



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:05 PM UTC

PDB ID : 4PS3 / pdb_00004ps3
Title : Structure of PI3K gamma in complex with 1-[6-(5-methoxypyridin-3-yl)-1,3-benzothiazol-2-yl]-3-[2-(1-propyl-1H-imidazol-4-yl)ethyl]urea
Authors : Griffith, J.P.
Deposited on : 2014-03-06
Resolution : 2.90 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

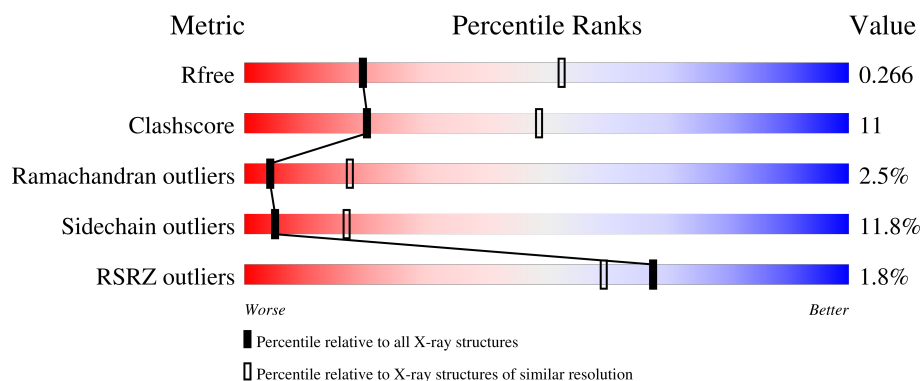
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	966	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6881 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.

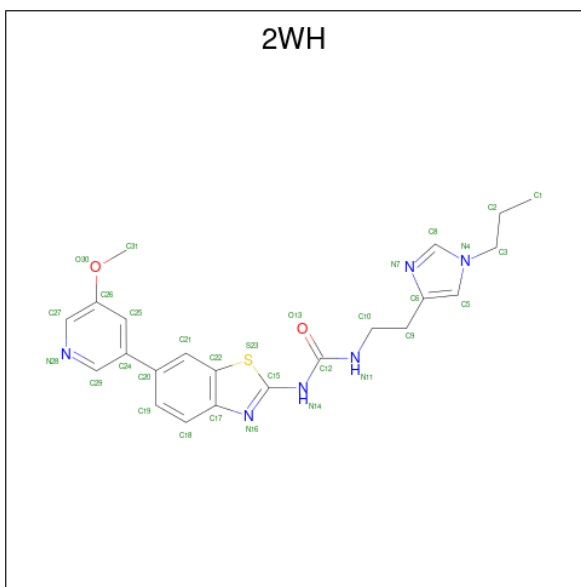
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	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 1-[6-(5-methoxypyridin-3-yl)-1,3-benzothiazol-2-yl]-3-[2-(1-propyl-1H-imidazol-4-yl)ethyl]urea (CCD ID: 2WH) (formula: C₂₂H₂₄N₆O₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			31	22	6	2	1		

