



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 02:53 am BST

PDB ID : 4PS7
Title : Structure of PI3K gamma in complex with N-[6-(pyridin-3-yl)-1,3-benzothiazol-2-yl]acetamide
Authors : Griffith, J.P.
Deposited on : 2014-03-06
Resolution : 2.69 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

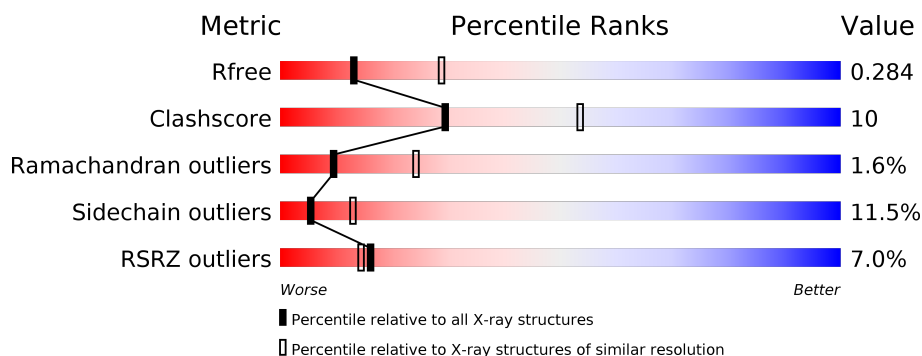
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7045 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.

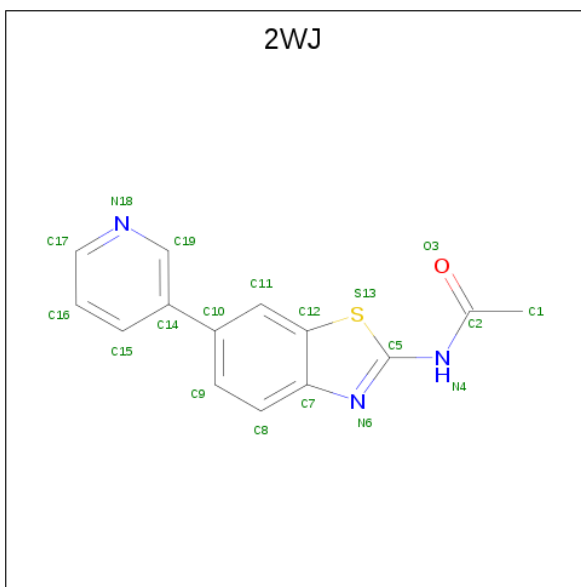
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic sub-unit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	843	Total	C	N	O	S	0	0	0
			6844	4395	1170	1244	35			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	MET	-	INITIATING METHIONINE	UNP P48736
A	459	ARG	GLN	CONFLICT	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 N-[6-(pyridin-3-yl)-1,3-benzothiazol-2-yl]acetamide (three-letter code: 2WJ) (formula: C₁₄H₁₁N₃OS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			19	14	3	1	1		

