



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:14 AM UTC

PDB ID : 5NGB / pdb_00005ngb
Title : X-Ray Diffraction Crystal Structure of the murine PI3K p110delta in complex with a pan inhibitor
Authors : Berndt, A.; Williams, R.L.
Deposited on : 2017-03-17
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

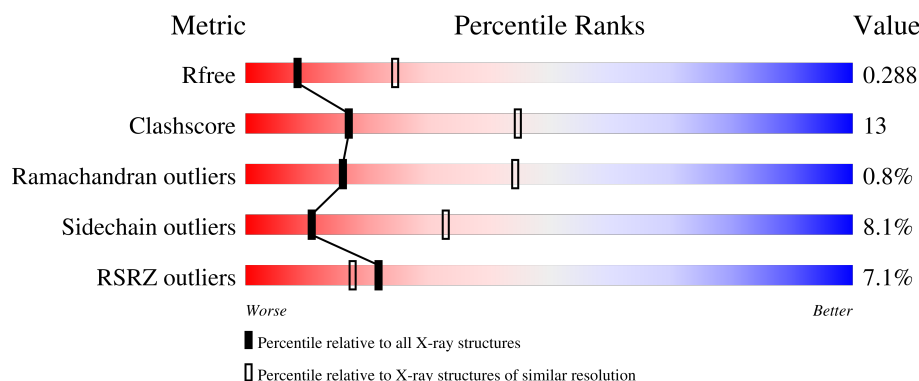
1 Overall quality at a glance

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	1079	5% 58% 15% • 24%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6625 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 delta isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	816	Total	C	N	O	S	0	0	0
			6593	4228	1120	1192	53			

There are 35 discrepancies between the modelled and reference sequences:

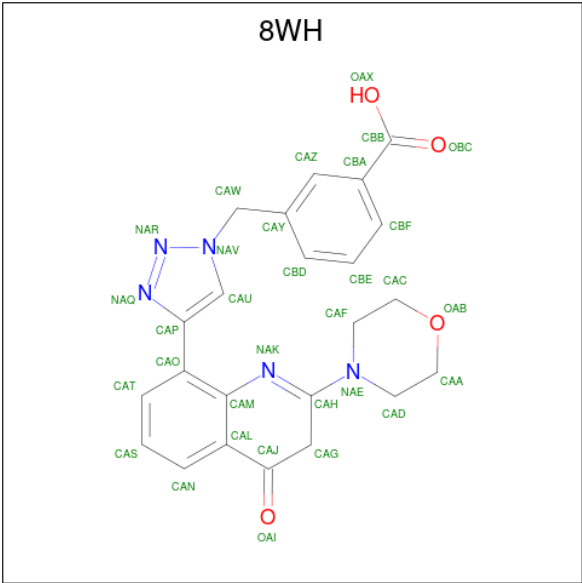
Chain	Residue	Modelled	Actual	Comment	Reference
A	-34	MET	-	initiating methionine	UNP Q3UDT3
A	-33	SER	-	expression tag	UNP Q3UDT3
A	-32	TYR	-	expression tag	UNP Q3UDT3
A	-31	TYR	-	expression tag	UNP Q3UDT3
A	-30	HIS	-	expression tag	UNP Q3UDT3
A	-29	HIS	-	expression tag	UNP Q3UDT3
A	-28	HIS	-	expression tag	UNP Q3UDT3
A	-27	HIS	-	expression tag	UNP Q3UDT3
A	-26	HIS	-	expression tag	UNP Q3UDT3
A	-25	HIS	-	expression tag	UNP Q3UDT3
A	-24	ASP	-	expression tag	UNP Q3UDT3
A	-23	TYR	-	expression tag	UNP Q3UDT3
A	-22	ASP	-	expression tag	UNP Q3UDT3
A	-21	ILE	-	expression tag	UNP Q3UDT3
A	-20	PRO	-	expression tag	UNP Q3UDT3
A	-19	THR	-	expression tag	UNP Q3UDT3
A	-18	THR	-	expression tag	UNP Q3UDT3
A	-17	GLU	-	expression tag	UNP Q3UDT3
A	-16	ASN	-	expression tag	UNP Q3UDT3
A	-15	LEU	-	expression tag	UNP Q3UDT3
A	-14	TYR	-	expression tag	UNP Q3UDT3
A	-13	PHE	-	expression tag	UNP Q3UDT3
A	-12	GLN	-	expression tag	UNP Q3UDT3
A	-11	GLY	-	expression tag	UNP Q3UDT3
A	-10	ALA	-	expression tag	UNP Q3UDT3
A	-9	MET	-	expression tag	UNP Q3UDT3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	ASP	-	expression tag	UNP Q3UDT3
A	-7	LEU	-	expression tag	UNP Q3UDT3
A	99	GLU	-	insertion	UNP Q3UDT3
A	100	ASN	-	insertion	UNP Q3UDT3
A	101	LEU	-	insertion	UNP Q3UDT3
A	102	TYR	-	insertion	UNP Q3UDT3
A	103	PHE	-	insertion	UNP Q3UDT3
A	104	GLN	-	insertion	UNP Q3UDT3
A	105	GLY	-	insertion	UNP Q3UDT3

