



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 01:06 PM UTC

PDB ID : 3MJW / pdb_00003mjw
Title : PI3 Kinase gamma with a benzofuranone inhibitor
Authors : Bard, J.; Svenson, K.
Deposited on : 2010-04-13
Resolution : 2.87 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

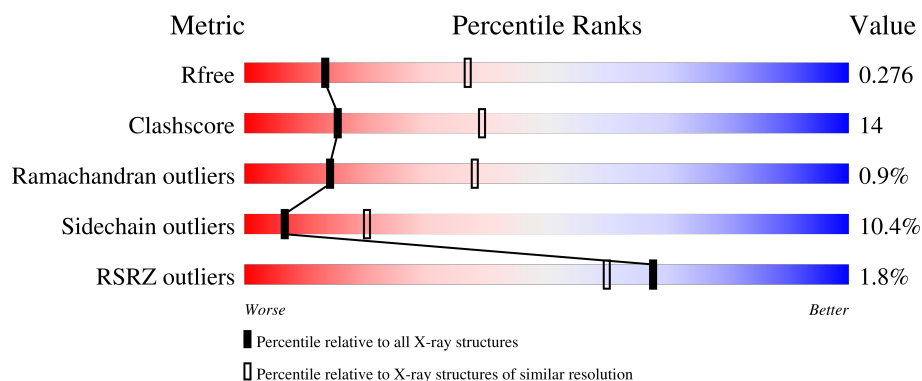
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.87 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	3557 (2.90-2.86)
Clashscore	190562	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)
RSRZ outliers	180081	3558 (2.90-2.86)

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 2 unique types of molecules in this entry. The entry contains 6472 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.

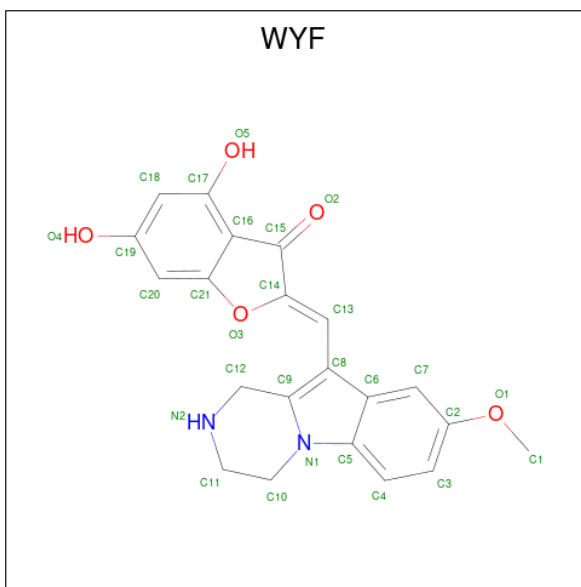
- Molecule 1 is a protein called Phosphatidylinositol-4,5-bisphosphate 3-kinase catalytic subunit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	819	Total	C	N	O	S	0	0	0
			6444	4133	1102	1177	32			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	MET	-	expression tag	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 (2Z)-4,6-dihydroxy-2-[(8-methoxy-1,2,3,4-tetrahydropyrazino[1,2-a]indol-10-yl)methylidene]-1-benzofuran-3(2H)-one (CCD ID: WYF) (formula: C₂₁H₁₈N₂O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	28	21	2	5	0	0

HIS
HIS
HIS
HIS

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	145.60Å 68.57Å 107.25Å 90.00° 95.02° 90.00°	Depositor
Resolution (Å)	36.23 – 2.87 36.23 – 2.87	Depositor EDS
% Data completeness (in resolution range)	86.3 (36.23-2.87) 86.6 (36.23-2.87)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.86Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.225 , 0.281 0.231 , 0.276	Depositor DCC
R_{free} test set	2000 reflections (9.00%)	wwPDB-VP
Wilson B-factor (Å ²)	70.4	Xtriage
Anisotropy	0.374	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 42.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6472	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.97% 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: WYF

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	0.26	0/6579	0.72	1/8926 (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	478	GLY	N-CA-C	5.60	117.99	110.43