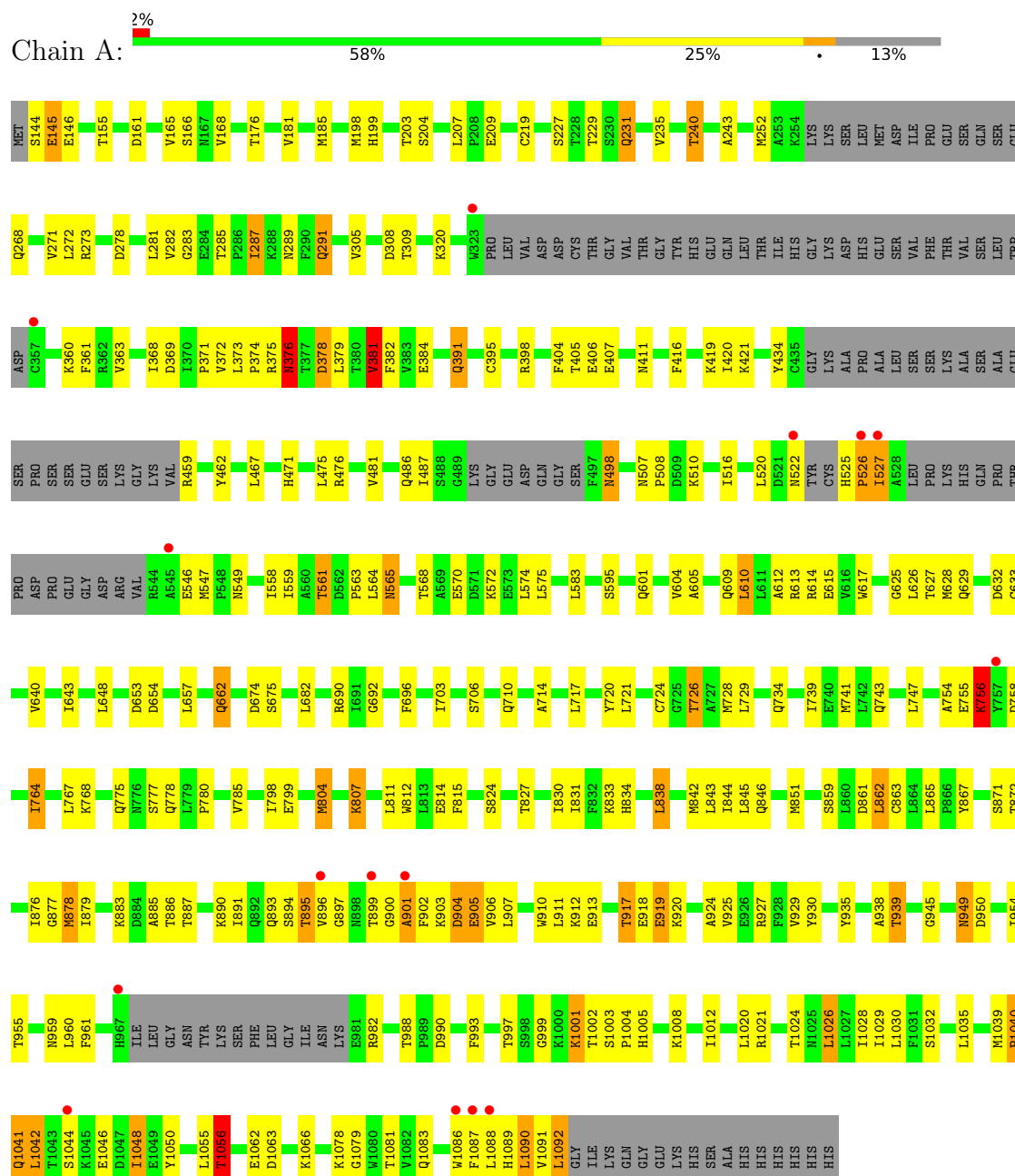
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total	O	0	0
			6	6		

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	143.69Å 67.79Å 106.12Å 90.00° 96.16° 90.00°	Depositor
Resolution (Å)	105.51 – 2.90 105.51 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (105.51-2.90) 99.8 (105.51-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.39 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.211 , 0.259 0.224 , 0.266	Depositor DCC
R_{free} test set	1164 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	72.6	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 64.9	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	6881	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.48% 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: 2WH

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	0.84	3/6992 (0.0%)	1.03	13/9457 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1078	LYS	C-O	10.06	1.37	1.24
1	A	904	ASP	CB-CG	8.01	1.72	1.52
1	A	904	ASP	CG-OD2	-5.03	1.15	1.25

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1056	THR	CB-CA-C	6.37	120.40	111.86
1	A	906	VAL	N-CA-C	6.00	116.74	110.62
1	A	824	SER	N-CA-C	5.60	117.36	108.79
1	A	546	GLU	N-CA-C	5.57	117.81	108.96
1	A	904	ASP	CA-CB-CG	5.57	118.17	112.60
1	A	547	MET	N-CA-C	5.51	116.83	109.83
1	A	559	ILE	CB-CA-C	-5.47	104.76	112.14
1	A	785	VAL	N-CA-C	-5.36	102.69	107.56
1	A	899	THR	N-CA-C	-5.35	105.55	111.71
1	A	381	VAL	N-CA-C	5.33	115.38	108.35
1	A	785	VAL	CA-C-N	5.23	125.28	119.32
1	A	785	VAL	C-N-CA	5.23	125.28	119.32
1	A	844	ILE	CB-CA-C	-5.03	105.54	111.97