- Molecule 2 is 3-[[4-(2-morpholin-4-yl-4-oxidanylidene-3 {H}-quinolin-8-yl)-1,2,3-triazol-1-yl]methyl]benzoic acid (CCD ID: 8WH) (formula: C₂₃H₂₁N₅O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			32	23	5	4		

R1024		
E1025		
S1026		
W1027		
LYS	THR	
	LYS	
	VAL	
	ASN	
	TRP	
	LEU	
	ALA	
	HIS	
	ASN	
	VAL	
	SER	
	LYS	
	ASP	
	ASN	
	ARG	
	GLN	

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	63.44Å 143.59Å 220.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.63 – 2.90 45.63 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.63-2.90) 99.9 (45.63-2.90)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	0.25	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.242 , 0.290 0.243 , 0.288	Depositor DCC
R_{free} test set	1170 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	48.7	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	6625	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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: 8WH

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	0.77	0/6734	0.95	3/9084 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	258	HIS	N-CA-C	-8.15	103.47	113.50
1	A	110	LYS	N-CA-C	-6.95	104.62	113.23
1	A	334	ASN	N-CA-C	5.72	116.95	108.60

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	6593	0	6573	167	1
2	A	32	0	0	2	0
All	All	6625	0	6573	168	1

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 13.

All (168) 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:369:PRO:HB2	1:A:371:TRP:CH2	1.61	1.33
1:A:954:GLU:HG2	1:A:957:ARG:NH1	1.60	1.15
1:A:746:VAL:O	1:A:748:GLN:N	1.83	1.12
1:A:341:LEU:HD21	1:A:365:VAL:HG13	1.34	1.08
1:A:224:LYS:HG3	1:A:228:PHE:CE2	1.87	1.08
1:A:369:PRO:O	1:A:371:TRP:CE3	2.06	1.06
1:A:330:GLY:C	1:A:369:PRO:HD2	1.83	1.03
1:A:369:PRO:HB2	1:A:371:TRP:CZ3	1.94	1.03
1:A:116:GLN:HE21	1:A:679:MET:CE	1.72	1.01
1:A:549:LEU:HG	1:A:564:MET:HE1	1.43	1.01
1:A:708:LYS:NZ	2:A:1101:8WH:OBC	1.94	1.00
1:A:224:LYS:HG3	1:A:228:PHE:CD2	1.99	0.97
1:A:339:MET:C	1:A:365:VAL:HG23	1.93	0.93
1:A:339:MET:O	1:A:365:VAL:HG23	1.69	0.92
1:A:369:PRO:CB	1:A:371:TRP:CH2	2.53	0.91
1:A:954:GLU:CG	1:A:957:ARG:NH1	2.33	0.91
1:A:218:ALA:O	1:A:222:ARG:HG3	1.73	0.87
