



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:20 PM UTC

PDB ID : 7KKE / pdb_00007kke
Title : Phosphoinositide 3-Kinase gamma bound to a thiazole inhibitor
Authors : Jacobs, M.D.; Griffith, J.P.
Deposited on : 2020-10-27
Resolution : 2.81 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

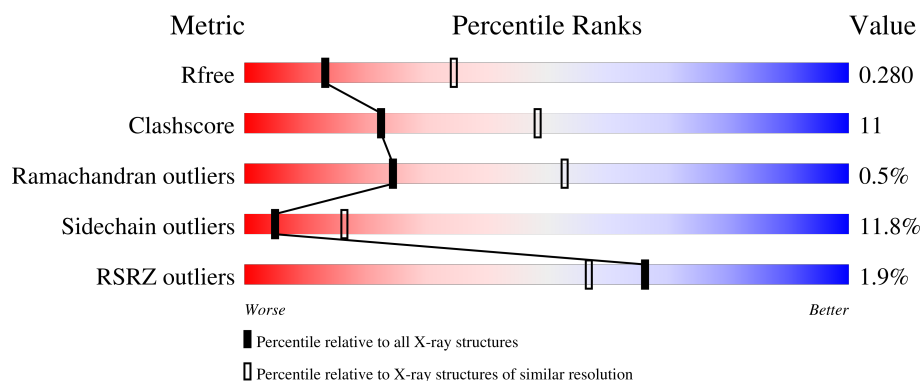
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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	971	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6825 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.

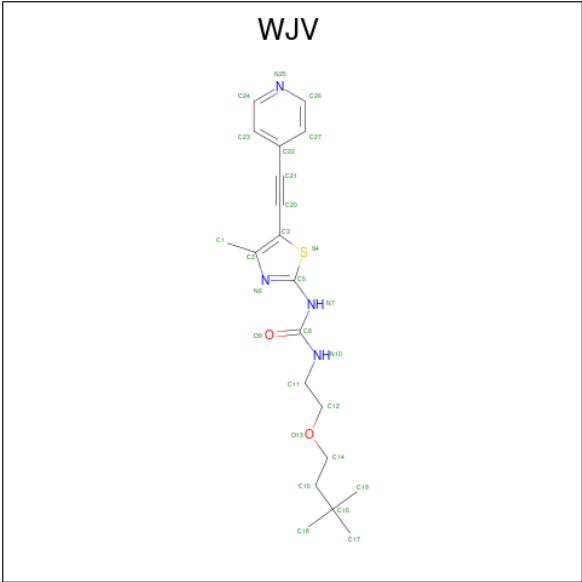
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	842	Total	C	N	O	S	0	0	0
			6775	4352	1149	1239	35			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	140	MET	-	expression tag	UNP P48736
A	141	PRO	-	expression tag	UNP P48736
A	142	MET	-	expression tag	UNP P48736
A	143	ALA	-	expression tag	UNP P48736
A	1103	LEU	-	expression tag	UNP P48736
A	1104	GLU	-	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
A	1109	HIS	-	expression tag	UNP P48736
A	1110	HIS	-	expression tag	UNP P48736

- Molecule 2 is N-[2-(3,3-dimethylbutoxy)ethyl]-N'-{4-methyl-5-[(pyridin-4-yl)ethynyl]-1,3-t hiazol-2-yl}urea (CCD ID: WJV) (formula: C₂₀H₂₆N₄O₂S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	27	20	4	2	1	0	0