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	155	0
2	A	31	0	24	8	0
3	A	6	0	0	3	0
All	All	6881	0	6910	156	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 (156) 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	1.35	1.03
1:A:851:MET:HE1	1:A:938:ALA:HA	1.57	0.85
1:A:176:THR:HG23	1:A:674:ASP:HB2	1.64	0.79
1:A:893:GLN:HA	1:A:897:GLY:CA	2.16	0.74
1:A:883:LYS:NZ	2:A:1201:2WH:H4	2.03	0.73
1:A:935:TYR:O	1:A:939:THR:HB	1.90	0.71
1:A:851:MET:HE1	1:A:938:ALA:CA	2.21	0.70
1:A:525:HIS:HB2	1:A:526:PRO:HD3	1.73	0.69
1:A:883:LYS:HZ3	2:A:1201:2WH:H4	1.56	0.67
1:A:867:TYR:OH	3:A:1302:HOH:O	2.13	0.66
1:A:1086:TRP:CE3	1:A:1087:PHE:HA	2.30	0.66
1:A:842:MET:HE2	1:A:871:SER:CB	2.27	0.65
1:A:1041:GLN:HE21	1:A:1041:GLN:HA	1.61	0.64
1:A:1035:LEU:HA	1:A:1039:MET:HG2	1.80	0.63
1:A:583:LEU:HD22	1:A:610:LEU:HD22	1.81	0.63
1:A:804:MET:HE2	1:A:812:TRP:HB2	1.82	0.62
1:A:842:MET:HE2	1:A:871:SER:HB2	1.81	0.62
1:A:919:GLU:OE2	1:A:920:LYS:N	2.33	0.62
1:A:949:ASN:H	1:A:1083:GLN:HE22	1.46	0.62
1:A:525:HIS:CB	1:A:526:PRO:HD3	2.32	0.58
1:A:851:MET:HE1	1:A:938:ALA:CB	2.33	0.58
1:A:918:GLU:O	1:A:918:GLU:OE1	2.22	0.58
1:A:804:MET:HE1	1:A:831:ILE:HG12	1.86	0.57
1:A:741:MET:HE1	1:A:778:GLN:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:893:GLN:CA	1:A:897:GLY:HA2	2.24	0.57
1:A:925:VAL:O	1:A:929:VAL:HG23	2.05	0.57
1:A:1021:ARG:O	1:A:1024:THR:OG1	2.17	0.56
1:A:863:CYS:SG	1:A:927:ARG:NH1	2.80	0.55
1:A:1086:TRP:CH2	1:A:1090:LEU:HD21	2.41	0.55
1:A:814:GLU:OE2	2:A:1201:2WH:H7	2.05	0.55
1:A:381:VAL:HG21	1:A:404:PHE:CD2	2.42	0.54
1:A:291:GLN:HA	1:A:291:GLN:HE21	1.72	0.54
1:A:851:MET:HE3	1:A:1020:LEU:HD11	1.90	0.54
1:A:1089:HIS:C	1:A:1091:VAL:N	2.63	0.54
1:A:807:LYS:NZ	3:A:1305:HOH:O	2.41	0.54
1:A:614:ARG:HG2	1:A:617:TRP:HB3	1.89	0.54
1:A:498:ASN:OD1	1:A:498:ASN:C	2.50	0.54
1:A:308:ASP:N	1:A:308:ASP:OD1	2.41	0.53
1:A:405:THR:O	1:A:407:GLU:N	2.41	0.53
1:A:1024:THR:HG22	1:A:1028:ILE:HD12	1.89	0.53
1:A:905:GLU:HG3	1:A:993:PHE:CE2	2.44	0.53
1:A:743:GLN:O	1:A:747:LEU:HD12	2.09	0.53
1:A:861:ASP:C	1:A:862:LEU:HD22	2.34	0.53
1:A:726:THR:HA	1:A:729:LEU:HD12	1.91	0.52
1:A:1005:HIS:O	1:A:1008:LYS:HB3	2.09	0.52
1:A:583:LEU:HD22	1:A:610:LEU:CD2	2.39	0.52
1:A:827:THR:O	1:A:883:LYS:NZ	2.43	0.52
1:A:271:VAL:HG23	1:A:282:VAL:CG1	2.40	0.52
1:A:997:THR:HG23	1:A:1001:LYS:HG3	1.91	0.52