1:A:224:LYS:CG	1:A:228:PHE:CD2	2.58	0.86
1:A:142:LYS:HE3	1:A:626:ASP:OD2	1.76	0.85
1:A:116:GLN:NE2	1:A:679:MET:CE	2.38	0.85
1:A:436:GLU:O	1:A:437:ARG:HD2	1.77	0.84
1:A:374:ARG:NH2	1:A:376:GLU:OE1	2.10	0.84
1:A:116:GLN:HE21	1:A:679:MET:HE1	1.42	0.84
1:A:916:LEU:O	1:A:918:ASN:N	2.09	0.84
1:A:224:LYS:O	1:A:228:PHE:HB2	1.77	0.84
1:A:954:GLU:CD	1:A:957:ARG:HH12	1.87	0.82
1:A:954:GLU:CG	1:A:957:ARG:HH12	1.90	0.81
1:A:435:GLY:O	1:A:475:LEU:N	2.13	0.79
1:A:369:PRO:O	1:A:371:TRP:CZ3	2.39	0.75
1:A:917:GLY:HA2	1:A:930:VAL:HG12	1.68	0.75
1:A:954:GLU:HG2	1:A:957:ARG:HH11	1.51	0.74
1:A:916:LEU:C	1:A:918:ASN:H	1.94	0.74
1:A:137:ASN:O	1:A:141:THR:HG23	1.87	0.74
1:A:368:GLU:OE1	1:A:368:GLU:N	2.23	0.71
1:A:165:TYR:CZ	1:A:641:ARG:HG3	2.26	0.71
1:A:435:GLY:HA3	1:A:475:LEU:O	1.91	0.71
1:A:895:HIS:H	1:A:898:ASN:HD21	1.40	0.69
1:A:951:GLU:OE2	1:A:955:ARG:NH1	2.25	0.69
1:A:330:GLY:N	1:A:369:PRO:HG2	2.07	0.69
1:A:746:VAL:O	1:A:749:CYS:N	2.24	0.69
1:A:386:ARG:HG3	1:A:387:MET:HE2	1.74	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:LEU:CG	1:A:564:MET:HE1	2.19	0.69
1:A:706:THR:OG1	1:A:710:GLN:OE1	2.11	0.68
1:A:435:GLY:C	1:A:475:LEU:H	2.03	0.67
1:A:116:GLN:HB3	1:A:679:MET:HE3	1.76	0.67
1:A:223:LYS:O	1:A:224:LYS:C	2.38	0.67
1:A:369:PRO:CB	1:A:371:TRP:CZ3	2.75	0.67
1:A:715:MET:HE1	1:A:750:THR:HA	1.77	0.66
1:A:746:VAL:C	1:A:748:GLN:N	2.53	0.66
1:A:435:GLY:CA	1:A:475:LEU:O	2.44	0.65
1:A:746:VAL:C	1:A:748:GLN:H	2.04	0.65
1:A:224:LYS:O	1:A:228:PHE:HD2	1.78	0.65
1:A:224:LYS:O	1:A:228:PHE:CD2	2.51	0.64
1:A:328:ILE:HB	1:A:472:VAL:HG23	1.80	0.64
1:A:339:MET:C	1:A:365:VAL:CG2	2.71	0.63
1:A:549:LEU:HG	1:A:564:MET:CE	2.24	0.63
1:A:224:LYS:HG2	1:A:228:PHE:CD2	2.34	0.63
1:A:246:ARG:NH1	1:A:248:GLU:OE1	2.32	0.63
1:A:330:GLY:O	1:A:369:PRO:HD2	1.97	0.62
1:A:285:MET:O	1:A:289:GLN:HG3	1.99	0.62
1:A:951:GLU:O	1:A:955:ARG:HG3	1.98	0.62
1:A:224:LYS:O	1:A:228:PHE:CB	2.47	0.62
1:A:325:ILE:HD11	1:A:375:LEU:HD12	1.82	0.61
1:A:245:GLY:HA3	1:A:768:ALA:HB2	1.81	0.61
1:A:116:GLN:HE21	1:A:679:MET:HE3	1.64	0.61
1:A:490:LYS:HD3	1:A:490:LYS:C	2.26	0.60
1:A:436:GLU:O	1:A:437:ARG:CD	2.49	0.60
1:A:341:LEU:CD2	1:A:365:VAL:HG13	2.21	0.59
1:A:553:THR:CG2	1:A:564:MET:HE3	2.32	0.59