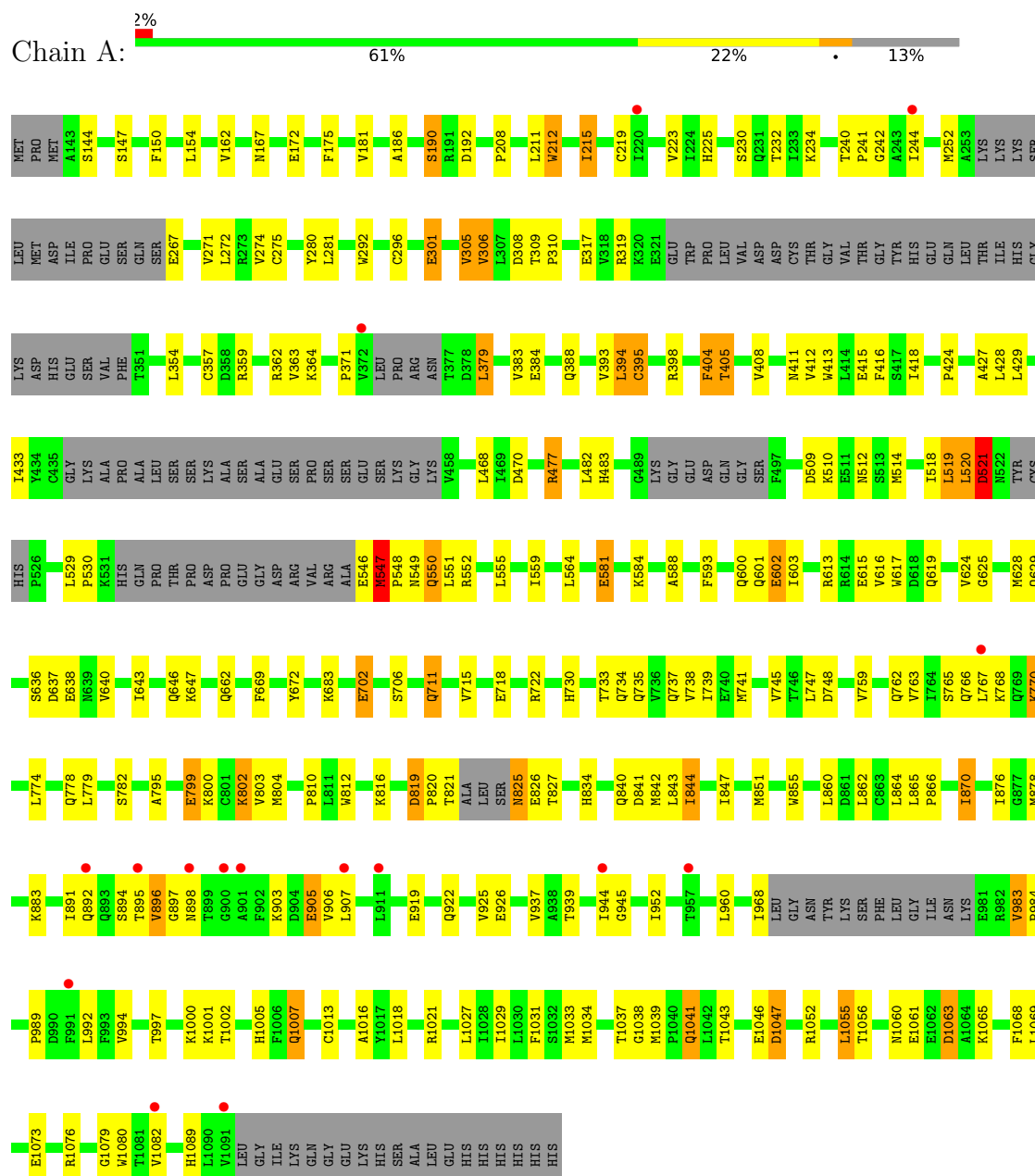
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	23	Total	O	0	0
			23	23		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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	141.46Å 67.05Å 107.40Å 90.00° 97.05° 90.00°	Depositor
Resolution (Å)	62.24 – 2.81 62.24 – 2.81	Depositor EDS
% Data completeness (in resolution range)	80.8 (62.24-2.81) 80.8 (62.24-2.81)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.81Å)	Xtriage
Refinement program	BUSTER	Depositor
R, R_{free}	0.194 , 0.264 0.210 , 0.280	Depositor DCC
R_{free} test set	937 reflections (3.81%)	wwPDB-VP
Wilson B-factor (Å ²)	75.3	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 68.7	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	6825	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.57% 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: WJV

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	0.81	4/6919 (0.1%)	1.16	25/9367 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	896	VAL	C-O	-9.57	1.14	1.24
1	A	826	GLU	CA-C	-7.70	1.43	1.52
1	A	897	GLY	C-O	-5.14	1.18	1.23
1	A	519	LEU	C-O	-5.11	1.17	1.23