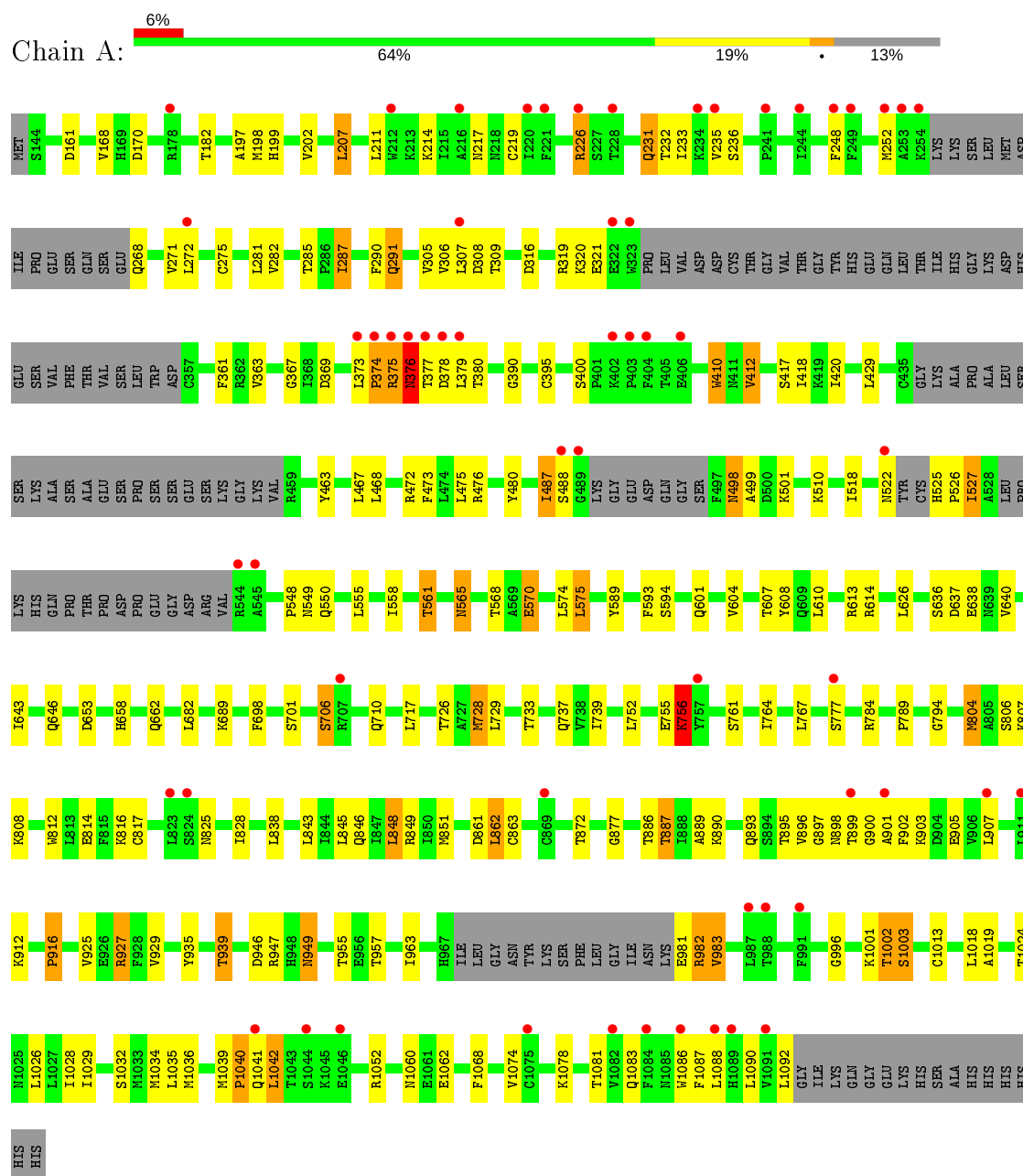
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	182	Total	O	0	0
			182	182		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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 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	143.97Å 67.71Å 106.70Å 90.00° 95.99° 90.00°	Depositor
Resolution (Å)	106.12 – 2.69 44.93 – 2.69	Depositor EDS
% Data completeness (in resolution range)	93.2 (106.12-2.69) 93.2 (44.93-2.69)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.211 , 0.274 0.227 , 0.284	Depositor DCC
R_{free} test set	1327 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	69.0	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 68.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7045	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.45% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 2WJ

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	0.55	0/6992	0.74	1/9457 (0.0%)

