



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 04:59 am BST

PDB ID : 4PS8
Title : Structure of PI3K gamma in complex with N-[6-(5,6-dimethoxypyridin-3-yl)-1,3-benzothiazol-2-yl]acetamide
Authors : Griffith, J.P.
Deposited on : 2014-03-06
Resolution : 2.99 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

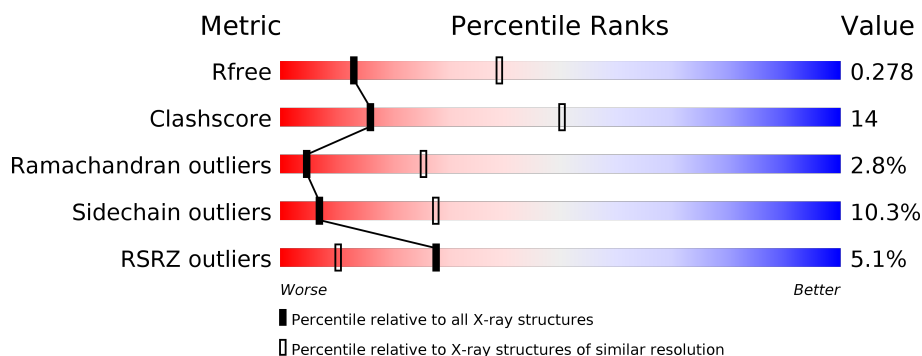
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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>4%</div> <div>54%</div> <div>28%</div> <div>5%</div> <div>13%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6869 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.

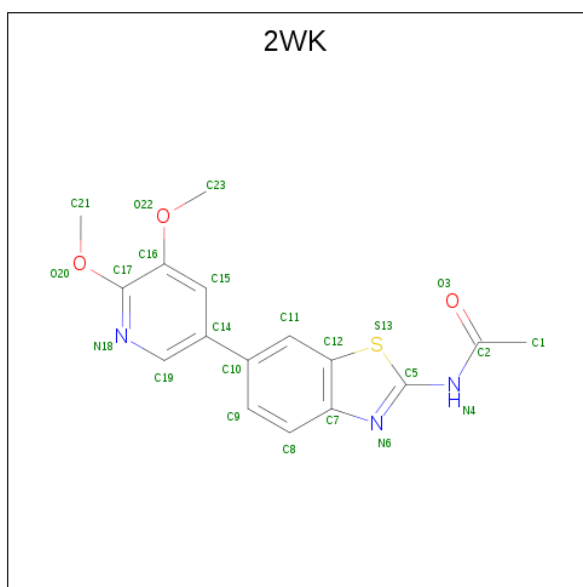
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic sub-unit gamma isoform.

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

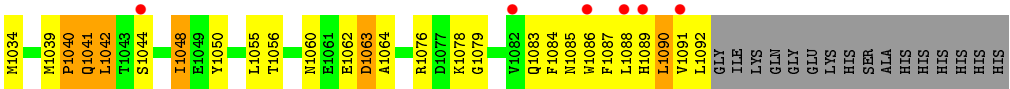
- Molecule 2 is N-[6-(5,6-dimethoxypyridin-3-yl)-1,3-benzothiazol-2-yl]acetamide (three-letter code: 2WK) (formula: C₁₆H₁₅N₃O₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			23	16	3	3	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	O	0	0
			2	2		



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	143.57Å 67.68Å 106.54Å 90.00° 96.21° 90.00°	Depositor
Resolution (Å)	105.92 – 2.99 44.92 – 2.99	Depositor EDS
% Data completeness (in resolution range)	89.9 (105.92-2.99) 90.0 (44.92-2.99)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.193 , 0.279 0.200 , 0.278	Depositor DCC
R_{free} test set	960 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	83.9	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 68.0	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	0.95	EDS
Total number of atoms	6869	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.49% 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: 2WK

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	0.69	2/6992 (0.0%)	0.86	3/9457 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	918	GLU	CG-CD	6.89	1.62	1.51
1	A	904	ASP	CG-OD2	6.52	1.40	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	632	ASP	CB-CG-OD1	-6.59	112.37	118.30
1	A	830	ILE	CB-CA-C	-6.31	98.97	111.60
1	A	152	ARG	NE-CZ-NH2	-5.07	117.76	120.30

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	6844	0	6886	199	0
2	A	23	0	15	0	0
3	A	2	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6869	0	6901	199	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 14.