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	PHE	CA-CB-CG	7.24	121.04	113.80
1	A	1031	PHE	CA-CB-CG	6.45	120.25	113.80
1	A	1038	GLY	N-CA-C	6.36	119.88	112.50
1	A	280	TYR	N-CA-C	6.19	118.50	108.41
1	A	521	ASP	N-CA-C	-6.11	97.79	110.80
1	A	470	ASP	CA-CB-CG	6.00	118.61	112.60
1	A	371	PRO	CA-C-N	5.71	131.97	121.70
1	A	371	PRO	C-N-CA	5.71	131.97	121.70
1	A	581	GLU	CA-C-N	5.49	128.65	120.31
1	A	581	GLU	C-N-CA	5.49	128.65	120.31
1	A	482	LEU	N-CA-C	5.32	117.39	108.73
1	A	819	ASP	CA-C-N	5.19	124.81	119.56
1	A	819	ASP	C-N-CA	5.19	124.81	119.56
1	A	593	PHE	CA-CB-CG	-5.15	108.65	113.80
1	A	181	VAL	CA-C-N	5.13	127.11	120.44
1	A	181	VAL	C-N-CA	5.13	127.11	120.44
1	A	547	MET	CA-C-N	5.11	125.09	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	547	MET	C-N-CA	5.11	125.09	120.03
1	A	1037	THR	CA-C-N	5.10	125.60	119.94
1	A	1037	THR	C-N-CA	5.10	125.60	119.94
1	A	601	GLN	CA-C-N	5.09	127.42	120.54
1	A	601	GLN	C-N-CA	5.09	127.42	120.54
1	A	702	GLU	CB-CG-CD	5.01	121.12	112.60
1	A	883	LYS	CA-C-N	5.01	131.10	121.54
1	A	883	LYS	C-N-CA	5.01	131.10	121.54

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	6775	0	6765	143	0
2	A	27	0	0	0	0
3	A	23	0	0	2	0
All	All	6825	0	6765	143	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 11.