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	6444	0	6306	171	0
2	A	28	0	17	4	0
All	All	6472	0	6323	173	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 (173) 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:217:ASN:HD22	1:A:219:CYS:HB3	1.52	0.75
1:A:404:PHE:CD1	1:A:404:PHE:N	2.55	0.72
1:A:887:THR:HG22	1:A:889:ALA:H	1.54	0.72
1:A:487:ILE:HG22	1:A:488:SER:H	1.59	0.67
1:A:613:ARG:HA	1:A:614:ARG:CB	2.26	0.65
1:A:240:THR:HG23	1:A:241:PRO:HD2	1.80	0.64
1:A:804:MET:HE2	1:A:812:TRP:HB2	1.79	0.63
1:A:793:ALA:HB2	1:A:828:ILE:HD12	1.80	0.63
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.82	0.62
1:A:219:CYS:HA	1:A:235:VAL:O	2.00	0.62
1:A:272:LEU:HB3	1:A:305:VAL:HG11	1.82	0.61
1:A:285:THR:HG22	1:A:289:ASN:HB2	1.82	0.61
1:A:404:PHE:N	1:A:404:PHE:HD1	1.97	0.61
1:A:303:ILE:HD12	1:A:303:ILE:H	1.66	0.60
1:A:174:GLU:O	1:A:178:ARG:HD2	2.01	0.60
1:A:613:ARG:HA	1:A:614:ARG:HB3	1.83	0.60
1:A:182:THR:HB	1:A:183:PRO:HD3	1.84	0.60
1:A:198:MET:HE2	1:A:282:VAL:HG21	1.83	0.60
1:A:998:SER:H	1:A:1001:LYS:HG3	1.66	0.59
1:A:198:MET:HE3	1:A:282:VAL:HG11	1.85	0.58
1:A:240:THR:HG22	1:A:242:GLY:H	1.68	0.58
1:A:239:ASP:O	1:A:286:PRO:HA	2.04	0.57
1:A:380:THR:HA	1:A:404:PHE:CD1	2.39	0.57
1:A:482:LEU:HB2	1:A:516:ILE:HG22	1.87	0.56
1:A:568:THR:HG22	1:A:570:GLU:H	1.69	0.56
1:A:629:GLN:HG2	1:A:1029:ILE:HG13	1.88	0.56
1:A:693:HIS:CD2	1:A:789:PRO:HG3	2.41	0.56
1:A:640:VAL:O	1:A:643:ILE:HG12	2.07	0.55
1:A:432:GLN:HB3	1:A:460:LEU:HD11	1.87	0.55
1:A:998:SER:H	1:A:1001:LYS:CG	2.19	0.55
1:A:660:LEU:O	1:A:664:VAL:HG23	2.06	0.55
1:A:273:ARG:HG2	1:A:274:VAL:N	2.22	0.54
1:A:210:TYR:HE2	1:A:859:SER:C	2.16	0.54
1:A:834:HIS:HB2	1:A:876:ILE:HD12	1.89	0.54
1:A:1003:SER:HB2	1:A:1004:PRO:HD2	1.88	0.54
1:A:225:HIS:ND1	1:A:225:HIS:N	2.55	0.54
1:A:467:LEU:HD13	1:A:672:TYR:CE2	2.43	0.54
1:A:737:GLN:O	1:A:741:MET:HG3	2.08	0.53
1:A:434:TYR:CZ	1:A:460:LEU:HD13	2.44	0.53
1:A:1035:LEU:HD12	1:A:1048:ILE:HG12	1.89	0.53
1:A:173:LEU:HD23	1:A:673:HIS:CD2	2.44	0.52
1:A:362:ARG:HG3	1:A:413:TRP:CE3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:811:LEU:HB3	1:A:813:LEU:CD1	2.40	0.52
1:A:180:LEU:C	1:A:183:PRO:HD2	2.35	0.52
1:A:779:LEU:HD12	1:A:796:LEU:HD12	1.92	0.52
1:A:948:HIS:HB2	1:A:1086:TRP:HD1	1.75	0.52
1:A:794:GLY:HA3	1:A:818:ALA:HB2	1.92	0.51
1:A:1060:ASN:C	1:A:1062:GLU:H	2.18	0.51
1:A:224:ILE:HD12	1:A:224:ILE:N	2.25	0.51
1:A:842:MET:HG2	1:A:869:CYS:O	2.11	0.51
1:A:229:THR:HG22	1:A:230:SER:N	2.26	0.51
1:A:395:CYS:SG	1:A:417:SER:HB2	2.50	0.51
1:A:583:LEU:HD21	1:A:614:ARG:H	1.75	0.51
1:A:753:SER:HB2	1:A:757:TYR:CB	2.40	0.51