All (199) 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:893:GLN:HA	1:A:897:GLY:HA2	1.37	1.06
1:A:834:HIS:HB2	1:A:876:ILE:HD12	1.46	0.97
1:A:395:CYS:HB2	1:A:418:ILE:HD11	1.56	0.86
1:A:893:GLN:HA	1:A:897:GLY:CA	2.07	0.85
1:A:1086:TRP:CE3	1:A:1087:PHE:HA	2.19	0.77
1:A:176:THR:HG23	1:A:674:ASP:HB2	1.74	0.70
1:A:217:ASN:ND2	1:A:219:CYS:SG	2.66	0.69
1:A:918:GLU:O	1:A:921:PHE:HB3	1.94	0.68
1:A:391:GLN:OE1	1:A:633:CYS:HB2	1.94	0.68
1:A:894:SER:OG	1:A:895:THR:N	2.27	0.68
1:A:935:TYR:O	1:A:939:THR:HB	1.95	0.66
1:A:863:CYS:SG	1:A:927:ARG:NH1	2.68	0.66
1:A:872:THR:OG1	1:A:877:GLY:HA2	1.95	0.66
1:A:207:LEU:HD22	1:A:208:PRO:CD	2.25	0.66
1:A:564:LEU:HD11	1:A:1048:ILE:HG22	1.79	0.65
1:A:395:CYS:HB2	1:A:418:ILE:CD1	2.25	0.65
1:A:525:HIS:HB2	1:A:526:PRO:HD3	1.80	0.63
1:A:1086:TRP:CH2	1:A:1090:LEU:HD21	2.34	0.62
1:A:291:GLN:HA	1:A:291:GLN:HE21	1.64	0.62
1:A:231:GLN:HE21	1:A:231:GLN:HA	1.62	0.62
1:A:525:HIS:CB	1:A:526:PRO:HD3	2.30	0.61
1:A:960:LEU:HD23	1:A:961:PHE:N	2.15	0.61
1:A:997:THR:HG23	1:A:1001:LYS:HG3	1.83	0.60
1:A:939:THR:HG23	1:A:945:GLY:HA2	1.84	0.60
1:A:988:THR:OG1	1:A:990:ASP:OD1	2.17	0.60
1:A:825:ASN:N	1:A:825:ASN:HD22	1.99	0.59
1:A:618:ASP:O	1:A:647:LYS:NZ	2.36	0.59
1:A:144:SER:OG	1:A:145:GLU:N	2.34	0.58
1:A:919:GLU:OE2	1:A:920:LYS:N	2.35	0.58
1:A:308:ASP:N	1:A:308:ASP:OD1	2.36	0.58
1:A:568:THR:HG22	1:A:570:GLU:H	1.70	0.57
1:A:181:VAL:HG12	1:A:185:MET:CE	2.34	0.57
1:A:1041:GLN:HA	1:A:1041:GLN:HE21	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:824:SER:OG	1:A:826:GLU:HB2	2.05	0.56
1:A:583:LEU:HD22	1:A:610:LEU:HD22	1.88	0.56
1:A:768:LYS:HE2	1:A:801:CYS:O	2.05	0.56
1:A:240:THR:HG22	1:A:243:ALA:H	1.70	0.56
1:A:174:GLU:O	1:A:178:ARG:HG2	2.06	0.55
1:A:811:LEU:O	1:A:831:ILE:HA	2.07	0.55
1:A:917:THR:OG1	1:A:919:GLU:OE2	2.25	0.55
1:A:703:ILE:HD11	1:A:714:ALA:HA	1.89	0.54
1:A:467:LEU:O	1:A:476:ARG:NH1	2.40	0.54
1:A:382:PHE:CE2	1:A:398:ARG:HD3	2.42	0.54
1:A:838:LEU:HD23	1:A:877:GLY:HA3	1.88	0.54
1:A:764:ILE:O	1:A:768:LYS:HG2	2.08	0.54
1:A:851:MET:HE1	1:A:938:ALA:HA	1.89	0.53
1:A:756:LYS:HG3	1:A:758:ASP:OD1	2.08	0.53
1:A:583:LEU:HD22	1:A:610:LEU:CD2	2.39	0.53
1:A:756:LYS:O	1:A:758:ASP:O	2.26	0.53
