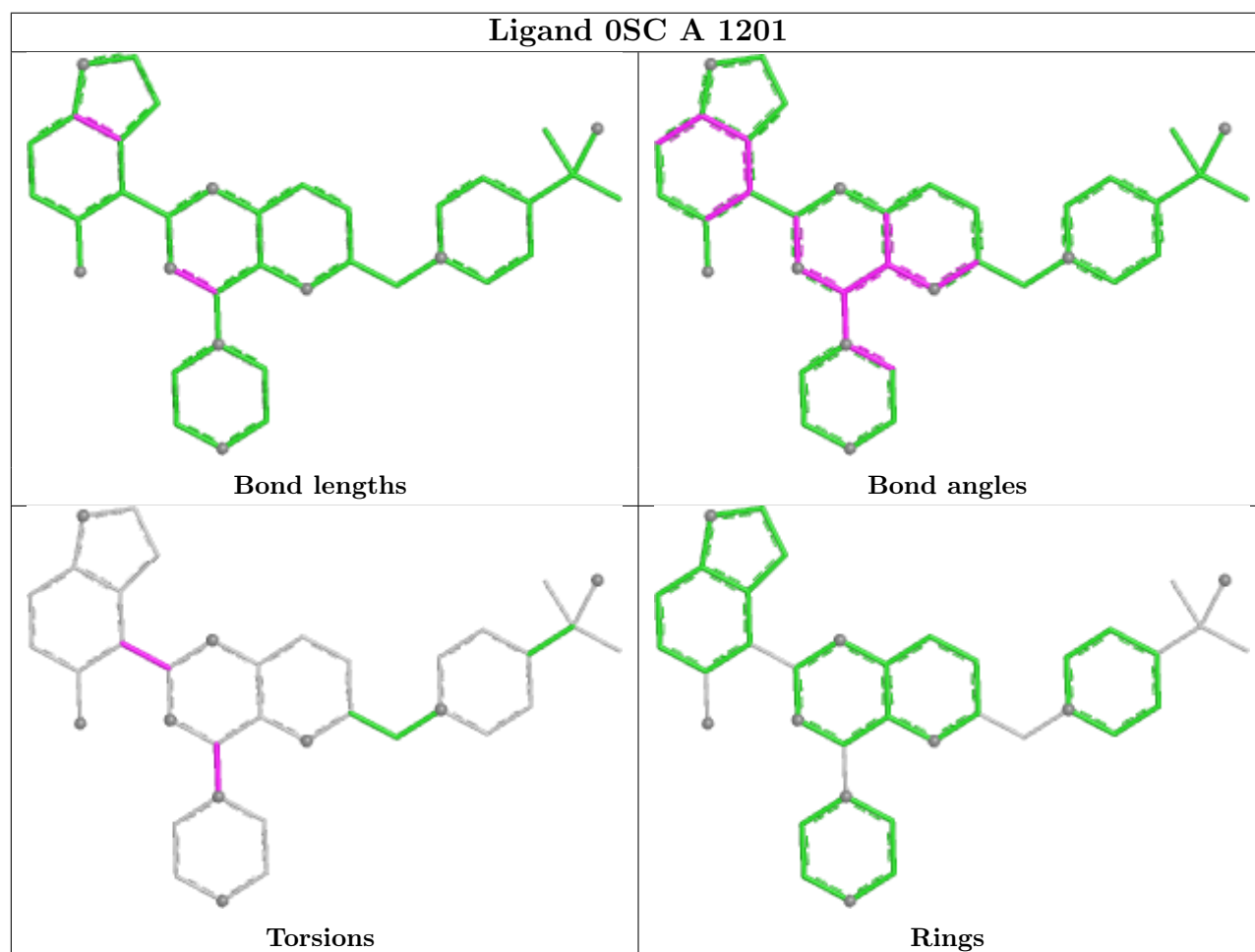
Mol	Chain	Res	Type	Atoms
2	A	1201	OSC	C14-C15-N6-C28
2	A	1201	OSC	N4-C16-C17-C18
2	A	1201	OSC	N3-C15-N6-C28
2	A	1201	OSC	N4-C16-C17-C24
2	A	1201	OSC	N3-C16-C17-C24