1:A:701:SER:O	1:A:705:GLN:HG2	2.11	0.50
1:A:424:PRO:HD2	1:A:427:ALA:HB2	1.94	0.50
1:A:303:ILE:HD12	1:A:303:ILE:N	2.26	0.50
1:A:287:ILE:HA	1:A:290:PHE:CD1	2.47	0.50
1:A:549:ASN:O	1:A:553:LYS:HG2	2.12	0.50
1:A:795:ALA:HB3	1:A:816:LYS:HE3	1.95	0.49
1:A:395:CYS:SG	1:A:418:ILE:HG13	2.53	0.49
1:A:567:LEU:HD21	1:A:591:LYS:HD2	1.95	0.49
1:A:807:LYS:CD	1:A:807:LYS:H	2.25	0.49
1:A:174:GLU:HB3	1:A:178:ARG:NH1	2.28	0.49
1:A:882:VAL:HG12	1:A:885:ALA:HB2	1.95	0.49
1:A:359:ARG:HG3	1:A:360:LYS:N	2.28	0.49
1:A:277:ARG:NH1	1:A:791:LEU:HG	2.28	0.48
1:A:829:GLY:HA3	1:A:881:ILE:HD12	1.96	0.48
1:A:558:ILE:HG21	1:A:575:LEU:HD21	1.96	0.48
1:A:779:LEU:HD22	1:A:780:PRO:O	2.14	0.48
1:A:853:SER:O	1:A:857:THR:HG23	2.13	0.48
2:A:1:WYF:O3	2:A:1:WYF:H7	2.14	0.47
1:A:282:VAL:HG23	1:A:283:GLY:N	2.28	0.47
1:A:804:MET:HE1	1:A:831:ILE:HG23	1.97	0.47
1:A:548:PRO:HG2	1:A:551:LEU:HD12	1.97	0.47
1:A:210:TYR:CD1	1:A:211:LEU:HG	2.50	0.47
1:A:997:THR:HA	1:A:1001:LYS:HD2	1.96	0.47
1:A:807:LYS:HD2	1:A:807:LYS:N	2.30	0.46
1:A:390:GLY:O	1:A:391:GLN:HB2	2.13	0.46
1:A:912:LYS:HE2	1:A:918:GLU:OE2	2.15	0.46
1:A:280:TYR:HB3	1:A:282:VAL:HG13	1.97	0.46
1:A:151:GLN:OE1	1:A:722:ARG:NH2	2.48	0.46
1:A:274:VAL:HG21	1:A:292:TRP:CD1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:LYS:HA	1:A:458:VAL:HA	1.79	0.46
1:A:273:ARG:O	1:A:305:VAL:HG13	2.16	0.46
1:A:387:ILE:HD12	1:A:418:ILE:HD12	1.97	0.46
1:A:484:MET:HE3	1:A:516:ILE:HB	1.96	0.46
1:A:888:ILE:HD11	1:A:952:ILE:CG2	2.46	0.46
1:A:948:HIS:HB2	1:A:1086:TRP:CD1	2.50	0.46
1:A:948:HIS:CB	1:A:1086:TRP:HD1	2.28	0.46
1:A:580:TYR:O	1:A:584:LYS:HD3	2.16	0.46
1:A:593:PHE:CE2	1:A:611:LEU:HD21	2.51	0.46
1:A:964:ASP:HA	2:A:1:WYF:C18	2.46	0.46
1:A:287:ILE:N	1:A:287:ILE:HD13	2.30	0.46
1:A:413:TRP:CH2	1:A:519:LEU:HD23	2.51	0.45
1:A:762:GLN:O	1:A:766:GLN:HG2	2.17	0.45
1:A:364:LYS:HA	1:A:412:VAL:O	2.16	0.45
1:A:390:GLY:C	1:A:392:GLN:H	2.25	0.45
1:A:418:ILE:HG22	1:A:419:LYS:O	2.17	0.45
1:A:208:PRO:HB3	1:A:210:TYR:CZ	2.51	0.45
1:A:613:ARG:CA	1:A:614:ARG:CB	2.94	0.45
1:A:1060:ASN:CG	1:A:1061:GLU:N	2.75	0.45
1:A:287:ILE:HD13	1:A:287:ILE:H	1.82	0.44
1:A:397:ARG:HB3	1:A:414:LEU:HD22	1.99	0.44
1:A:191:ARG:O	1:A:191:ARG:HG3	2.18	0.44
1:A:998:SER:O	1:A:999:GLY:C	2.60	0.44
1:A:1062:GLU:C	1:A:1064:ALA:H	2.25	0.44
1:A:198:MET:CE	1:A:282:VAL:HG21	2.47	0.44
1:A:223:VAL:HG12	1:A:225:HIS:CE1	2.53	0.44
1:A:989:PRO:HD3	1:A:1079:GLY:HA2	1.98	0.44
1:A:1003:SER:CB	1:A:1004:PRO:HD2	2.46	0.44
1:A:423:LEU:HA	1:A:424:PRO:HD3	1.81	0.44
1:A:317:GLU:HG2	1:A:318:VAL:N	2.33	0.44
1:A:629:GLN:CG	1:A:1029:ILE:HG13	2.47	0.44
1:A:1060:ASN:CG	1:A:1061:GLU:H	2.25	0.44