1:A:655:ASP:O	1:A:656:VAL:C	2.46	0.53
1:A:207:LEU:HD22	1:A:208:PRO:HD2	1.90	0.53
1:A:1055:LEU:O	1:A:1056:THR:HG22	2.09	0.53
1:A:154:LEU:O	1:A:157:LEU:N	2.42	0.53
1:A:391:GLN:OE1	1:A:633:CYS:SG	2.67	0.53
1:A:155:THR:HG23	1:A:161:ASP:HA	1.91	0.52
1:A:467:LEU:HD13	1:A:672:TYR:CE1	2.45	0.52
1:A:760:SER:OG	1:A:763:VAL:HG23	2.11	0.51
1:A:1026:LEU:O	1:A:1030:LEU:HG	2.11	0.50
1:A:564:LEU:HD11	1:A:1048:ILE:CG2	2.39	0.50
1:A:640:VAL:O	1:A:643:ILE:HG12	2.11	0.50
1:A:741:MET:O	1:A:744:LYS:HB2	2.12	0.50
1:A:966:GLY:HA3	3:A:1302:HOH:O	2.11	0.50
1:A:966:GLY:O	1:A:967:HIS:O	2.30	0.50
1:A:598:TRP:CE3	1:A:604:VAL:HG22	2.47	0.50
1:A:726:THR:HA	1:A:729:LEU:HB2	1.92	0.50
1:A:562:ASP:OD1	1:A:565:ASN:N	2.45	0.50
1:A:898:ASN:OD1	1:A:901:ALA:HB3	2.11	0.50
1:A:181:VAL:HG12	1:A:185:MET:HE2	1.93	0.50
1:A:1000:LYS:HA	1:A:1076:ARG:NH2	2.27	0.49
1:A:1050:TYR:C	1:A:1050:TYR:CD1	2.84	0.49
1:A:593:PHE:CE1	1:A:611:LEU:HD21	2.48	0.49
1:A:165:VAL:O	1:A:165:VAL:HG12	2.12	0.49
1:A:274:VAL:HG11	1:A:292:TRP:CE2	2.48	0.49
1:A:283:GLY:O	1:A:285:THR:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:ASN:O	1:A:411:ASN:CG	2.51	0.48
1:A:207:LEU:HD22	1:A:208:PRO:HD3	1.94	0.48
1:A:391:GLN:OE1	1:A:633:CYS:CB	2.60	0.48
1:A:851:MET:O	1:A:852:GLU:C	2.52	0.48
1:A:291:GLN:NE2	1:A:291:GLN:HA	2.28	0.47
1:A:157:LEU:HD21	1:A:733:THR:HA	1.97	0.47
1:A:395:CYS:SG	1:A:417:SER:OG	2.71	0.47
1:A:287:ILE:HA	1:A:290:PHE:HD2	1.79	0.47
1:A:706:SER:O	1:A:710:GLN:HB3	2.15	0.47
1:A:396:GLN:HG2	1:A:397:ARG:N	2.28	0.47
1:A:614:ARG:HG2	1:A:617:TRP:HB3	1.96	0.47
1:A:743:GLN:O	1:A:747:LEU:HD12	2.15	0.47
1:A:674:ASP:OD1	1:A:674:ASP:C	2.52	0.46
1:A:604:VAL:O	1:A:605:ALA:C	2.50	0.46
1:A:830:ILE:HG22	1:A:831:ILE:N	2.29	0.46
1:A:806:SER:HB2	1:A:810:PRO:HD3	1.97	0.46
1:A:271:VAL:HG23	1:A:282:VAL:HG13	1.97	0.46
1:A:626:LEU:HD23	1:A:626:LEU:HA	1.72	0.46
1:A:878:MET:C	1:A:879:ILE:HG13	2.36	0.46
1:A:1033:MET:O	1:A:1034:MET:C	2.54	0.46
1:A:645:VAL:HA	1:A:648:LEU:HD12	1.97	0.46
1:A:653:ASP:O	1:A:654:ASP:C	2.53	0.46
1:A:1039:MET:HB3	1:A:1040:PRO:HD2	1.98	0.46
1:A:466:LEU:HD21	1:A:476:ARG:HD3	1.98	0.46
1:A:629:GLN:HG2	1:A:1029:ILE:HG13	1.97	0.46
1:A:887:THR:O	1:A:888:ILE:C	2.53	0.46