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	653	ASP	CB-CG-OD1	5.13	122.92	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	6844	0	6886	131	0
2	A	19	0	11	0	0
3	A	182	0	0	34	0
All	All	7045	0	6897	131	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 (131) 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:594:SER:HB3	3:A:1357:HOH:O	1.27	1.27
1:A:817:CYS:SG	3:A:1415:HOH:O	2.16	1.04
1:A:275:CYS:SG	3:A:1316:HOH:O	2.27	0.92
1:A:380:THR:HA	3:A:1450:HOH:O	1.78	0.82
1:A:893:GLN:HA	1:A:897:GLY:CA	2.10	0.81
1:A:863:CYS:SG	1:A:927:ARG:NH1	2.60	0.75
1:A:784:ARG:NH1	1:A:789:PRO:O	2.21	0.73
1:A:594:SER:CB	3:A:1357:HOH:O	2.05	0.71
1:A:410:TRP:CE3	3:A:1399:HOH:O	2.45	0.69
1:A:983:VAL:HA	3:A:1445:HOH:O	1.91	0.68
1:A:232:THR:HG23	3:A:1470:HOH:O	1.94	0.68
1:A:527:ILE:HG12	3:A:1403:HOH:O	1.92	0.68
1:A:689:LYS:HE3	3:A:1420:HOH:O	1.95	0.67
1:A:231:GLN:HA	1:A:231:GLN:HE21	1.61	0.66
1:A:608:TYR:OH	1:A:637:ASP:OD1	2.15	0.63
1:A:804:MET:CE	1:A:812:TRP:HB2	2.29	0.62
1:A:410:TRP:HE3	3:A:1399:HOH:O	1.79	0.61
1:A:957:THR:HG22	3:A:1347:HOH:O	2.01	0.60
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.83	0.60
1:A:168:VAL:HG13	1:A:170:ASP:O	2.02	0.60
1:A:561:THR:CG2	1:A:565:ASN:HB3	2.32	0.60
1:A:872:THR:OG1	1:A:877:GLY:HA2	2.02	0.60
1:A:568:THR:HG22	1:A:570:GLU:N	2.16	0.60
1:A:898:ASN:OD1	1:A:901:ALA:HB3	2.02	0.59
1:A:1039:MET:HB3	1:A:1040:PRO:HD2	1.84	0.59
1:A:935:TYR:O	1:A:939:THR:HB	2.01	0.59
1:A:640:VAL:O	1:A:643:ILE:HG12	2.03	0.59
1:A:1002:THR:O	1:A:1003:SER:HB3	2.04	0.58
1:A:526:PRO:O	1:A:527:ILE:HB	2.06	0.56
1:A:846:GLN:OE1	1:A:849:ARG:NH1	2.38	0.56
1:A:1042:LEU:O	1:A:1042:LEU:HD22	2.07	0.55
1:A:1086:TRP:CZ3	1:A:1090:LEU:HD21	2.42	0.55
1:A:981:GLU:N	1:A:982:ARG:CZ	2.70	0.55
1:A:1086:TRP:HB3	3:A:1374:HOH:O	2.06	0.55
1:A:893:GLN:HA	1:A:897:GLY:HA3	1.89	0.54
1:A:374:PRO:O	1:A:376:ASN:N	2.41	0.54
1:A:410:TRP:HB3	1:A:412:VAL:HG22	1.91	0.53
1:A:1087:PHE:O	1:A:1090:LEU:N	2.34	0.53
1:A:550:GLN:HB2	3:A:1456:HOH:O	2.09	0.52
1:A:527:ILE:CG1	3:A:1403:HOH:O	2.54	0.52
1:A:689:LYS:HG2	1:A:728:MET:CE	2.40	0.52
1:A:498:ASN:C	1:A:498:ASN:OD1	2.48	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1035:LEU:HB3	1:A:1042:LEU:HG	1.92	0.52
1:A:848:LEU:HD12	1:A:851:MET:CE	2.41	0.51
1:A:1060:ASN:OD1	1:A:1062:GLU:HB2	2.10	0.51
1:A:843:LEU:HG	1:A:1034:MET:HG3	1.93	0.51
1:A:901:ALA:C	3:A:1381:HOH:O	2.48	0.51
1:A:981:GLU:N	1:A:982:ARG:NH2	2.59	0.50
1:A:900:GLY:N	3:A:1376:HOH:O	2.44	0.50
1:A:561:THR:HG23	1:A:565:ASN:HB3	1.94	0.50
1:A:197:ALA:HA	3:A:1420:HOH:O	2.12	0.50
1:A:726:THR:HA	1:A:729:LEU:HD12	1.94	0.50
1:A:1032:SER:CB	3:A:1400:HOH:O	2.59	0.50
1:A:291:GLN:HA	1:A:291:GLN:HE21	1.77	0.50
1:A:321:GLU:HB3	3:A:1359:HOH:O	2.12	0.50
1:A:198:MET:O	1:A:199:HIS:C	2.50	0.49
1:A:804:MET:HE2	1:A:812:TRP:HB2	1.93	0.49
1:A:558:ILE:O	1:A:561:THR:HB	2.13	0.49
1:A:498:ASN:N	3:A:1355:HOH:O	2.45	0.49
1:A:887:THR:HG22	1:A:890:LYS:H	1.78	0.49
1:A:893:GLN:HA	1:A:897:GLY:HA2	1.91	0.49
1:A:1018:LEU:HD12	1:A:1019:ALA:N	2.28	0.48
1:A:361:PHE:HB2	1:A:420:ILE:HD13	1.95	0.48