1:A:614:ARG:O	1:A:615:GLU:C	2.52	0.52
1:A:434:TYR:HA	1:A:459:ARG:O	2.10	0.51
1:A:565:ASN:C	1:A:565:ASN:ND2	2.69	0.51
1:A:764:ILE:O	1:A:768:LYS:HG2	2.09	0.51
1:A:391:GLN:OE1	1:A:633:CYS:HB2	2.10	0.51
1:A:378:ASP:N	1:A:378:ASP:OD1	2.44	0.51
1:A:692:GLY:HA3	1:A:720:TYR:OH	2.10	0.51
1:A:1050:TYR:C	1:A:1050:TYR:CD1	2.88	0.50
1:A:181:VAL:O	1:A:185:MET:HG3	2.11	0.50
1:A:240:THR:HG22	1:A:243:ALA:H	1.76	0.50
1:A:363:VAL:HG13	1:A:363:VAL:O	2.11	0.50
1:A:674:ASP:OD1	1:A:674:ASP:C	2.55	0.50
1:A:272:LEU:HB3	1:A:305:VAL:HG11	1.94	0.50
1:A:814:GLU:OE2	2:A:1201:2WH:C3	2.60	0.49
1:A:231:GLN:HE21	1:A:231:GLN:HA	1.77	0.49
1:A:384:GLU:OE2	1:A:398:ARG:NH1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1086:TRP:CZ3	1:A:1090:LEU:HD21	2.47	0.49
1:A:1026:LEU:O	1:A:1030:LEU:HG	2.13	0.49
2:A:1201:2WH:S23	2:A:1201:2WH:O13	2.70	0.49
1:A:419:LYS:O	1:A:420:ILE:C	2.56	0.49
1:A:475:LEU:HD21	1:A:522:ASN:HB2	1.95	0.48
1:A:887:THR:CG2	1:A:950:ASP:HA	2.44	0.48
1:A:883:LYS:NZ	2:A:1201:2WH:C2	2.75	0.48
1:A:564:LEU:HD11	1:A:1048:ILE:HG22	1.95	0.48
1:A:939:THR:HG23	1:A:945:GLY:CA	2.44	0.48
1:A:885:ALA:H	2:A:1201:2WH:H10	1.79	0.47
1:A:911:LEU:HD22	1:A:924:ALA:HB1	1.96	0.47
1:A:935:TYR:CE2	1:A:961:PHE:HA	2.50	0.47
1:A:558:ILE:O	1:A:561:THR:HB	2.13	0.47
1:A:703:ILE:HD11	1:A:714:ALA:HA	1.96	0.47
1:A:734:GLN:NE2	1:A:780:PRO:HB3	2.30	0.47
1:A:988:THR:OG1	1:A:990:ASP:OD1	2.30	0.47
1:A:1021:ARG:HE	1:A:1056:THR:HG22	1.79	0.47
1:A:901:ALA:O	1:A:902:PHE:CG	2.68	0.46
1:A:361:PHE:HB2	1:A:420:ILE:HD13	1.97	0.46
1:A:706:SER:O	1:A:710:GLN:HB3	2.16	0.46
1:A:939:THR:HG23	1:A:945:GLY:HA2	1.96	0.46
1:A:609:GLN:O	1:A:612:ALA:HB3	2.16	0.46
1:A:181:VAL:HG12	1:A:185:MET:HE2	1.98	0.46
1:A:1055:LEU:O	1:A:1056:THR:HG22	2.16	0.46
1:A:917:THR:OG1	1:A:919:GLU:OE2	2.34	0.46
1:A:918:GLU:O	1:A:918:GLU:CD	2.59	0.46
1:A:1042:LEU:HD22	1:A:1042:LEU:O	2.16	0.46
1:A:1092:LEU:O	1:A:1092:LEU:HD13	2.16	0.46
1:A:411:ASN:O	1:A:411:ASN:ND2	2.50	0.45
1:A:838:LEU:HD23	1:A:877:GLY:HA3	1.97	0.45
1:A:421:LYS:HE3	1:A:527:ILE:HD12	1.98	0.45
1:A:954:ILE:HA	1:A:960:LEU:HA	1.98	0.45
1:A:155:THR:HG23	1:A:161:ASP:HA	1.99	0.45
1:A:755:GLU:O	1:A:756:LYS:C	2.59	0.45
1:A:878:MET:C	1:A:879:ILE:HG13	2.42	0.45
1:A:960:LEU:C	1:A:960:LEU:HD23	2.41	0.45
1:A:930:TYR:CE2	1:A:1012:ILE:HD13	2.52	0.44
1:A:376:ASN:OD1	1:A:376:ASN:C	2.59	0.44
1:A:568:THR:HG22	1:A:570:GLU:H	1.82	0.44