1:A:915:PHE:C	1:A:915:PHE:CD1	2.81	0.59
1:A:154:ARG:HA	1:A:157:LEU:HG	1.84	0.59
1:A:915:PHE:C	1:A:915:PHE:HD1	2.12	0.58
1:A:387:MET:HE3	1:A:590:CYS:HB3	1.86	0.57
1:A:716:HIS:O	1:A:720:ARG:HG3	2.05	0.57
1:A:870:ARG:NH2	1:A:874:GLU:OE2	2.35	0.57
1:A:914:HIS:HB3	1:A:918:ASN:O	2.05	0.57
1:A:116:GLN:NE2	1:A:679:MET:HE1	2.11	0.56
1:A:256:LEU:O	1:A:262:ILE:HB	2.06	0.56
1:A:332:LYS:HE3	1:A:333:VAL:N	2.20	0.56
1:A:834:ILE:HD11	1:A:901:ILE:HG23	1.88	0.56
1:A:918:ASN:ND2	1:A:927:ARG:HG3	2.22	0.55
1:A:116:GLN:CB	1:A:679:MET:HE3	2.37	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:700:LYS:HE2	1:A:756:MET:HA	1.90	0.54
1:A:934:LEU:O	1:A:1026:SER:HB2	2.08	0.54
1:A:916:LEU:C	1:A:918:ASN:N	2.62	0.53
1:A:330:GLY:CA	1:A:369:PRO:HG2	2.39	0.53
1:A:553:THR:HG21	1:A:564:MET:HE3	1.91	0.53
1:A:837:ILE:O	1:A:839:LEU:N	2.42	0.52
1:A:194:VAL:HG21	1:A:216:LEU:HD21	1.91	0.52
1:A:113:ILE:O	1:A:117:ILE:HG13	2.10	0.52
1:A:330:GLY:CA	1:A:369:PRO:HD2	2.41	0.51
1:A:750:THR:OG1	1:A:751:PHE:N	2.44	0.51
1:A:339:MET:HB2	1:A:365:VAL:HG21	1.92	0.50
1:A:1009:GLU:OE2	1:A:1009:GLU:HA	2.09	0.50
1:A:393:ALA:HB2	1:A:453:LEU:HD12	1.93	0.50
1:A:583:LEU:HD11	1:A:600:LEU:HD11	1.94	0.50
1:A:515:LEU:C	1:A:517:ARG:H	2.20	0.50
1:A:535:ARG:HB2	1:A:567:LEU:HD11	1.94	0.50
1:A:142:LYS:CE	1:A:626:ASP:OD2	2.56	0.49
2:A:1101:8WH:NAQ	2:A:1101:8WH:NAK	2.61	0.49
1:A:223:LYS:O	1:A:226:THR:N	2.46	0.48
1:A:693:LYS:HE2	1:A:780:ASN:HD21	1.78	0.48
1:A:895:HIS:H	1:A:898:ASN:ND2	2.09	0.48
1:A:330:GLY:O	1:A:368:GLU:HG3	2.14	0.48
1:A:330:GLY:CA	1:A:369:PRO:CG	2.92	0.48
1:A:223:LYS:O	1:A:225:ALA:N	2.46	0.47
1:A:788:MET:O	1:A:792:GLN:HB2	2.14	0.47
1:A:435:GLY:HA2	1:A:475:LEU:O	2.14	0.47
1:A:701:VAL:O	1:A:705:LYS:HD2	2.14	0.47
1:A:746:VAL:O	1:A:747:GLU:C	2.53	0.47
1:A:894:ARG:NH2	1:A:911:ASP:O	2.46	0.47
1:A:329:GLU:HG2	1:A:472:VAL:CG2	2.45	0.47
1:A:530:LEU:CD1	1:A:534:MET:HG3	2.44	0.47
1:A:855:LEU:CD2	1:A:901:ILE:HD13	2.44	0.47
1:A:1020:ASN:O	1:A:1024:ARG:HG3	2.15	0.47
1:A:222:ARG:O	1:A:225:ALA:HB3	2.15	0.47
1:A:535:ARG:HB2	1:A:567:LEU:CD1	2.45	0.46
1:A:330:GLY:HA3	1:A:369:PRO:CG	2.44	0.46
1:A:435:GLY:HA2	1:A:475:LEU:HB2	1.97	0.46
1:A:165:TYR:OH	1:A:641:ARG:HG3	2.15	0.46