1:A:321:GLU:CB	3:A:1359:HOH:O	2.61	0.48
1:A:947:ARG:NH2	1:A:963:ILE:O	2.46	0.48
1:A:916:PRO:HB2	3:A:1407:HOH:O	2.13	0.48
1:A:814:GLU:HA	1:A:828:ILE:O	2.14	0.47
1:A:1035:LEU:HA	1:A:1039:MET:HG2	1.96	0.47
1:A:565:ASN:HD22	1:A:565:ASN:C	2.18	0.47
1:A:794:GLY:N	1:A:816:LYS:O	2.39	0.47
1:A:949:ASN:H	1:A:1083:GLN:HE22	1.63	0.46
1:A:861:ASP:C	1:A:862:LEU:HD22	2.36	0.46
1:A:1074:VAL:HG12	3:A:1445:HOH:O	2.15	0.46
1:A:565:ASN:C	1:A:565:ASN:ND2	2.68	0.46
1:A:843:LEU:CG	1:A:1034:MET:HG3	2.46	0.46
1:A:887:THR:CG2	1:A:889:ALA:HB3	2.46	0.46
1:A:899:THR:HG23	1:A:899:THR:O	2.16	0.46
1:A:410:TRP:N	3:A:1399:HOH:O	2.49	0.45
1:A:271:VAL:HG23	1:A:282:VAL:CG1	2.45	0.45
1:A:400:SER:O	1:A:410:TRP:NE1	2.45	0.45
1:A:862:LEU:N	1:A:862:LEU:CD2	2.80	0.45
1:A:946:ASP:OD2	1:A:983:VAL:N	2.46	0.45
1:A:843:LEU:HD23	1:A:1034:MET:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:GLY:N	1:A:636:SER:OG	2.48	0.45
1:A:614:ARG:NH1	1:A:643:ILE:HG22	2.32	0.45
1:A:755:GLU:O	1:A:756:LYS:C	2.55	0.44
1:A:463:TYR:CE2	1:A:501:LYS:HA	2.52	0.44
1:A:525:HIS:CB	1:A:526:PRO:HD3	2.46	0.44
1:A:1083:GLN:HA	1:A:1083:GLN:NE2	2.32	0.44
1:A:480:TYR:HB2	1:A:518:ILE:HG13	1.98	0.44
1:A:658:HIS:CD2	3:A:1344:HOH:O	2.71	0.44
1:A:893:GLN:HA	1:A:897:GLY:N	2.33	0.44
1:A:1086:TRP:CE3	1:A:1087:PHE:HA	2.51	0.44
1:A:525:HIS:HB2	1:A:526:PRO:HD3	1.99	0.44
1:A:308:ASP:OD1	1:A:308:ASP:N	2.51	0.44
1:A:1035:LEU:HA	1:A:1039:MET:CG	2.48	0.43
1:A:467:LEU:O	1:A:476:ARG:NH1	2.51	0.43
1:A:487:ILE:HG23	1:A:488:SER:N	2.33	0.43
1:A:955:THR:HB	3:A:1347:HOH:O	2.18	0.43
1:A:843:LEU:CD2	1:A:1034:MET:HG3	2.48	0.43
1:A:472:ARG:O	1:A:473:PHE:HB2	2.19	0.43
1:A:1002:THR:O	1:A:1003:SER:CB	2.66	0.43
1:A:498:ASN:OD1	1:A:499:ALA:N	2.52	0.43
1:A:380:THR:CA	3:A:1450:HOH:O	2.52	0.43
1:A:925:VAL:O	1:A:929:VAL:HG23	2.19	0.43
1:A:380:THR:CB	3:A:1450:HOH:O	2.66	0.42
1:A:1024:THR:HG22	1:A:1028:ILE:HD12	2.02	0.42
1:A:1036:MET:HA	1:A:1042:LEU:HD11	2.01	0.42
1:A:226:ARG:NH2	3:A:1422:HOH:O	2.53	0.42
1:A:1013:CYS:HB3	1:A:1068:PHE:CE2	2.54	0.42
1:A:589:TYR:CD2	1:A:593:PHE:HE2	2.37	0.42
1:A:316:ASP:CG	3:A:1420:HOH:O	2.58	0.42
1:A:555:LEU:HD11	1:A:575:LEU:HD12	2.01	0.42
1:A:248:PHE:CE2	1:A:252:MET:HG3	2.55	0.41
1:A:363:VAL:O	1:A:363:VAL:HG13	2.20	0.41
1:A:706:SER:O	1:A:710:GLN:HB3	2.20	0.41
1:A:271:VAL:N	1:A:308:ASP:O	2.51	0.41
1:A:1034:MET:HG2	1:A:1039:MET:CE	2.51	0.41
1:A:233:ILE:HD12	1:A:233:ILE:N	2.35	0.41
1:A:367:GLY:HA2	3:A:1399:HOH:O	2.20	0.41
1:A:161:ASP:C	1:A:161:ASP:OD1	2.59	0.41
1:A:207:LEU:HD22	1:A:211:LEU:HB2	2.02	0.41
1:A:902:PHE:N	3:A:1381:HOH:O	2.53	0.41
1:A:475:LEU:HD21	1:A:522:ASN:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:733:THR:O	1:A:737:GLN:HG3	2.21	0.41
1:A:217:ASN:OD1	1:A:217:ASN:N	2.55	0.40
1:A:287:ILE:HA	1:A:290:PHE:HD1	1.85	0.40
1:A:548:PRO:HG2	3:A:1305:HOH:O	2.21	0.40
1:A:604:VAL:O	1:A:607:THR:HB	2.21	0.40
1:A:698:PHE:O	1:A:701:SER:HB3	2.22	0.40
1:A:272:LEU:HD22	1:A:305:VAL:HG11	2.03	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	827/966 (86%)	746 (90%)	68 (8%)	13 (2%)	9	24