1:A:419:LYS:O	1:A:420:ILE:C	2.54	0.46
1:A:734:GLN:HE22	1:A:780:PRO:HB3	1.81	0.45
1:A:1056:THR:HG21	1:A:1064:ALA:CB	2.45	0.45
1:A:1041:GLN:HA	1:A:1041:GLN:NE2	2.31	0.45
1:A:935:TYR:CE2	1:A:961:PHE:HA	2.51	0.45
1:A:1028:ILE:O	1:A:1032:SER:HB3	2.15	0.45
1:A:851:MET:HE2	1:A:938:ALA:HB2	1.99	0.45
1:A:1024:THR:HG22	1:A:1028:ILE:HD12	1.97	0.45
1:A:270:PHE:CD2	1:A:309:THR:HG23	2.51	0.45
1:A:760:SER:O	1:A:763:VAL:HB	2.17	0.45
1:A:917:THR:O	1:A:920:LYS:N	2.50	0.45
1:A:947:ARG:NH2	1:A:963:ILE:O	2.49	0.45
1:A:568:THR:O	1:A:571:ASP:HB2	2.17	0.45
1:A:1089:HIS:C	1:A:1091:VAL:N	2.69	0.44
1:A:273:ARG:NH1	1:A:277:ARG:O	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:623:ASP:HB3	1:A:626:LEU:HB2	1.99	0.44
1:A:758:ASP:OD1	1:A:758:ASP:N	2.48	0.44
1:A:895:THR:OG1	1:A:896:VAL:HG22	2.18	0.44
1:A:1021:ARG:HE	1:A:1056:THR:CG2	2.31	0.44
1:A:1060:ASN:ND2	1:A:1063:ASP:OD2	2.50	0.44
1:A:825:ASN:N	1:A:825:ASN:ND2	2.63	0.44
1:A:1055:LEU:O	1:A:1056:THR:CG2	2.65	0.44
1:A:243:ALA:O	1:A:246:GLN:HB2	2.18	0.44
1:A:434:TYR:CE1	1:A:460:LEU:HB2	2.53	0.44
1:A:558:ILE:O	1:A:561:THR:HB	2.18	0.43
1:A:586:PRO:O	1:A:626:LEU:HD11	2.18	0.43
1:A:692:GLY:HA3	1:A:720:TYR:OH	2.19	0.43
1:A:861:ASP:C	1:A:862:LEU:HD22	2.38	0.43
1:A:1086:TRP:CE3	1:A:1087:PHE:CA	2.95	0.43
1:A:572:LYS:HD3	1:A:595:SER:HA	2.00	0.43
1:A:890:LYS:HA	1:A:893:GLN:HB2	2.00	0.43
1:A:932:CYS:O	1:A:936:CYS:SG	2.74	0.43
1:A:1042:LEU:HD13	1:A:1042:LEU:N	2.34	0.43
1:A:743:GLN:O	1:A:744:LYS:C	2.56	0.43
1:A:565:ASN:HA	1:A:566:PRO:HD3	1.92	0.43
1:A:614:ARG:O	1:A:615:GLU:C	2.55	0.43
1:A:997:THR:HG23	1:A:1001:LYS:CG	2.47	0.43
1:A:588:ALA:O	1:A:589:TYR:C	2.57	0.43
1:A:635:PHE:O	1:A:641:ARG:HD2	2.18	0.43
1:A:743:GLN:NE2	1:A:876:ILE:HG12	2.34	0.43
1:A:925:VAL:O	1:A:929:VAL:HG23	2.19	0.43
1:A:937:VAL:O	1:A:941:VAL:HG23	2.19	0.43
1:A:920:LYS:O	1:A:923:ALA:HB3	2.19	0.43
1:A:1055:LEU:C	1:A:1056:THR:HG22	2.38	0.42
1:A:609:GLN:O	1:A:612:ALA:HB3	2.19	0.42
1:A:171:ASP:OD1	1:A:471:HIS:NE2	2.50	0.42
1:A:368:ILE:HG22	1:A:516:ILE:HB	2.00	0.42
1:A:557:ALA:O	1:A:558:ILE:C	2.58	0.42
1:A:955:THR:HG1	1:A:959:ASN:H	1.65	0.42
1:A:989:PRO:HA	1:A:992:LEU:HD12	2.01	0.42
1:A:1056:THR:HG21	1:A:1064:ALA:HB1	2.00	0.42