1:A:324:SER:HA	1:A:375:LEU:O	2.15	0.46
1:A:791:LEU:HD11	1:A:813:TYR:CE1	2.51	0.46
1:A:716:HIS:CE1	1:A:747:GLU:HA	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:ALA:O	1:A:230:GLN:N	2.49	0.45
1:A:838:GLN:NE2	1:A:937:ASP:OD2	2.49	0.45
1:A:256:LEU:O	1:A:262:ILE:CB	2.65	0.45
1:A:317:TRP:HA	1:A:382:CYS:HB2	1.98	0.45
1:A:340:LYS:N	1:A:365:VAL:HG23	2.32	0.45
1:A:285:MET:HE2	1:A:285:MET:HB3	1.88	0.44
1:A:1002:LEU:HB3	1:A:1004:LEU:HD23	1.98	0.44
1:A:530:LEU:O	1:A:534:MET:HG3	2.17	0.44
1:A:746:VAL:O	1:A:748:GLN:CA	2.64	0.44
1:A:326:GLU:HB3	1:A:474:TYR:HB3	2.00	0.44
1:A:343:VAL:H	1:A:360:SER:HB2	1.83	0.44
1:A:898:ASN:HD22	1:A:898:ASN:C	2.25	0.43
1:A:860:LYS:HG2	1:A:868:LEU:HD22	2.00	0.43
1:A:341:LEU:HG	1:A:365:VAL:HG22	2.01	0.43
1:A:523:LEU:HB2	1:A:527:GLU:OE1	2.18	0.43
1:A:679:MET:O	1:A:683:MET:HG3	2.19	0.43
1:A:221:LEU:HD23	1:A:221:LEU:HA	1.82	0.43
1:A:213:PRO:O	1:A:217:MET:HG3	2.19	0.43
1:A:330:GLY:HA3	1:A:369:PRO:HG2	2.01	0.43
1:A:434:THR:HA	1:A:435:GLY:HA2	1.76	0.43
1:A:1024:ARG:O	1:A:1027:TRP:CZ3	2.72	0.42
1:A:224:LYS:O	1:A:228:PHE:N	2.52	0.42
1:A:716:HIS:CD2	1:A:746:VAL:CG1	3.03	0.41
1:A:147:CYS:SG	1:A:638:LEU:HD11	2.60	0.41
1:A:532:TRP:HZ3	1:A:564:MET:HE2	1.84	0.41
1:A:548:ARG:HA	1:A:548:ARG:HD2	1.79	0.41
1:A:855:LEU:HD21	1:A:901:ILE:HD13	2.02	0.41
1:A:530:LEU:HD13	1:A:534:MET:HG3	2.01	0.41
1:A:1009:GLU:O	1:A:1010:GLU:C	2.62	0.41
1:A:143:MET:O	1:A:144:ARG:C	2.59	0.41
1:A:349:HIS:NE2	1:A:588:PRO:HG2	2.34	0.41
1:A:136:VAL:HG13	1:A:666:LEU:HD11	2.02	0.41
1:A:340:LYS:CA	1:A:365:VAL:HG23	2.51	0.41
1:A:833:THR:OG1	1:A:836:ASN:HB2	2.19	0.41
1:A:254:TYR:HA	1:A:255:PRO:HD2	1.94	0.41
1:A:437:ARG:O	1:A:472:VAL:HA	2.21	0.41
1:A:523:LEU:O	1:A:523:LEU:HD23	2.20	0.41
1:A:713:GLU:OE2	1:A:713:GLU:HA	2.21	0.41
1:A:223:LYS:C	1:A:225:ALA:N	2.77	0.41
1:A:553:THR:HG22	1:A:564:MET:HE3	2.01	0.41
1:A:341:LEU:HD21	1:A:365:VAL:CG1	2.25	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:786:GLN:NE2	1:A:913:GLY:O	2.53	0.41
1:A:859:LEU:HD21	1:A:905:GLY:HA2	2.03	0.40
1:A:419:ALA:HB3	1:A:441:MET:HE3	2.03	0.40
1:A:432:LEU:HB3	1:A:483:VAL:HG23	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:948:ASN:ND2	1:A:948:ASN:ND2[3_655]	2.02	0.18