1:A:883:LYS:HD3	2:A:1201:2WH:H4	1.99	0.44
1:A:507:ASN:HA	1:A:508:PRO:HD2	1.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:756:LYS:O	1:A:758:ASP:O	2.36	0.44
1:A:891:ILE:HG12	1:A:910:TRP:CD1	2.53	0.44
1:A:368:ILE:HG22	1:A:516:ILE:HB	1.99	0.44
1:A:628:MET:HE1	1:A:662:GLN:HB3	1.99	0.44
1:A:632:ASP:C	1:A:632:ASP:OD1	2.60	0.44
1:A:1089:HIS:O	1:A:1091:VAL:N	2.51	0.44
1:A:165:VAL:HG12	1:A:165:VAL:O	2.18	0.44
1:A:572:LYS:HD3	1:A:595:SER:HA	1.99	0.44
1:A:955:THR:OG1	1:A:959:ASN:N	2.41	0.43
1:A:283:GLY:O	1:A:285:THR:N	2.50	0.43
1:A:481:VAL:O	1:A:481:VAL:HG12	2.17	0.43
1:A:862:LEU:N	1:A:862:LEU:CD2	2.81	0.43
1:A:872:THR:OG1	1:A:877:GLY:HA2	2.19	0.43
1:A:842:MET:HE2	1:A:871:SER:HB3	1.97	0.43
1:A:811:LEU:O	1:A:831:ILE:HA	2.18	0.43
1:A:627:THR:HG21	1:A:648:LEU:CD2	2.48	0.43
1:A:657:LEU:HD11	1:A:690:ARG:HD3	2.01	0.43
1:A:1089:HIS:O	1:A:1090:LEU:C	2.61	0.43
1:A:144:SER:OG	1:A:145:GLU:N	2.50	0.43
1:A:198:MET:O	1:A:199:HIS:C	2.60	0.42
1:A:625:GLY:O	1:A:629:GLN:HG3	2.18	0.42
1:A:653:ASP:O	1:A:654:ASP:C	2.60	0.42
1:A:756:LYS:HA	1:A:756:LYS:NZ	2.34	0.42
1:A:894:SER:OG	1:A:895:THR:N	2.52	0.42
1:A:1003:SER:HB2	1:A:1004:PRO:HD2	2.00	0.42
1:A:834:HIS:HB2	1:A:876:ILE:HD12	2.01	0.42
1:A:1039:MET:HB3	1:A:1040:PRO:HD2	2.01	0.42
1:A:462:TYR:CD1	1:A:486:GLN:HA	2.53	0.42
1:A:395:CYS:HG	1:A:416:PHE:HD1	1.67	0.42
1:A:640:VAL:O	1:A:643:ILE:HG12	2.20	0.42
1:A:382:PHE:CD2	1:A:382:PHE:C	2.97	0.42
1:A:721:LEU:HA	1:A:724:CYS:SG	2.60	0.42
1:A:734:GLN:HE22	1:A:780:PRO:HB3	1.85	0.41
1:A:833:LYS:CE	3:A:1304:HOH:O	2.69	0.41
1:A:949:ASN:H	1:A:1083:GLN:NE2	2.17	0.41
1:A:527:ILE:HD11	1:A:601:GLN:OE1	2.21	0.41
1:A:563:PRO:HD2	1:A:1028:ILE:HG21	2.03	0.41
1:A:815:PHE:CE1	1:A:830:ILE:HD12	2.56	0.41
1:A:1032:SER:HB2	1:A:1048:ILE:HG21	2.02	0.41
1:A:1062:GLU:O	1:A:1063:ASP:C	2.63	0.41
1:A:604:VAL:O	1:A:605:ALA:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:696:PHE:CD1	1:A:696:PHE:C	2.99	0.41
1:A:273:ARG:O	1:A:305:VAL:HG13	2.20	0.41
1:A:467:LEU:O	1:A:476:ARG:NH1	2.54	0.40
1:A:198:MET:C	1:A:199:HIS:CG	2.99	0.40
1:A:411:ASN:O	1:A:411:ASN:CG	2.64	0.40
1:A:209:GLU:HB2	1:A:859:SER:HB3	2.03	0.40
1:A:287:ILE:C	1:A:289:ASN:N	2.77	0.40
1:A:614:ARG:NH1	1:A:643:ILE:HG22	2.36	0.40
1:A:804:MET:HB2	1:A:804:MET:HE3	1.81	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%)	737 (89%)	69 (8%)	21 (2%)	4 17