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	375	ARG
1	A	527	ILE
1	A	756	LYS
1	A	1003	SER
1	A	1040	PRO
1	A	374	PRO
1	A	376	ASN
1	A	949	ASN
1	A	561	THR
1	A	498	ASN
1	A	777	SER
1	A	996	GLY
1	A	916	PRO

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	757/864 (88%)	670 (88%)	87 (12%)	5 13

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	182	THR
1	A	202	VAL
1	A	207	LEU
1	A	214	LYS
1	A	219	CYS
1	A	226	ARG
1	A	231	GLN
1	A	235	VAL
1	A	236	SER
1	A	268	GLN
1	A	281	LEU
1	A	285	THR
1	A	287	ILE
1	A	291	GLN
1	A	306	VAL
1	A	307	LEU
1	A	309	THR
1	A	319	ARG
1	A	320	LYS
1	A	369	ASP
1	A	373	LEU
1	A	375	ARG
1	A	376	ASN
1	A	377	THR
1	A	378	ASP
1	A	379	LEU
1	A	395	CYS
1	A	410	TRP
1	A	412	VAL
1	A	417	SER

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Mol	Chain	Res	Type
1	A	418	ILE
1	A	487	ILE
1	A	510	LYS
1	A	549	ASN
1	A	565	ASN
1	A	570	GLU
1	A	574	LEU
1	A	575	LEU
1	A	601	GLN
1	A	610	LEU
1	A	613	ARG
1	A	626	LEU
1	A	638	GLU
1	A	646	GLN
1	A	662	GLN
1	A	682	LEU
1	A	706	SER
1	A	717	LEU
1	A	728	MET
1	A	739	ILE
1	A	752	LEU
1	A	756	LYS
1	A	761	SER
1	A	764	ILE
1	A	767	LEU
1	A	804	MET
1	A	806	SER
1	A	807	LYS
1	A	808	LYS
1	A	825	ASN
1	A	838	LEU
1	A	845	LEU
1	A	848	LEU
1	A	862	LEU
1	A	886	THR
1	A	887	THR
1	A	895	THR
1	A	896	VAL
1	A	903	LYS
1	A	905	GLU
1	A	907	LEU
1	A	912	LYS

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Mol	Chain	Res	Type
1	A	927	ARG
1	A	939	THR
1	A	982	ARG
1	A	983	VAL
1	A	1001	LYS
1	A	1002	THR
1	A	1026	LEU
1	A	1029	ILE
1	A	1041	GLN
1	A	1042	LEU
1	A	1052	ARG
1	A	1078	LYS
1	A	1081	THR
1	A	1088	LEU
1	A	1092	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	GLN
1	A	218	ASN
1	A	231	GLN
1	A	291	GLN
1	A	304	HIS
1	A	549	ASN
1	A	565	ASN
1	A	601	GLN
1	A	710	GLN
1	A	743	GLN
1	A	762	GLN
1	A	766	GLN
1	A	773	ASN
1	A	776	ASN
1	A	959	ASN
1	A	1023	HIS
1	A	1083	GLN