All (143) 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:895:THR:HG21	1:A:906:VAL:HG12	1.34	1.09
1:A:167:ASN:HD22	1:A:711:GLN:HE22	1.06	0.97
1:A:819:ASP:OD2	1:A:820:PRO:HD2	1.67	0.93
1:A:477:ARG:CZ	1:A:521:ASP:OD1	2.22	0.87
1:A:483:HIS:CD2	1:A:510:LYS:HA	2.09	0.86
1:A:741:MET:HE1	1:A:779:LEU:CB	2.08	0.83
1:A:895:THR:CG2	1:A:906:VAL:HG12	2.10	0.81
1:A:741:MET:HE1	1:A:779:LEU:HB2	1.63	0.80
1:A:477:ARG:NH2	1:A:521:ASP:OD1	2.16	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:825:ASN:N	1:A:825:ASN:OD1	2.17	0.77
1:A:477:ARG:NH1	1:A:521:ASP:OD1	2.18	0.76
1:A:774:LEU:HB3	1:A:779:LEU:HD23	1.65	0.75
1:A:483:HIS:HD2	1:A:510:LYS:HA	1.51	0.75
1:A:364:LYS:HE2	1:A:413:TRP:NE1	2.04	0.73
1:A:274:VAL:HG11	1:A:292:TRP:CD1	2.24	0.72
1:A:778:GLN:HG2	1:A:778:GLN:O	1.92	0.69
1:A:997:THR:HG23	1:A:1001:LYS:HB3	1.74	0.69
1:A:816:LYS:HA	1:A:827:THR:HG22	1.72	0.69
1:A:1043:THR:HB	1:A:1047:ASP:HB2	1.74	0.69
1:A:241:PRO:HA	1:A:244:ILE:HG12	1.75	0.69
1:A:424:PRO:HD2	1:A:427:ALA:HB2	1.76	0.67
1:A:741:MET:HE1	1:A:779:LEU:HB3	1.77	0.67
1:A:223:VAL:HG12	1:A:225:HIS:NE2	2.10	0.66
1:A:1021:ARG:HE	1:A:1056:THR:HB	1.60	0.66
1:A:395:CYS:HB2	1:A:418:ILE:HD11	1.76	0.66
1:A:738:VAL:HA	1:A:741:MET:HE2	1.76	0.66
1:A:394:LEU:HD23	1:A:394:LEU:N	2.12	0.65
1:A:319:ARG:HH12	1:A:722:ARG:NH1	1.94	0.65
1:A:1002:THR:HG22	1:A:1007:GLN:HE21	1.62	0.64
1:A:550:GLN:C	1:A:550:GLN:HE21	2.06	0.64
1:A:1000:LYS:H	1:A:1076:ARG:NH1	1.97	0.63
1:A:741:MET:SD	1:A:779:LEU:HB3	2.39	0.62
1:A:271:VAL:HG13	1:A:310:PRO:HG3	1.80	0.62
1:A:1013:CYS:HG	1:A:1068:PHE:HE2	1.48	0.61
1:A:354:LEU:HD12	1:A:529:LEU:HD13	1.83	0.61
1:A:167:ASN:HD22	1:A:711:GLN:NE2	1.89	0.60
1:A:903:LYS:HE3	1:A:905:GLU:HB3	1.83	0.60
1:A:296:CYS:HA	1:A:301:GLU:HG3	1.82	0.60
1:A:379:LEU:HB2	1:A:404:PHE:HD2	1.67	0.59
1:A:219:CYS:HB3	1:A:234:LYS:HG2	1.83	0.59
1:A:617:TRP:O	1:A:647:LYS:HE2	2.03	0.59
1:A:741:MET:CE	1:A:779:LEU:HB3	2.33	0.57
1:A:1013:CYS:SG	1:A:1068:PHE:HE2	2.26	0.57
1:A:843:LEU:HD13	1:A:1034:MET:HB2	1.85	0.57
1:A:208:PRO:HD2	1:A:211:LEU:HD12	1.86	0.57
1:A:795:ALA:HB3	1:A:816:LYS:HD2	1.86	0.57
1:A:891:ILE:O	1:A:894:SER:HB2	2.04	0.57
1:A:896:VAL:HG13	1:A:896:VAL:O	2.04	0.57
1:A:799:GLU:H	1:A:799:GLU:CD	2.12	0.56
1:A:521:ASP:OD2	3:A:1301:HOH:O	2.17	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:LEU:HD23	1:A:718:GLU:HG3	1.86	0.56
1:A:802:LYS:HG2	1:A:812:TRP:HB3	1.87	0.56
1:A:150:PHE:HE2	1:A:722:ARG:NH1	2.05	0.55
1:A:864:LEU:O	1:A:866:PRO:HD3	2.07	0.55
1:A:395:CYS:HB3	1:A:416:PHE:HD1	1.73	0.54
1:A:223:VAL:CG1	1:A:225:HIS:NE2	2.70	0.54
1:A:903:LYS:HB3	1:A:906:VAL:HG13	1.88	0.54
1:A:983:VAL:HG22	1:A:984:PRO:HD2	1.89	0.53
1:A:1073:GLU:HA	1:A:1076:ARG:HG3	1.90	0.53
1:A:167:ASN:ND2	1:A:711:GLN:HE22	1.90	0.53
1:A:150:PHE:CE2	1:A:722:ARG:NH1	2.77	0.52
1:A:362:ARG:HG3	1:A:413:TRP:CZ3	2.45	0.51
1:A:779:LEU:HD12	1:A:779:LEU:O	2.11	0.51
1:A:405:THR:HG23	1:A:408:VAL:HG22	1.92	0.51
1:A:272:LEU:HB3	1:A:305:VAL:HG21	1.93	0.51
1:A:550:GLN:CA	1:A:550:GLN:NE2	2.73	0.51
1:A:804:MET:HB2	1:A:810:PRO:HD2	1.93	0.51
1:A:637:ASP:HB3	1:A:640:VAL:HB	1.93	0.50
1:A:741:MET:CE	1:A:779:LEU:CB	2.87	0.50
1:A:212:TRP:HA	1:A:215:ILE:HD12	1.92	0.50
1:A:240:THR:HG22	1:A:242:GLY:H	1.77	0.49
1:A:384:GLU:HG3	1:A:398:ARG:HG2	1.92	0.49