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	227	SER
1	A	374	PRO
1	A	406	GLU
1	A	527	ILE
1	A	754	ALA
1	A	949	ASN
1	A	376	ASN
1	A	471	HIS
1	A	726	THR
1	A	756	LYS
1	A	1090	LEU
1	A	900	GLY

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Mol	Chain	Res	Type
1	A	1040	PRO
1	A	371	PRO
1	A	901	ALA
1	A	999	GLY
1	A	391	GLN
1	A	252	MET
1	A	526	PRO
1	A	777	SER
1	A	1079	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	757/864 (88%)	668 (88%)	89 (12%)	5 17

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145	GLU
1	A	146	GLU
1	A	166	SER
1	A	168	VAL
1	A	203	THR
1	A	204	SER
1	A	207	LEU
1	A	219	CYS
1	A	229	THR
1	A	231	GLN
1	A	235	VAL
1	A	240	THR
1	A	268	GLN
1	A	278	ASP
1	A	281	LEU
1	A	287	ILE
1	A	291	GLN

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Mol	Chain	Res	Type
1	A	309	THR
1	A	320	LYS
1	A	360	LYS
1	A	369	ASP
1	A	372	VAL
1	A	373	LEU
1	A	375	ARG
1	A	376	ASN
1	A	378	ASP
1	A	379	LEU
1	A	381	VAL
1	A	487	ILE
1	A	498	ASN
1	A	510	LYS
1	A	520	LEU
1	A	549	ASN
1	A	561	THR
1	A	565	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	756	LYS
1	A	764	ILE
1	A	767	LEU
1	A	775	GLN
1	A	798	ILE
1	A	799	GLU
1	A	804	MET
1	A	807	LYS
1	A	838	LEU
1	A	843	LEU
1	A	845	LEU
1	A	846	GLN
1	A	862	LEU

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Mol	Chain	Res	Type
1	A	865	LEU
1	A	878	MET
1	A	886	THR
1	A	890	LYS
1	A	895	THR
1	A	896	VAL
1	A	903	LYS
1	A	904	ASP
1	A	905	GLU
1	A	907	LEU
1	A	912	LYS
1	A	913	GLU
1	A	917	THR
1	A	919	GLU
1	A	939	THR
1	A	982	ARG
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	1044	SER
1	A	1046	GLU
1	A	1048	ILE
1	A	1056	THR
1	A	1066	LYS
1	A	1081	THR
1	A	1088	LEU
1	A	1092	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	GLN
1	A	225	HIS
1	A	231	GLN
1	A	291	GLN
1	A	295	HIS
1	A	304	HIS
1	A	386	ASN
1	A	389	HIS