1:A:434:TYR:HA	1:A:459:ARG:O	2.18	0.42
1:A:784:ARG:NH1	1:A:789:PRO:O	2.53	0.42
1:A:851:MET:CE	1:A:938:ALA:HB2	2.49	0.42
1:A:872:THR:HG1	1:A:877:GLY:HA2	1.82	0.42
1:A:1089:HIS:O	1:A:1091:VAL:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:GLY:O	1:A:245:LEU:HB2	2.19	0.42
1:A:721:LEU:HA	1:A:724:CYS:SG	2.60	0.42
1:A:928:PHE:CD1	1:A:928:PHE:C	2.93	0.42
1:A:1062:GLU:O	1:A:1063:ASP:C	2.58	0.42
1:A:386:ASN:OD1	1:A:396:GLN:HG3	2.20	0.42
1:A:632:ASP:OD1	1:A:632:ASP:C	2.56	0.42
1:A:905:GLU:HG3	1:A:993:PHE:CE2	2.55	0.42
1:A:1083:GLN:O	1:A:1084:PHE:C	2.58	0.42
1:A:381:VAL:HG21	1:A:404:PHE:CD2	2.54	0.42
1:A:887:THR:CG2	1:A:950:ASP:HA	2.49	0.42
1:A:232:THR:C	1:A:233:ILE:HD12	2.39	0.42
1:A:411:ASN:ND2	1:A:411:ASN:O	2.52	0.42
1:A:198:MET:O	1:A:199:HIS:C	2.58	0.42
1:A:280:TYR:CD1	1:A:280:TYR:N	2.88	0.41
1:A:689:LYS:HG2	1:A:728:MET:HE2	2.02	0.41
1:A:732:PHE:O	1:A:733:THR:C	2.58	0.41
1:A:656:VAL:HG11	1:A:691:ILE:HD13	2.02	0.41
1:A:1021:ARG:HE	1:A:1056:THR:HG23	1.85	0.41
1:A:770:LYS:O	1:A:773:ASN:HB2	2.19	0.41
1:A:466:LEU:HD11	1:A:476:ARG:HD3	2.02	0.41
1:A:364:LYS:HA	1:A:412:VAL:O	2.21	0.41
1:A:579:ARG:HB2	1:A:610:LEU:HD11	2.03	0.41
1:A:271:VAL:HG22	1:A:272:LEU:N	2.36	0.41
1:A:171:ASP:C	1:A:171:ASP:OD1	2.58	0.41
1:A:667:VAL:O	1:A:712:ARG:NH1	2.54	0.41
1:A:988:THR:CB	1:A:990:ASP:OD1	2.69	0.41
1:A:1012:ILE:O	1:A:1013:CYS:C	2.59	0.41
1:A:696:PHE:C	1:A:696:PHE:CD1	2.94	0.41
1:A:561:THR:CG2	1:A:565:ASN:HB3	2.51	0.41
1:A:920:LYS:O	1:A:921:PHE:C	2.58	0.41
1:A:945:GLY:O	1:A:985:PHE:HA	2.19	0.41
1:A:1005:HIS:O	1:A:1008:LYS:HB3	2.20	0.41
1:A:930:TYR:CE2	1:A:1012:ILE:HD13	2.56	0.41
1:A:209:GLU:HB2	1:A:859:SER:HB3	2.03	0.40
1:A:990:ASP:OD1	1:A:990:ASP:N	2.54	0.40
1:A:1042:LEU:HD22	1:A:1042:LEU:O	2.21	0.40
1:A:851:MET:CE	1:A:938:ALA:CB	2.99	0.40
1:A:738:VAL:HG22	1:A:780:PRO:HD2	2.04	0.40
1:A:744:LYS:O	1:A:748:ASP:OD1	2.39	0.40
1:A:851:MET:HE1	1:A:938:ALA:CA	2.51	0.40
1:A:271:VAL:CG2	1:A:272:LEU:N	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:586:PRO:C	1:A:626:LEU:HD11	2.42	0.40
1:A:613:ARG:HB3	1:A:613:ARG:NH1	2.36	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%)	713 (86%)	91 (11%)	23 (3%)	5	25