1:A:748:ASP:HB3	1:A:770:LYS:HZ1	1.77	0.49
1:A:1027:LEU:HD12	1:A:1055:LEU:HD21	1.94	0.49
1:A:730:HIS:NE2	1:A:734:GLN:NE2	2.61	0.49
1:A:640:VAL:O	1:A:643:ILE:HG12	2.12	0.49
1:A:584:LYS:HA	1:A:616:VAL:HG21	1.95	0.49
1:A:144:SER:HB3	1:A:147:SER:HB2	1.95	0.48
1:A:840:GLN:O	1:A:844:ILE:HD12	2.13	0.48
1:A:842:MET:HE3	1:A:870:ILE:HA	1.95	0.48
1:A:275:CYS:SG	1:A:306:VAL:HG12	2.54	0.48
1:A:892:GLN:C	1:A:894:SER:H	2.21	0.48
1:A:1002:THR:CG2	1:A:1007:GLN:HE21	2.26	0.48
1:A:395:CYS:HB2	1:A:418:ILE:CD1	2.43	0.48
1:A:363:VAL:HG23	1:A:520:LEU:HD23	1.95	0.48
1:A:319:ARG:HH12	1:A:722:ARG:HH11	1.61	0.48
1:A:855:TRP:HB3	1:A:860:LEU:HB2	1.96	0.47
1:A:364:LYS:HZ3	1:A:411:ASN:ND2	2.12	0.47
1:A:989:PRO:HD2	1:A:1080:TRP:CE2	2.49	0.47
1:A:477:ARG:NH2	1:A:521:ASP:CG	2.72	0.47
1:A:150:PHE:CE2	1:A:319:ARG:NH1	2.83	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:GLN:C	1:A:550:GLN:NE2	2.72	0.47
1:A:870:ILE:HD11	1:A:878:MET:HE3	1.95	0.47
1:A:1000:LYS:H	1:A:1076:ARG:HH12	1.61	0.47
1:A:552:ARG:HH21	1:A:581:GLU:CD	2.23	0.46
1:A:745:VAL:HG21	1:A:774:LEU:HD11	1.97	0.46
1:A:862:LEU:HD11	1:A:1016:ALA:HB2	1.97	0.46
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.98	0.46
1:A:1013:CYS:SG	1:A:1068:PHE:CE2	3.04	0.46
1:A:937:VAL:HG22	1:A:1068:PHE:CZ	2.50	0.46
1:A:364:LYS:NZ	1:A:411:ASN:ND2	2.64	0.46
1:A:1039:MET:SD	1:A:1041:GLN:NE2	2.89	0.46
1:A:1060:ASN:ND2	1:A:1063:ASP:H	2.14	0.46
1:A:779:LEU:HD12	1:A:779:LEU:C	2.41	0.46
1:A:319:ARG:NH1	1:A:722:ARG:NH1	2.63	0.45
1:A:767:LEU:HD22	1:A:803:VAL:HG23	1.98	0.45
1:A:925:VAL:HG23	1:A:994:VAL:HG12	1.98	0.45
1:A:669:PHE:HE2	1:A:1033:MET:HE3	1.81	0.45
1:A:364:LYS:HE2	1:A:413:TRP:CE2	2.51	0.45
1:A:433:ILE:HG21	1:A:514:MET:HE3	1.98	0.45
1:A:774:LEU:CB	1:A:779:LEU:HD23	2.40	0.44
1:A:602:GLU:H	1:A:602:GLU:CD	2.25	0.44
1:A:821:THR:O	1:A:821:THR:HG22	2.17	0.44
1:A:847:ILE:HG22	1:A:851:MET:HE3	1.98	0.44
1:A:223:VAL:CG1	1:A:225:HIS:HE2	2.30	0.44
1:A:477:ARG:CZ	1:A:521:ASP:CG	2.91	0.44
1:A:834:HIS:HB2	1:A:876:ILE:HD13	1.99	0.44
1:A:1000:LYS:N	1:A:1076:ARG:HH12	2.16	0.43
1:A:306:VAL:HG22	1:A:308:ASP:HB2	2.01	0.43
1:A:274:VAL:CG1	1:A:292:TRP:CD1	2.98	0.43
1:A:702:GLU:O	1:A:706:SER:HB3	2.18	0.43
1:A:230:SER:O	1:A:230:SER:OG	2.27	0.43
1:A:735:GLN:O	1:A:739:ILE:HG12	2.19	0.43
1:A:559:ILE:HG12	1:A:588:ALA:HB2	2.01	0.42
1:A:296:CYS:HA	1:A:301:GLU:CG	2.48	0.42
1:A:547:MET:HE2	1:A:551:LEU:C	2.45	0.42
1:A:223:VAL:HG12	1:A:225:HIS:CD2	2.54	0.42
1:A:364:LYS:HB3	1:A:519:LEU:HB3	2.01	0.42
1:A:388:GLN:HG2	1:A:393:VAL:HG22	2.02	0.42
1:A:737:GLN:O	1:A:741:MET:HG3	2.20	0.42
1:A:306:VAL:HG11	1:A:821:THR:HG21	2.01	0.42
1:A:564:LEU:HB2	1:A:1052:ARG:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:555:LEU:O	1:A:559:ILE:HG13	2.20	0.41
1:A:509:ASP:OD2	1:A:512:ASN:HB2	2.20	0.41
1:A:625:GLY:O	1:A:629:GLN:HG3	2.20	0.41
1:A:672:TYR:HA	3:A:1305:HOH:O	2.20	0.41
1:A:186:ALA:O	1:A:190:SER:HB2	2.20	0.41
1:A:765:SER:HA	1:A:768:LYS:HG2	2.02	0.41
1:A:939:THR:HB	1:A:945:GLY:HA2	2.03	0.41
1:A:529:LEU:HA	1:A:530:PRO:HD3	1.94	0.41
1:A:547:MET:HA	1:A:548:PRO:HD2	1.94	0.40
1:A:870:ILE:HG13	1:A:878:MET:HG2	2.02	0.40
1:A:1073:GLU:HA	1:A:1076:ARG:CG	2.51	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	822/971 (85%)	773 (94%)	45 (6%)	4 (0%)	24 53