5.3.3 RNA ⓘ

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	2WJ	A	1201	-	18,21,21	0.75	0	22,29,29	1.60	3 (13%)

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	2WJ	A	1201	-	-	0/6/8/8	0/3/3/3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	2WJ	C17-N18-C19	4.48	124.60	116.85
2	A	1201	2WJ	C1-C2-N4	3.06	119.47	114.98
2	A	1201	2WJ	C11-C12-S13	2.41	129.93	125.10

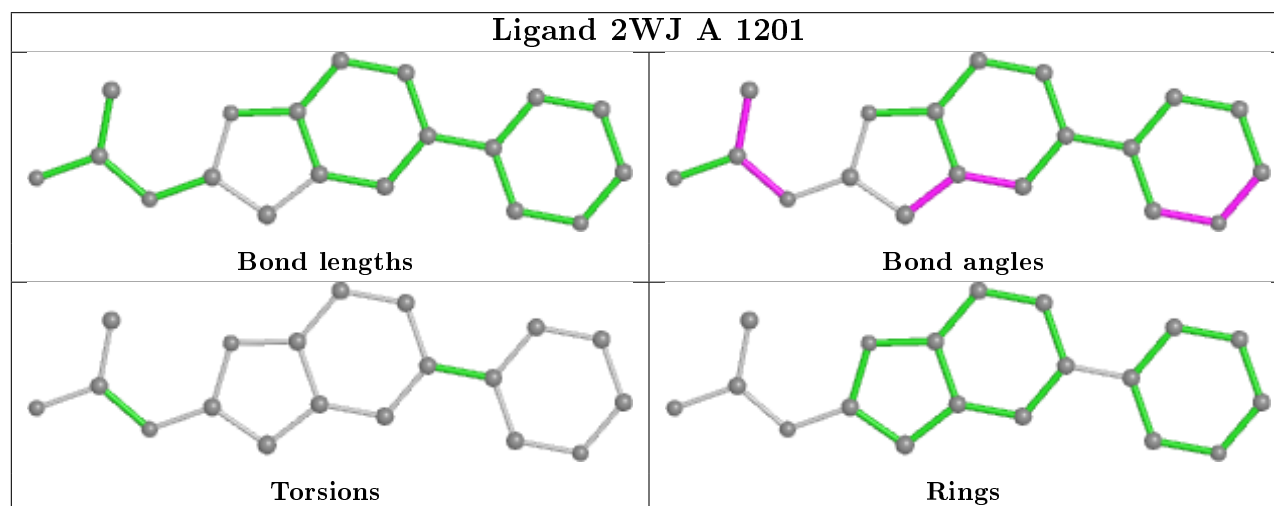
There are no chirality outliers.

There are no torsion outliers.

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	843/966 (87%)	0.29	59 (6%) 16 14	35, 78, 134, 185	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1088	LEU	10.7
1	A	1044	SER	9.3
1	A	899	THR	8.2
1	A	374	PRO	7.3
1	A	323	TRP	6.7
1	A	1091	VAL	6.1
1	A	216	ALA	5.6
1	A	375	ARG	5.4
1	A	322	GLU	5.1
1	A	248	PHE	5.1
1	A	1089	HIS	5.0
1	A	404	PHE	4.9
1	A	373	LEU	4.7
1	A	1084	PHE	4.3
1	A	377	THR	4.2
1	A	221	PHE	3.8
1	A	823	LEU	3.8
1	A	376	ASN	3.4
1	A	378	ASP	3.3
1	A	403	PRO	3.3
1	A	254	LYS	3.3
1	A	212	TRP	3.1
1	A	757	TYR	3.1
1	A	228	THR	2.9
1	A	488	SER	2.9
1	A	241	PRO	2.9
1	A	991	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	1086	TRP	2.8
1	A	234	LYS	2.8
1	A	1082	VAL	2.8
1	A	307	LEU	2.8
1	A	252	MET	2.8
1	A	544	ARG	2.7
1	A	406	GLU	2.7
1	A	522	ASN	2.7
1	A	1041	GLN	2.6
1	A	1075	CYS	2.6
1	A	489	GLY	2.5
1	A	777	SER	2.5
1	A	220	ILE	2.4
1	A	907	LEU	2.4
1	A	235	VAL	2.3
1	A	1046	GLU	2.3
1	A	253	ALA	2.3
1	A	226	ARG	2.3
1	A	545	ALA	2.3
1	A	901	ALA	2.2
1	A	244	ILE	2.2
1	A	911	LEU	2.2
1	A	988	THR	2.2
1	A	272	LEU	2.1
1	A	987	LEU	2.1
1	A	402	LYS	2.1
1	A	869	CYS	2.1
1	A	707	ARG	2.1
1	A	379	LEU	2.1
1	A	824	SER	2.0
1	A	249	PHE	2.0
1	A	178	ARG	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](#)