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	227	SER
1	A	374	PRO
1	A	406	GLU
1	A	471	HIS
1	A	949	ASN
1	A	371	PRO
1	A	376	ASN
1	A	756	LYS
1	A	867	TYR
1	A	1085	ASN
1	A	1090	LEU
1	A	391	GLN
1	A	754	ALA
1	A	1063	ASP
1	A	526	PRO
1	A	900	GLY
1	A	901	ALA
1	A	1040	PRO
1	A	1044	SER

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Mol	Chain	Res	Type
1	A	601	GLN
1	A	757	TYR
1	A	1079	GLY
1	A	424	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%)	679 (90%)	78 (10%)	7 28

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145	GLU
1	A	168	VAL
1	A	182	THR
1	A	203	THR
1	A	219	CYS
1	A	226	ARG
1	A	231	GLN
1	A	232	THR
1	A	240	THR
1	A	268	GLN
1	A	278	ASP
1	A	282	VAL
1	A	287	ILE
1	A	291	GLN
1	A	309	THR
1	A	320	LYS
1	A	359	ARG
1	A	373	LEU
1	A	375	ARG
1	A	376	ASN
1	A	379	LEU
1	A	395	CYS

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Mol	Chain	Res	Type
1	A	404	PHE
1	A	487	ILE
1	A	498	ASN
1	A	510	LYS
1	A	520	LEU
1	A	549	ASN
1	A	574	LEU
1	A	575	LEU
1	A	610	LEU
1	A	613	ARG
1	A	626	LEU
1	A	662	GLN
1	A	675	SER
1	A	682	LEU
1	A	717	LEU
1	A	728	MET
1	A	739	ILE
1	A	761	SER
1	A	767	LEU
1	A	775	GLN
1	A	798	ILE
1	A	804	MET
1	A	807	LYS
1	A	825	ASN
1	A	838	LEU
1	A	843	LEU
1	A	845	LEU
1	A	852	GLU
1	A	853	SER
1	A	862	LEU
1	A	865	LEU
1	A	869	CYS
1	A	871	SER
1	A	886	THR
1	A	895	THR
1	A	896	VAL
1	A	903	LYS
1	A	905	GLU
1	A	912	LYS
1	A	917	THR
1	A	919	GLU
1	A	927	ARG

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Mol	Chain	Res	Type
1	A	939	THR
1	A	982	ARG
1	A	998	SER
1	A	1001	LYS
1	A	1002	THR
1	A	1026	LEU
1	A	1029	ILE
1	A	1032	SER
1	A	1041	GLN
1	A	1042	LEU
1	A	1048	ILE
1	A	1078	LYS
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	153	GLN
1	A	217	ASN
1	A	218	ASN
1	A	231	GLN
1	A	291	GLN
1	A	304	HIS
1	A	565	ASN
1	A	585	HIS
1	A	734	GLN
1	A	743	GLN
1	A	766	GLN
1	A	773	ASN
1	A	825	ASN
1	A	1007	GLN
1	A	1041	GLN
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	2WK	A	1201	-	21,25,25	0.75	0	26,35,35	1.71	10 (38%)

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	2WK	A	1201	-	-	4/10/12/12	0/3/3/3