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	792/1079 (73%)	757 (96%)	29 (4%)	6 (1%)	16	44

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	746	VAL
1	A	747	GLU
1	A	917	GLY
1	A	229	ARG
1	A	364	ASN
1	A	435	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	724/957 (76%)	665 (92%)	59 (8%)	11	33

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	VAL
1	A	110	LYS
1	A	111	LYS
1	A	132	ARG
1	A	141	THR
1	A	142	LYS
1	A	154	ARG
1	A	190	LEU
1	A	201	GLU
1	A	206	GLN
1	A	229	ARG
1	A	263	CYS
1	A	317	TRP
1	A	332	LYS
1	A	340	LYS
1	A	352	GLU
1	A	356	LYS
1	A	360	SER
1	A	366	CYS
1	A	368	GLU
1	A	373	GLN
1	A	415	ASP
1	A	423	LEU
1	A	453	LEU
1	A	490	LYS
1	A	514	ILE
1	A	516	GLU
1	A	522	GLU
1	A	523	LEU
1	A	530	LEU
1	A	534	MET
1	A	537	GLU
1	A	548	ARG
1	A	553	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	631	LYS
1	A	634	LEU
1	A	641	ARG
1	A	705	LYS
1	A	713	GLU
1	A	720	ARG
1	A	726	GLU
1	A	743	GLU
1	A	748	GLN
1	A	752	MET
1	A	755	LYS
1	A	756	MET
1	A	788	MET
1	A	836	ASN
1	A	839	LEU
1	A	847	THR
1	A	855	LEU
1	A	898	ASN
1	A	911	ASP
1	A	915	PHE
1	A	927	ARG
1	A	930	VAL
1	A	1004	LEU
1	A	1008	GLU
1	A	1021	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	GLN
1	A	170	GLN
1	A	193	ASN
1	A	206	GLN
1	A	273	HIS
1	A	278	HIS
1	A	291	ASN
1	A	344	GLN
1	A	536	HIS
1	A	539	GLN
1	A	617	GLN
1	A	721	GLN
1	A	773	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	780	ASN
1	A	795	GLN
1	A	895	HIS
1	A	898	ASN
1	A	914	HIS
1	A	918	ASN
1	A	976	HIS

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	8WH	A	1101	-	36,36,36	3.67	10 (27%)	44,51,51	1.83	12 (27%)