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	898	ASN
1	A	521	ASP
1	A	547	MET
1	A	1079	GLY

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	746/868 (86%)	658 (88%)	88 (12%)	5 16

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	162	VAL
1	A	172	GLU
1	A	190	SER
1	A	192	ASP
1	A	212	TRP
1	A	215	ILE
1	A	232	THR
1	A	252	MET
1	A	267	GLU
1	A	281	LEU
1	A	301	GLU
1	A	305	VAL
1	A	306	VAL
1	A	309	THR
1	A	317	GLU
1	A	357	CYS
1	A	359	ARG
1	A	379	LEU
1	A	383	VAL
1	A	394	LEU
1	A	395	CYS
1	A	404	PHE
1	A	405	THR
1	A	412	VAL
1	A	415	GLU
1	A	428	LEU
1	A	477	ARG
1	A	518	ILE
1	A	520	LEU
1	A	546	GLU
1	A	549	ASN
1	A	550	GLN
1	A	600	GLN
1	A	602	GLU

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Mol	Chain	Res	Type
1	A	603	ILE
1	A	613	ARG
1	A	615	GLU
1	A	619	GLN
1	A	624	VAL
1	A	628	MET
1	A	636	SER
1	A	638	GLU
1	A	646	GLN
1	A	662	GLN
1	A	683	LYS
1	A	711	GLN
1	A	715	VAL
1	A	733	THR
1	A	747	LEU
1	A	759	VAL
1	A	762	GLN
1	A	763	VAL
1	A	766	GLN
1	A	770	LYS
1	A	782	SER
1	A	799	GLU
1	A	800	LYS
1	A	802	LYS
1	A	825	ASN
1	A	841	ASP
1	A	844	ILE
1	A	865	LEU
1	A	870	ILE
1	A	905	GLU
1	A	907	LEU
1	A	919	GLU
1	A	922	GLN
1	A	926	GLU
1	A	944	ILE
1	A	952	ILE
1	A	960	LEU
1	A	968	ILE
1	A	983	VAL
1	A	992	LEU
1	A	1005	HIS
1	A	1007	GLN