1:A:224:ILE:C	1:A:225:HIS:ND1	2.76	0.44
1:A:462:TYR:HA	1:A:485:TRP:O	2.18	0.44
1:A:739:ILE:HD12	1:A:739:ILE:C	2.43	0.44
1:A:935:TYR:CE1	1:A:961:PHE:HA	2.52	0.44
1:A:157:LEU:HD21	1:A:733:THR:HA	2.00	0.44
1:A:366:ARG:HG3	1:A:517:SER:C	2.42	0.44
1:A:1031:PHE:O	1:A:1035:LEU:HG	2.18	0.44
1:A:226:ARG:O	1:A:227:SER:HB2	2.18	0.43
1:A:661:LEU:O	1:A:665:GLN:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:742:LEU:HD22	1:A:813:LEU:HD21	2.01	0.43
1:A:953:MET:HE1	2:A:1:WYF:C4	2.49	0.43
1:A:954:ILE:HG13	1:A:955:THR:O	2.19	0.43
2:A:1:WYF:H7	2:A:1:WYF:H1B	1.78	0.43
1:A:363:VAL:HG12	1:A:416:PHE:HE1	1.84	0.43
1:A:838:LEU:O	1:A:842:MET:HG3	2.19	0.43
1:A:717:LEU:HD22	1:A:721:LEU:HG	2.01	0.42
1:A:1048:ILE:C	1:A:1050:TYR:N	2.77	0.42
1:A:579:ARG:H	1:A:579:ARG:HG3	1.55	0.42
1:A:867:TYR:OH	1:A:963:ILE:HA	2.20	0.42
1:A:926:GLU:O	1:A:929:VAL:HG22	2.20	0.42
1:A:794:GLY:CA	1:A:818:ALA:HB2	2.48	0.42
1:A:197:ALA:HB2	1:A:316:ASP:OD2	2.19	0.42
1:A:395:CYS:HB3	1:A:416:PHE:HD2	1.85	0.42
1:A:434:TYR:HB3	1:A:458:VAL:CG2	2.50	0.42
1:A:287:ILE:HA	1:A:290:PHE:HD1	1.83	0.42
1:A:431:LEU:HD13	1:A:516:ILE:HD12	2.01	0.42
1:A:779:LEU:HD23	1:A:780:PRO:HD2	2.01	0.42
1:A:801:CYS:HA	1:A:812:TRP:O	2.20	0.42
1:A:201:TRP:CE2	1:A:291:GLN:HG3	2.55	0.41
1:A:738:VAL:HG21	1:A:783:PHE:CG	2.55	0.41
1:A:360:LYS:HB3	1:A:416:PHE:O	2.19	0.41
1:A:514:MET:HG3	1:A:515:SER:N	2.34	0.41
1:A:767:LEU:HG	1:A:803:VAL:CG2	2.51	0.41
1:A:607:THR:O	1:A:610:LEU:HB2	2.19	0.41
1:A:593:PHE:CZ	1:A:611:LEU:HD21	2.56	0.41
1:A:737:GLN:HB3	1:A:741:MET:HE3	2.02	0.41
1:A:628:MET:HB2	1:A:1029:ILE:HG21	2.02	0.41
1:A:236:SER:HB3	1:A:239:ASP:OD1	2.21	0.41
1:A:583:LEU:HD12	1:A:610:LEU:HD22	2.03	0.41
1:A:999:GLY:O	1:A:1000:LYS:CB	2.68	0.41
1:A:769:GLN:C	1:A:772:GLU:HG2	2.46	0.41
1:A:862:LEU:HB3	1:A:934:GLY:HA3	2.03	0.41
1:A:996:GLY:O	1:A:1003:SER:HB3	2.21	0.41
1:A:207:LEU:HD21	1:A:211:LEU:C	2.47	0.40
1:A:830:ILE:CG2	1:A:878:MET:HB2	2.50	0.40
1:A:921:PHE:O	1:A:925:VAL:HG23	2.19	0.40
1:A:935:TYR:O	1:A:939:THR:HG23	2.21	0.40
1:A:364:LYS:O	1:A:518:ILE:HA	2.21	0.40
1:A:863:CYS:SG	1:A:930:TYR:HB3	2.61	0.40
1:A:154:LEU:O	1:A:158:ILE:HG13	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:803:VAL:O	1:A:804:MET:C	2.64	0.40
1:A:1048:ILE:C	1:A:1050:TYR:H	2.30	0.40
1:A:319:ARG:HG3	1:A:320:LYS:N	2.36	0.40
1:A:614:ARG:HG2	1:A:617:TRP:HB3	2.03	0.40
1:A:819:ASP:HA	1:A:820:PRO:HD3	1.86	0.40
1:A:807:LYS:CD	1:A:807:LYS:N	2.84	0.40
1:A:817:CYS:C	1:A:819:ASP:H	2.29	0.40
1:A:1058:GLY:O	1:A:1059:LYS:C	2.64	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	801/966 (83%)	720 (90%)	74 (9%)	7 (1%)	14	38