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	8WH	A	1101	-	-	1/16/36/36	0/4/5/5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	8WH	CAG-CAH	-11.16	1.39	1.49
2	A	1101	8WH	NAQ-NAR	-9.60	1.16	1.32
2	A	1101	8WH	CAO-CAP	-7.80	1.33	1.47
2	A	1101	8WH	CAL-CAJ	-6.96	1.39	1.48
2	A	1101	8WH	CAH-NAK	6.09	1.40	1.29
2	A	1101	8WH	NAV-NAR	-5.20	1.26	1.34
2	A	1101	8WH	CAW-CAY	-5.15	1.42	1.51
2	A	1101	8WH	CBA-CBB	-4.55	1.39	1.49
2	A	1101	8WH	CAW-NAV	4.40	1.54	1.47
2	A	1101	8WH	CAU-CAP	-3.84	1.30	1.37

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	8WH	NAV-NAR-NAQ	4.38	110.96	107.02
2	A	1101	8WH	CAA-CAD-NAE	4.16	118.57	109.82
2	A	1101	8WH	CAL-CAM-NAK	-3.79	118.59	122.33
2	A	1101	8WH	CAD-NAE-CAF	3.36	119.54	112.68
2	A	1101	8WH	CAG-CAJ-CAL	3.32	121.03	116.49
2	A	1101	8WH	CAY-CAW-NAV	3.21	117.95	112.14
2	A	1101	8WH	OAB-CAC-CAF	-2.94	105.43	111.77
2	A	1101	8WH	OAX-CBB-CBA	2.82	122.08	114.84
2	A	1101	8WH	OAX-CBB-OBC	-2.57	117.82	123.35
2	A	1101	8WH	OAI-CAJ-CAG	-2.54	116.95	120.92
2	A	1101	8WH	CAU-NAV-NAR	-2.23	108.59	110.75
2	A	1101	8WH	CAW-NAV-NAR	2.14	123.03	120.03

There are no chirality outliers.

All (1) torsion outliers are listed below:

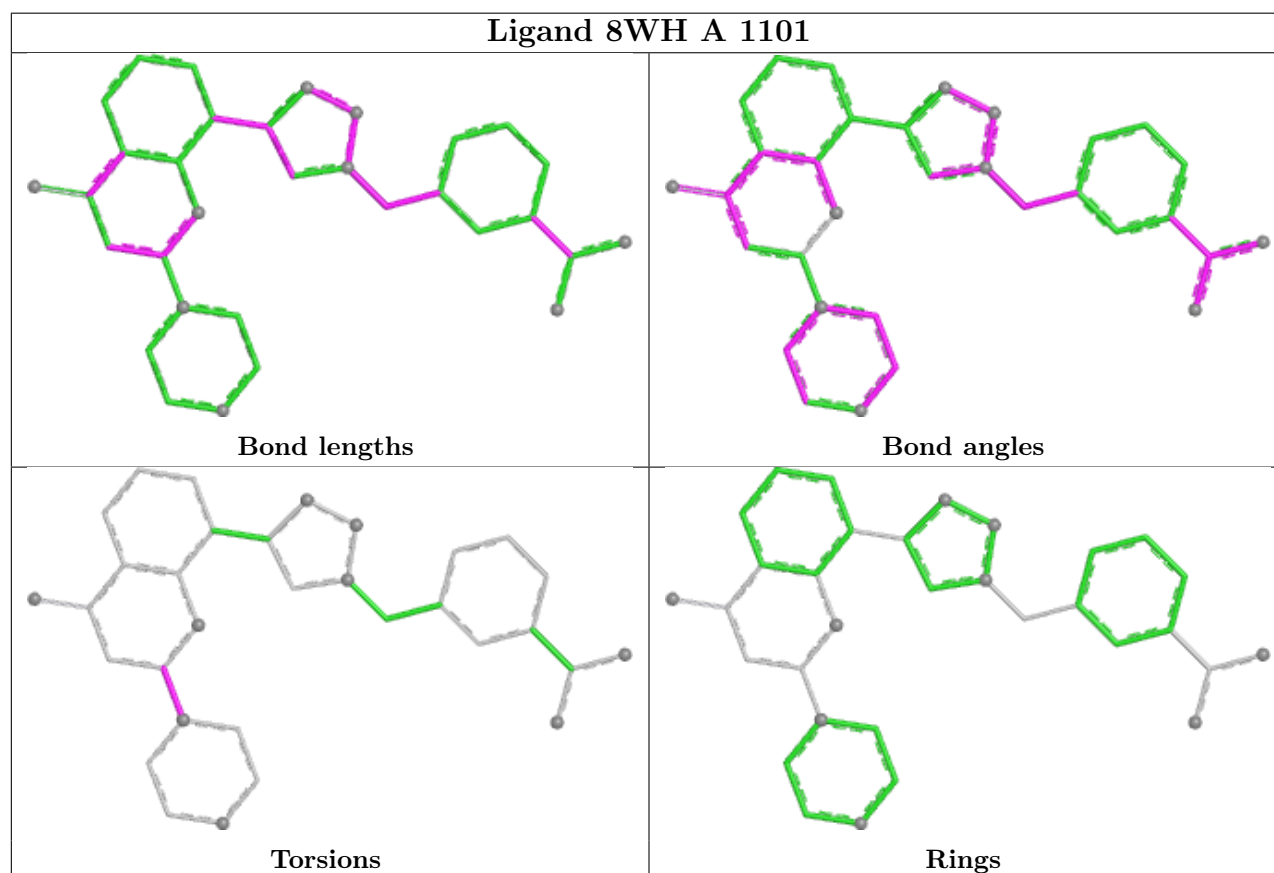
Mol	Chain	Res	Type	Atoms
2	A	1101	8WH	CAG-CAH-NAE-CAD