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Mol	Chain	Res	Type
1	A	1018	LEU
1	A	1029	ILE
1	A	1041	GLN
1	A	1046	GLU
1	A	1047	ASP
1	A	1055	LEU
1	A	1061	GLU
1	A	1063	ASP
1	A	1065	LYS
1	A	1069	LEU
1	A	1082	VAL
1	A	1089	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	217	ASN
1	A	299	ASN
1	A	386	ASN
1	A	388	GLN
1	A	411	ASN
1	A	430	ASN
1	A	432	GLN
1	A	483	HIS
1	A	550	GLN
1	A	554	GLN
1	A	585	HIS
1	A	600	GLN
1	A	711	GLN
1	A	734	GLN
1	A	769	GLN
1	A	778	GLN
1	A	825	ASN
1	A	959	ASN
1	A	1007	GLN
1	A	1022	HIS
1	A	1071	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 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	WJV	A	1201	-	27,28,28	1.09	3 (11%)	35,37,37	2.99	9 (25%)

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	WJV	A	1201	-	-	4/19/19/19	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	WJV	C2-N6	-3.00	1.32	1.38
2	A	1201	WJV	C5-S4	-2.96	1.68	1.73
2	A	1201	WJV	C20-C21	-2.42	1.16	1.20

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	WJV	C5-N6-C2	12.89	118.24	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	WJV	S4-C5-N6	-7.44	109.12	115.78
2	A	1201	WJV	C5-S4-C3	4.38	91.08	88.35
2	A	1201	WJV	C3-C2-N6	-3.86	112.32	115.00
2	A	1201	WJV	C1-C2-N6	2.94	125.22	119.32
2	A	1201	WJV	C26-N25-C24	2.90	123.49	116.86
2	A	1201	WJV	C20-C3-S4	2.77	125.47	119.02
2	A	1201	WJV	N7-C5-N6	2.15	124.89	121.18
2	A	1201	WJV	C23-C24-N25	-2.03	120.13	123.60

There are no chirality outliers.

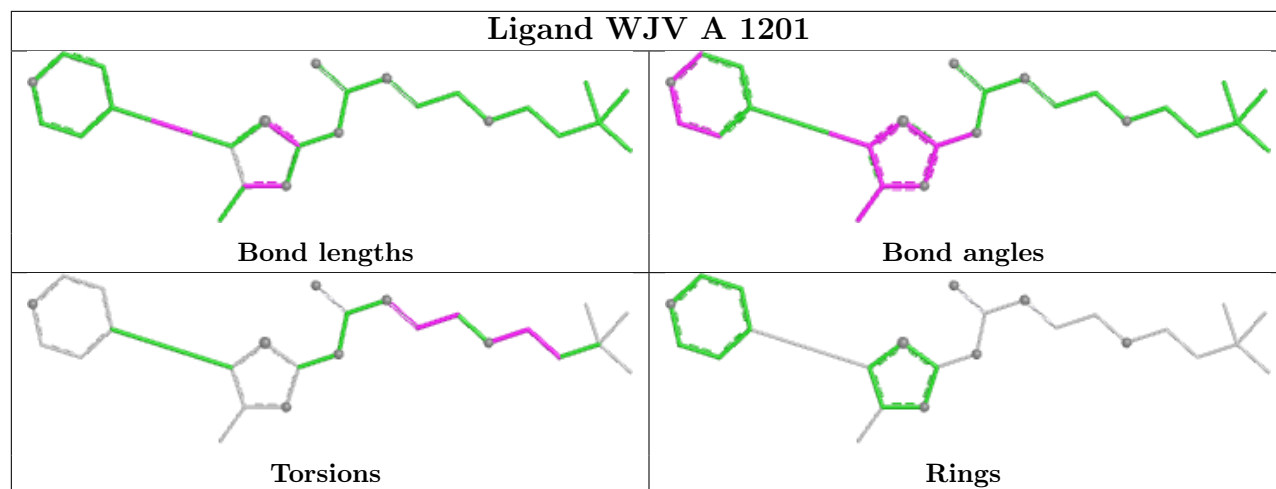
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201	WJV	O13-C14-C15-C16
2	A	1201	WJV	N10-C11-C12-O13
2	A	1201	WJV	C12-C11-N10-C8
2	A	1201	WJV	C15-C14-O13-C12