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	2WK	O22-C16-C15	-3.35	118.35	124.12
2	A	1201	2WK	C7-C12-S13	-2.82	108.11	111.85
2	A	1201	2WK	O3-C2-C1	-2.67	117.11	122.06
2	A	1201	2WK	C12-C7-N6	2.47	113.78	108.04
2	A	1201	2WK	C19-N18-C17	2.37	122.36	116.27
2	A	1201	2WK	C11-C12-S13	2.31	129.72	125.10
2	A	1201	2WK	O20-C17-C16	2.24	120.82	116.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	2WK	C8-C7-C12	-2.14	116.76	120.53
2	A	1201	2WK	C14-C19-N18	-2.05	120.94	124.32
2	A	1201	2WK	C15-C14-C10	-2.00	117.55	120.86

There are no chirality outliers.

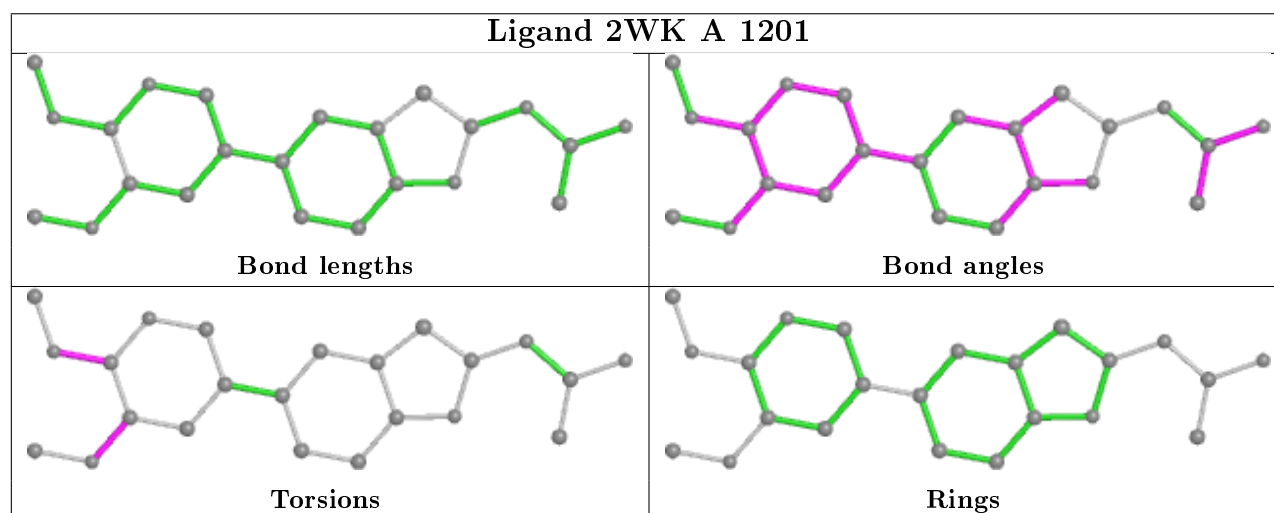
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201	2WK	C17-C16-O22-C23
2	A	1201	2WK	C15-C16-O22-C23
2	A	1201	2WK	N18-C17-O20-C21
2	A	1201	2WK	C16-C17-O20-C21

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

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	843/966 (87%)	0.15	43 (5%) 28 10	45, 90, 153, 192	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	374	PRO	8.1
1	A	1088	LEU	7.9
1	A	322	GLU	7.6
1	A	254	LYS	7.3
1	A	1044	SER	6.1
1	A	375	ARG	6.0
1	A	323	TRP	6.0
1	A	377	THR	5.5
1	A	995	MET	5.5
1	A	253	ALA	4.9
1	A	376	ASN	4.8
1	A	907	LEU	4.3
1	A	991	PHE	4.2
1	A	404	PHE	3.8
1	A	1091	VAL	3.8
1	A	1086	TRP	3.7
1	A	899	THR	3.7
1	A	373	LEU	3.7
1	A	212	TRP	3.4
1	A	320	LYS	3.4
1	A	998	SER	3.3
1	A	967	HIS	3.3
1	A	1089	HIS	3.2
1	A	220	ILE	3.1
1	A	993	PHE	3.0
1	A	252	MET	2.9
1	A	489	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	757	TYR	2.7
1	A	999	GLY	2.7
1	A	235	VAL	2.6
1	A	221	PHE	2.5
1	A	1082	VAL	2.5
1	A	234	LYS	2.5
1	A	987	LEU	2.4
1	A	378	ASP	2.4
1	A	1000	LYS	2.4
1	A	233	ILE	2.3
1	A	270	PHE	2.3
1	A	248	PHE	2.3
1	A	992	LEU	2.2
1	A	281	LEU	2.2
1	A	997	THR	2.2
1	A	216	ALA	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](#)