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	966	GLY
1	A	999	GLY
1	A	206	PRO
1	A	269	ASP
1	A	303	ILE
1	A	227	SER
1	A	1000	LYS

5.3.2 Protein sidechains [i](#)

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	685/864 (79%)	614 (90%)	71 (10%)	7 20

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	GLU
1	A	214	LYS
1	A	217	ASN
1	A	225	HIS
1	A	245	LEU
1	A	251	LYS
1	A	271	VAL
1	A	282	VAL
1	A	287	ILE
1	A	306	VAL
1	A	319	ARG
1	A	321	GLU
1	A	357	CYS
1	A	359	ARG
1	A	362	ARG
1	A	369	ASP
1	A	370	ILE
1	A	381	VAL
1	A	393	VAL
1	A	404	PHE
1	A	408	VAL
1	A	420	ILE
1	A	477	ARG
1	A	487	ILE
1	A	502	LEU
1	A	511	GLU
1	A	516	ILE
1	A	570	GLU
1	A	579	ARG
1	A	583	LEU
1	A	609	GLN
1	A	616	VAL
1	A	647	LYS
1	A	651	LEU

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Mol	Chain	Res	Type
1	A	682	LEU
1	A	717	LEU
1	A	759	VAL
1	A	763	VAL
1	A	772	GLU
1	A	775	GLN
1	A	779	LEU
1	A	796	LEU
1	A	798	ILE
1	A	806	SER
1	A	807	LYS
1	A	826	GLU
1	A	838	LEU
1	A	843	LEU
1	A	864	LEU
1	A	865	LEU
1	A	876	ILE
1	A	878	MET
1	A	888	ILE
1	A	890	LYS
1	A	892	GLN
1	A	902	PHE
1	A	908	ASN
1	A	917	THR
1	A	926	GLU
1	A	927	ARG
1	A	954	ILE
1	A	988	THR
1	A	997	THR
1	A	998	SER
1	A	1001	LYS
1	A	1026	LEU
1	A	1029	ILE
1	A	1049	GLU
1	A	1056	THR
1	A	1072	ILE
1	A	1086	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	217	ASN

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Mol	Chain	Res	Type
1	A	392	GLN
1	A	600	GLN
1	A	665	GLN
1	A	710	GLN
1	A	825	ASN
1	A	1007	GLN

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	WYF	A	1	-	32,32,32	1.20	2 (6%)	42,48,48	1.39	7 (16%)

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	WYF	A	1	-	-	3/6/25/25	0/5/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	WYF	C12-N2	4.74	1.51	1.46
2	A	1	WYF	C16-C17	-2.02	1.38	1.41