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Mol	Chain	Res	Type
1	A	392	GLN
1	A	396	GLN
1	A	411	ASN
1	A	522	ASN
1	A	565	ASN
1	A	634	ASN
1	A	710	GLN
1	A	730	HIS
1	A	734	GLN
1	A	766	GLN
1	A	773	ASN
1	A	776	ASN
1	A	825	ASN
1	A	893	GLN
1	A	951	ASN
1	A	962	HIS
1	A	1007	GLN
1	A	1022	HIS
1	A	1041	GLN
1	A	1083	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	2WH	A	1201	-	34,34,34	0.88	1 (2%)	46,46,46	1.99	10 (21%)

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	2WH	A	1201	-	-	6/19/19/19	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	2WH	C17-N16	-2.51	1.34	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	2WH	N4-C8-N7	-5.78	107.75	112.35
2	A	1201	2WH	S23-C15-N16	-5.29	110.70	117.06
2	A	1201	2WH	C5-N4-C8	4.93	109.13	106.71
2	A	1201	2WH	C29-N28-C27	3.73	122.58	117.51
2	A	1201	2WH	C17-N16-C15	3.69	117.41	108.66
2	A	1201	2WH	C9-C10-N11	-3.24	105.11	112.00
2	A	1201	2WH	C9-C6-C5	-2.47	125.48	130.26
2	A	1201	2WH	N14-C15-N16	2.21	124.65	120.87
2	A	1201	2WH	C6-C5-N4	-2.10	105.06	106.53
2	A	1201	2WH	O13-C12-N11	-2.05	118.95	122.47

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201	2WH	C27-C26-O30-C31
2	A	1201	2WH	C25-C26-O30-C31
2	A	1201	2WH	C5-C6-C9-C10
2	A	1201	2WH	N7-C6-C9-C10

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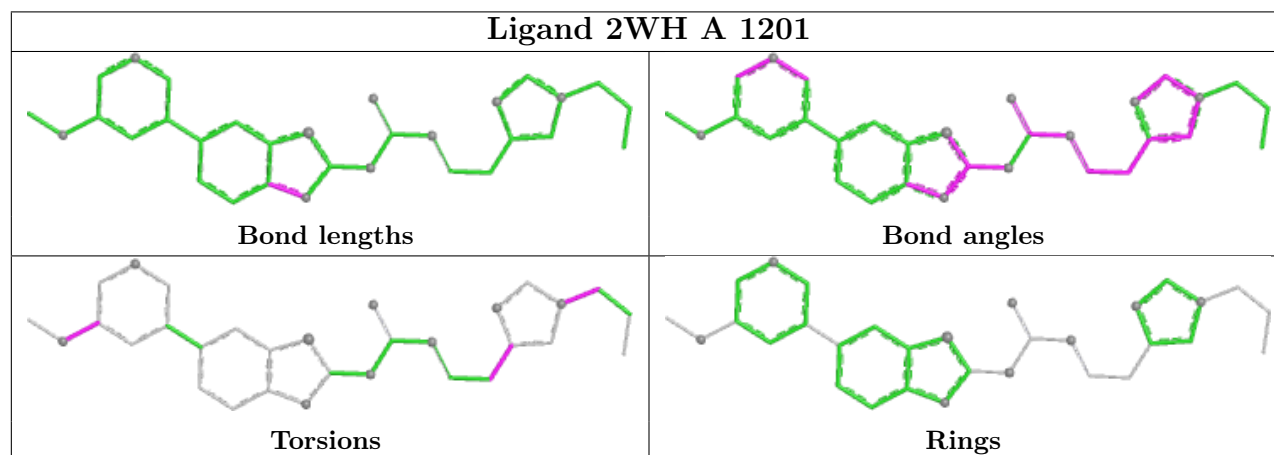
Mol	Chain	Res	Type	Atoms
2	A	1201	2WH	C2-C3-N4-C5
2	A	1201	2WH	C2-C3-N4-C8