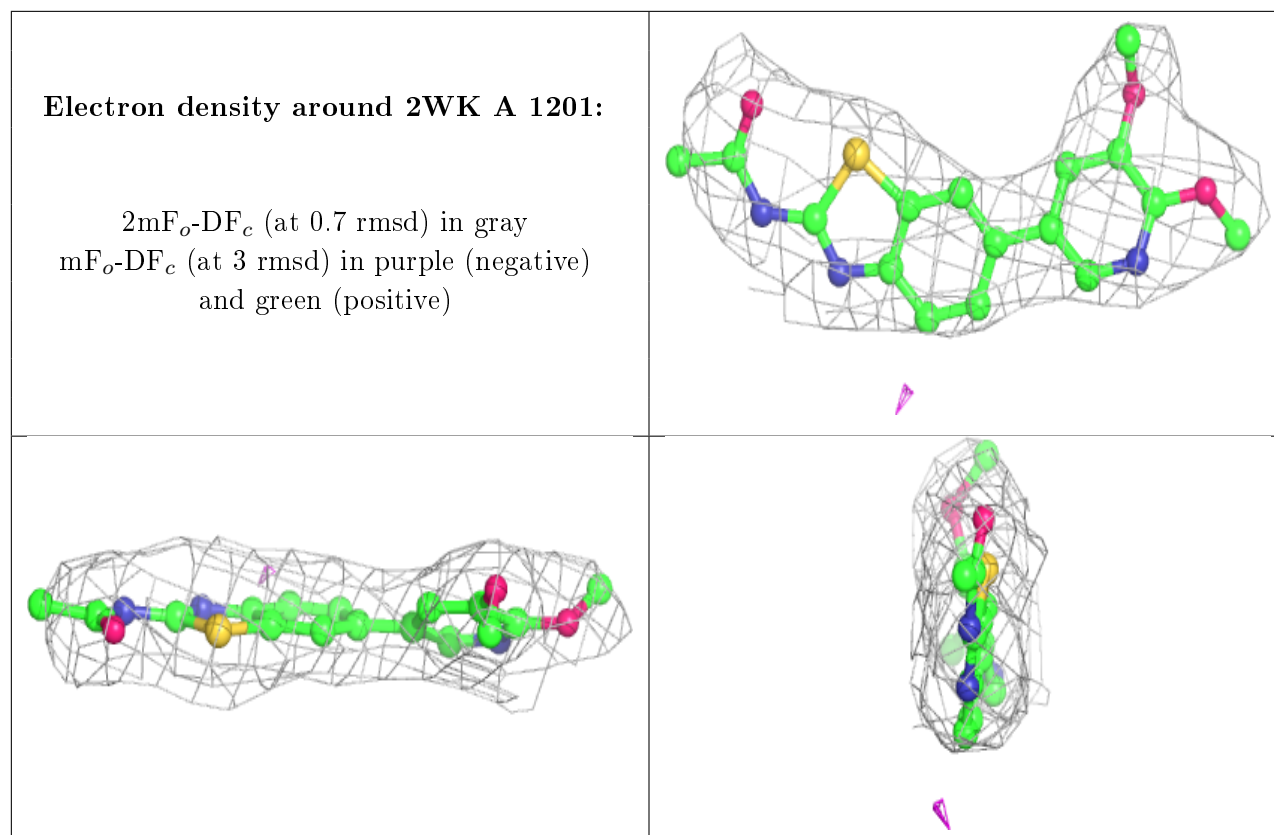
There are no carbohydrates in this entry.

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	2WK	A	1201	23/23	0.97	0.16	59,72,80,83	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.