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	WYF	C13-C14-C15	-3.85	121.92	126.73
2	A	1	WYF	O3-C14-C13	3.06	127.61	124.20
2	A	1	WYF	C12-N2-C11	2.68	115.81	112.06
2	A	1	WYF	O3-C21-C16	2.49	113.18	110.69
2	A	1	WYF	C18-C17-C16	-2.44	118.18	120.92
2	A	1	WYF	C20-C21-C16	-2.44	121.65	124.74
2	A	1	WYF	O2-C15-C14	2.40	128.34	126.21

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	WYF	C7-C2-O1-C1
2	A	1	WYF	C3-C2-O1-C1
2	A	1	WYF	C14-C13-C8-C6

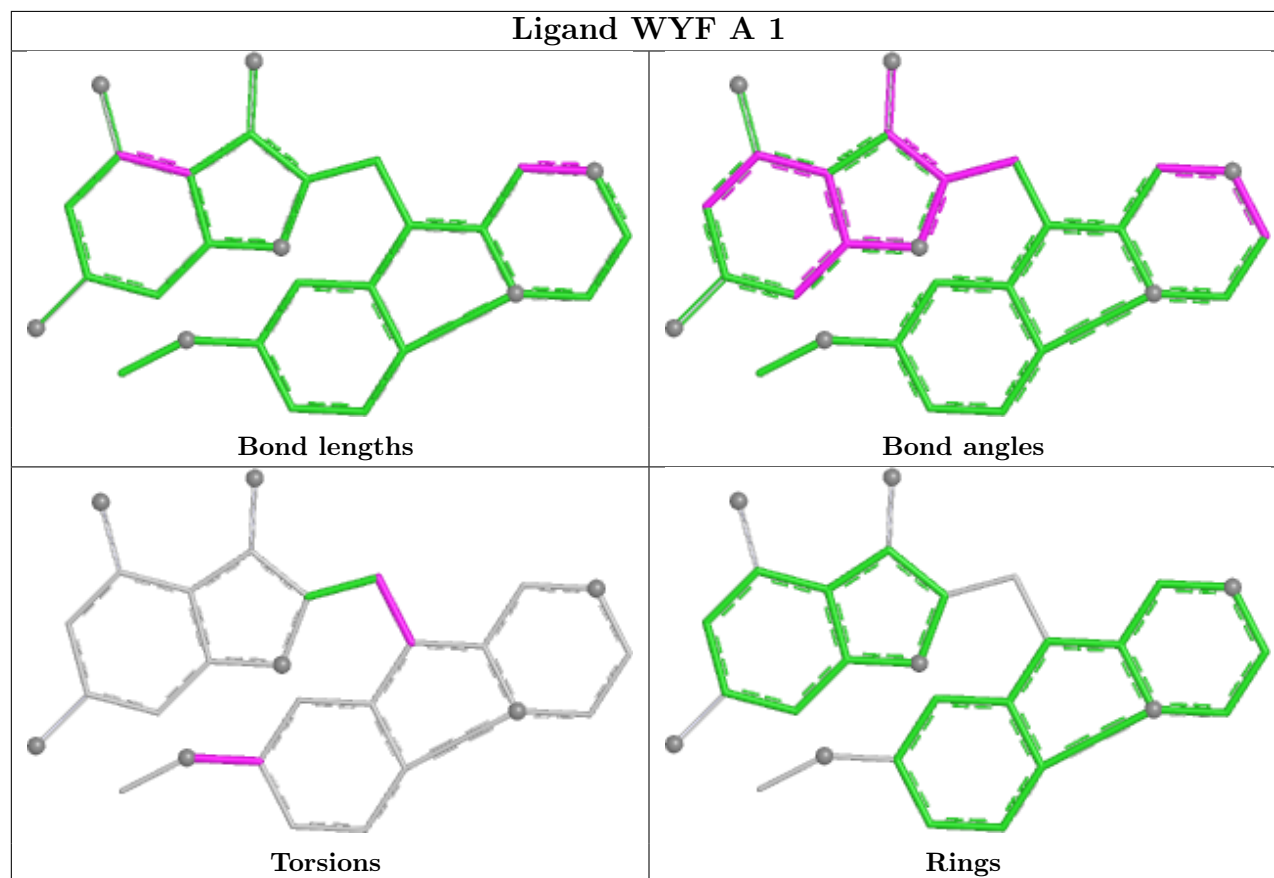
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	WYF	4	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	819/966 (84%)	0.21	15 (1%) 67 60	41, 77, 115, 138	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	435	CYS	3.3
1	A	767	LEU	3.0
1	A	581	GLU	2.7
1	A	380	THR	2.5
1	A	1085	ASN	2.5
1	A	582	SER	2.3
1	A	1075	CYS	2.2
1	A	1086	TRP	2.2
1	A	1070	ASP	2.2
1	A	902	PHE	2.2
1	A	272	LEU	2.1
1	A	162	VAL	2.0
1	A	401	PRO	2.0
1	A	218	ASN	2.0
1	A	404	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