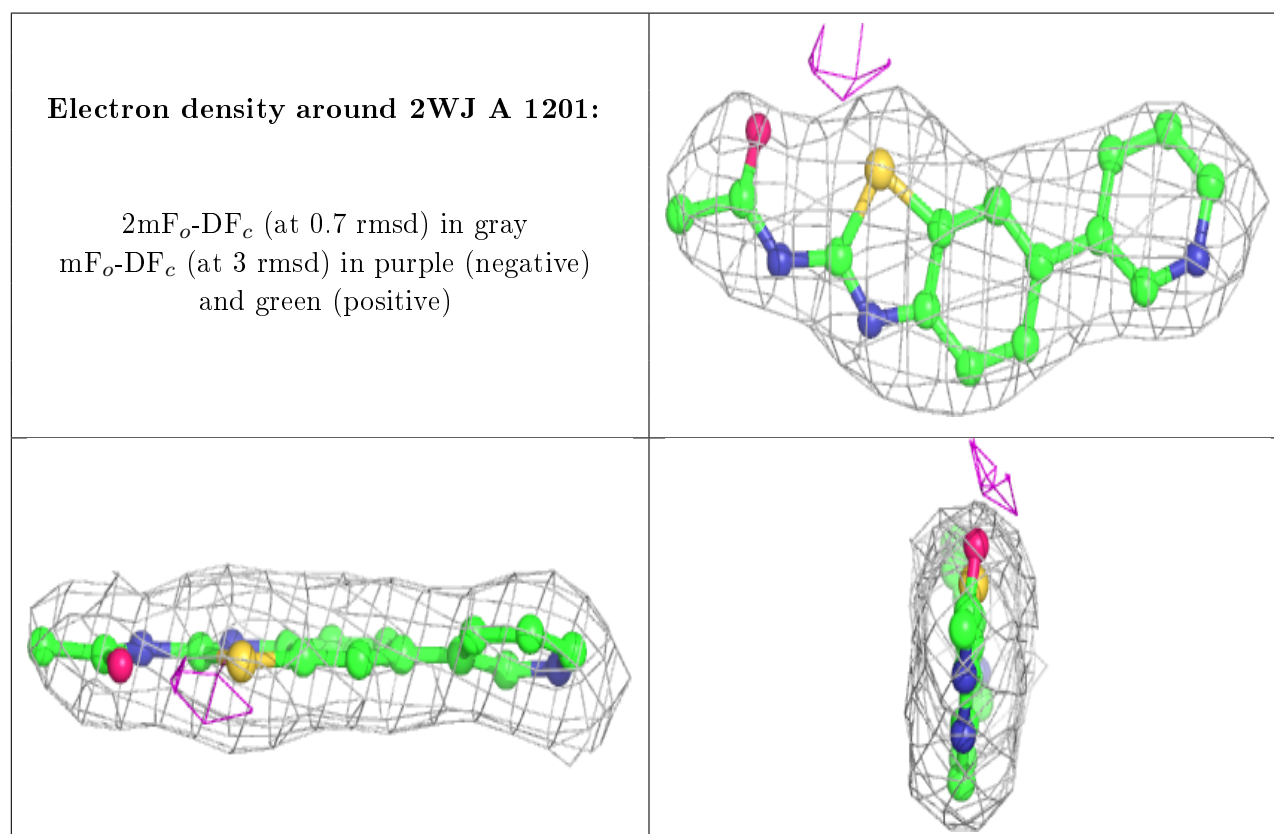
There are no carbohydrates in this entry.

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	2WJ	A	1201	19/19	0.97	0.15	46,53,70,71	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.