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	2WH	8	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	843/966 (87%)	-0.01	15 (1%) 67 59	31, 75, 135, 176	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1088	LEU	4.3
1	A	1086	TRP	3.6
1	A	357	CYS	3.4
1	A	899	THR	3.3
1	A	1087	PHE	2.7
1	A	526	PRO	2.7
1	A	967	HIS	2.7
1	A	527	ILE	2.6
1	A	1044	SER	2.5
1	A	757	TYR	2.2
1	A	896	VAL	2.2
1	A	545	ALA	2.2
1	A	522	ASN	2.0
1	A	901	ALA	2.0
1	A	323	TRP	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](#)

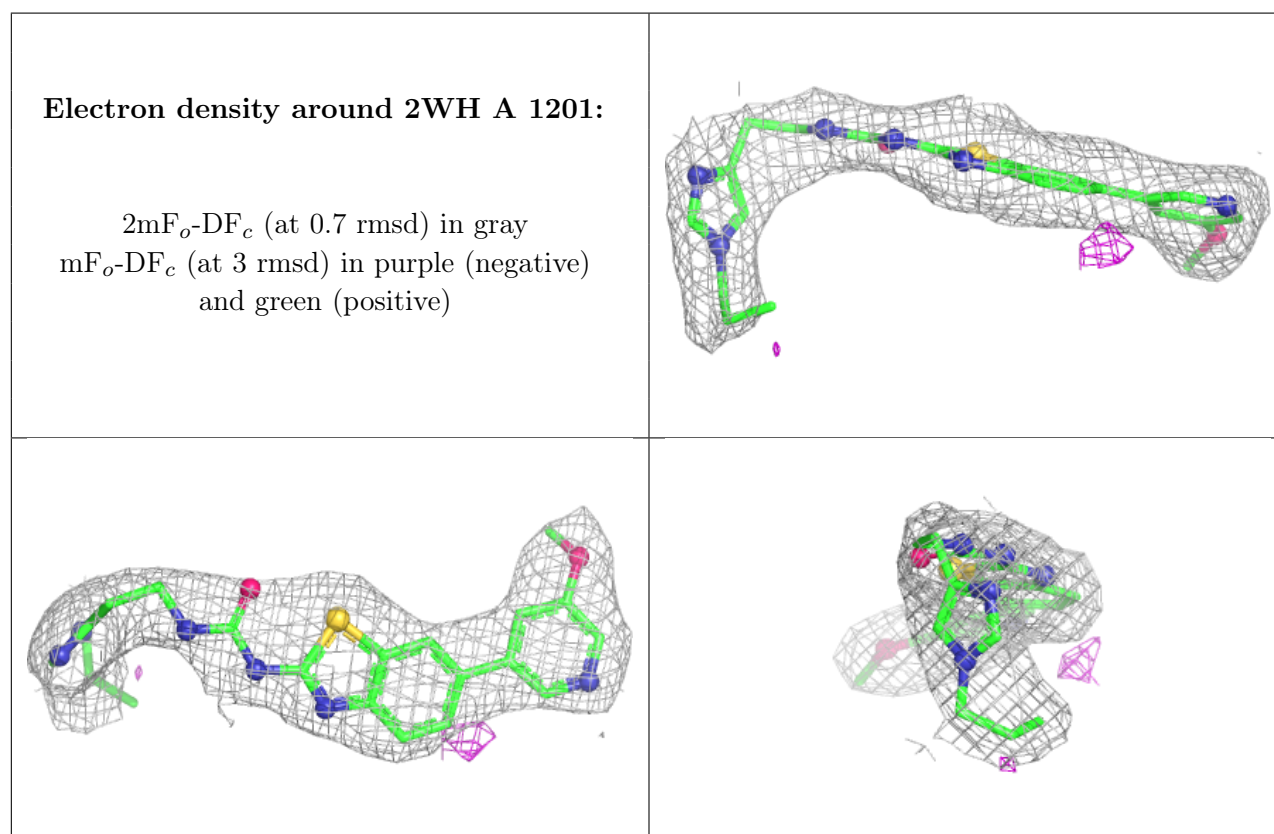
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
2	2WH	A	1201	31/31	0.94	0.08	50,60,74,77	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.