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 [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	842/971 (86%)	0.00	16 (1%) 66 57	39, 82, 130, 150	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	892	GLN	3.8
1	A	898	ASN	2.7
1	A	911	LEU	2.6
1	A	220	ILE	2.4
1	A	991	PHE	2.4
1	A	895	THR	2.4
1	A	944	ILE	2.3
1	A	901	ALA	2.3
1	A	244	ILE	2.3
1	A	907	LEU	2.3
1	A	900	GLY	2.2
1	A	1082	VAL	2.1
1	A	767	LEU	2.1
1	A	957	THR	2.1
1	A	372	VAL	2.0
1	A	1091	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

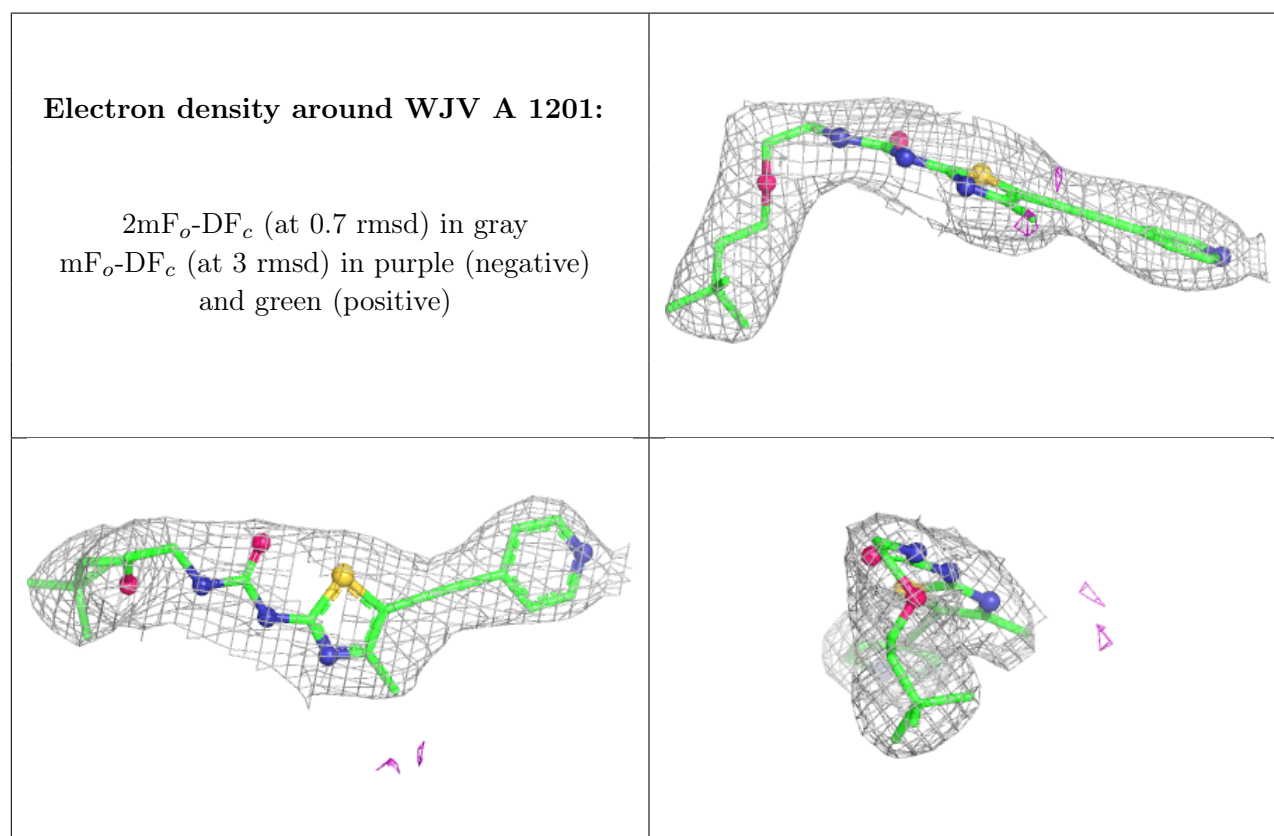
There are no oligosaccharides in this entry.

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(Å ²)	Q<0.9
2	WJV	A	1201	27/27	0.96	0.08	64,66,67,68	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.