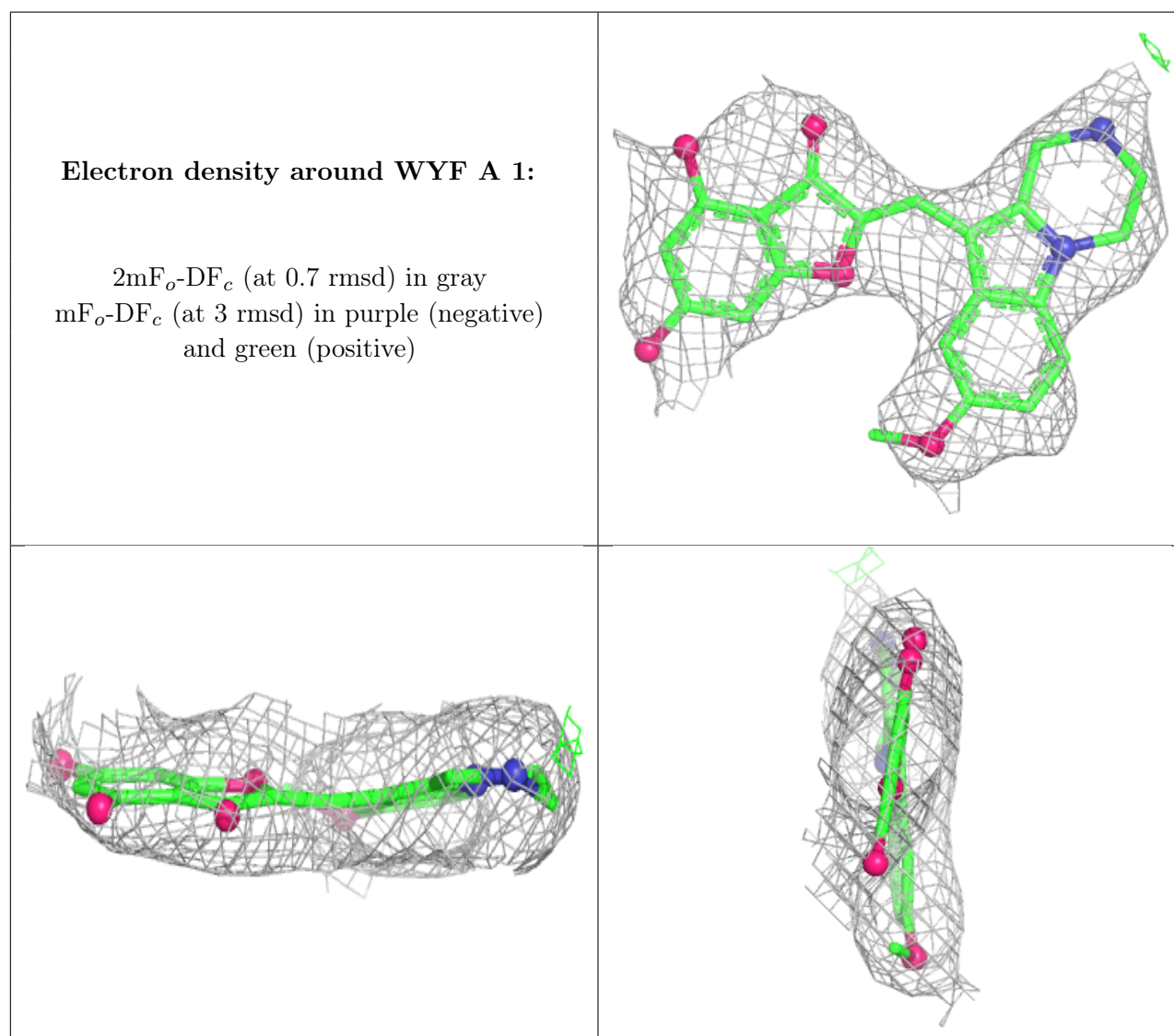
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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(Å ²)	Q<0.9
2	WYF	A	1	28/28	0.86	0.12	69,85,92,96	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.