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 ⓘ

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%)	0.27	25 (2%)	52 48	28, 66, 106, 148	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	754	ALA	5.7
1	A	757	TYR	5.4
1	A	1044	SER	4.2
1	A	526	PRO	3.9
1	A	374	PRO	3.7
1	A	1093	GLY	3.4
1	A	1040	PRO	3.4
1	A	756	LYS	3.2
1	A	1045	LYS	3.1
1	A	752	LEU	3.0
1	A	758	ASP	3.0
1	A	373	LEU	2.9
1	A	1084	PHE	2.8
1	A	807	LYS	2.8
1	A	377	THR	2.5
1	A	730	HIS	2.5
1	A	751	SER	2.5
1	A	753	SER	2.4
1	A	1009	PHE	2.3
1	A	409	LEU	2.3
1	A	823	LEU	2.2
1	A	749	ILE	2.2
1	A	525	HIS	2.1
1	A	759	VAL	2.1
1	A	806	SER	2.1

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](#)

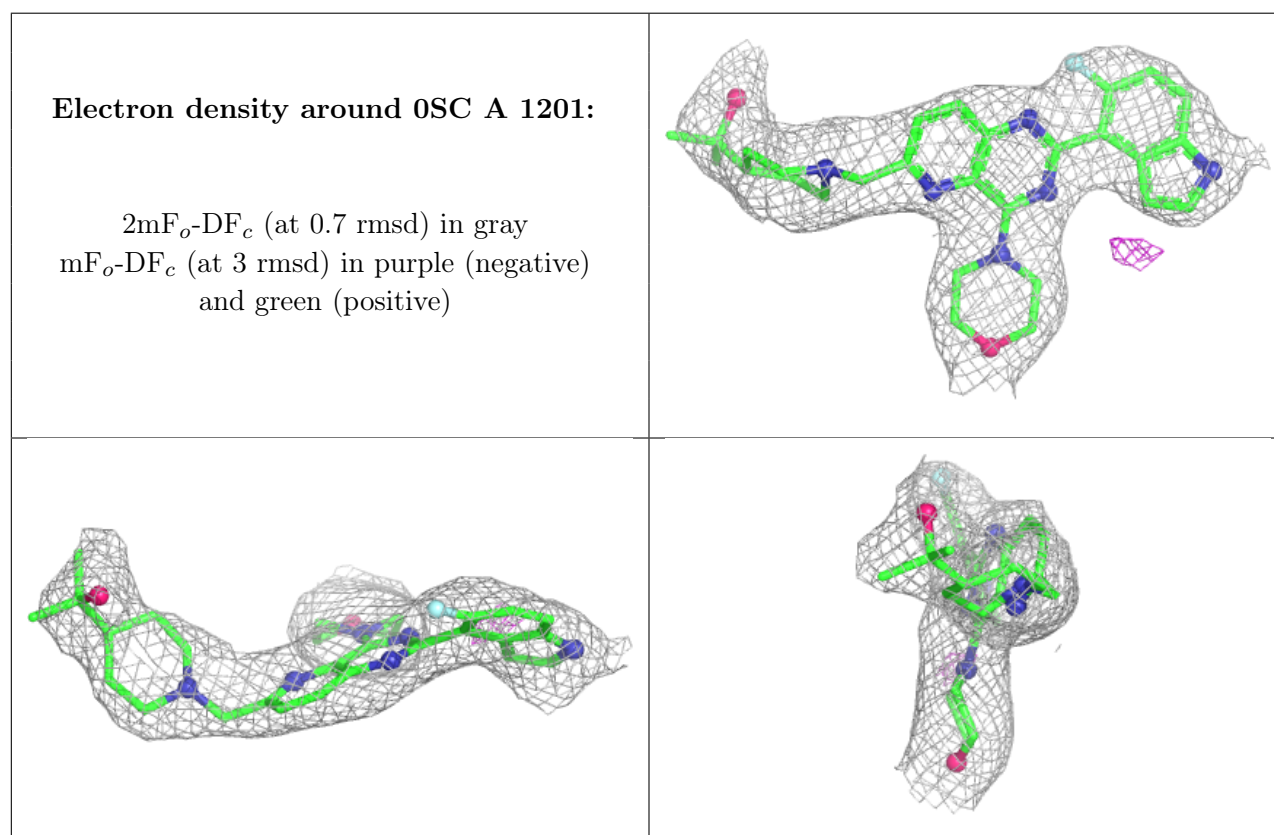
There are no oligosaccharides in this entry.

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	OSC	A	1201	37/37	0.91	0.10	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 ⓘ

There are no such residues in this entry.