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	8WH	2	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

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	816/1079 (75%)	0.50	58 (7%)	22 17	19, 49, 85, 140	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	369	PRO	6.0
1	A	317	TRP	5.8
1	A	365	VAL	5.1
1	A	332	LYS	4.5
1	A	511	LEU	4.4
1	A	366	CYS	4.1
1	A	839	LEU	4.0
1	A	109	VAL	4.0
1	A	334	ASN	4.0
1	A	228	PHE	4.0
1	A	367	SER	3.8
1	A	316	LEU	3.8
1	A	479	ALA	3.7
1	A	335	ALA	3.7
1	A	341	LEU	3.6
1	A	173	PRO	3.4
1	A	445	VAL	3.3
1	A	512	ARG	3.3
1	A	1027	TRP	3.2
1	A	358	VAL	3.2
1	A	397	VAL	3.1
1	A	398	VAL	3.0
1	A	488	LEU	2.9
1	A	472	VAL	2.8
1	A	206	GLN	2.8
1	A	190	LEU	2.7
1	A	187	ASN	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	370	VAL	2.7
1	A	476	PRO	2.7
1	A	932	PHE	2.7
1	A	267	HIS	2.6
1	A	226	THR	2.6
1	A	260	GLN	2.6
1	A	937	ASP	2.6
1	A	363	VAL	2.5
1	A	155	GLN	2.5
1	A	364	ASN	2.4
1	A	484	TYR	2.4
1	A	491	ILE	2.4
1	A	482	PRO	2.4
1	A	938	PHE	2.3
1	A	426	PHE	2.3
1	A	927	ARG	2.3
1	A	433	LYS	2.3
1	A	474	TYR	2.3
1	A	470	ALA	2.2
1	A	266	LEU	2.2
1	A	483	VAL	2.2
1	A	838	GLN	2.1
1	A	959	TYR	2.1
1	A	342	VAL	2.1
1	A	253	ASN	2.0
1	A	514	ILE	2.0
1	A	162	TRP	2.0
1	A	333	VAL	2.0
1	A	558	HIS	2.0
1	A	851	ASN	2.0
1	A	262	ILE	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](#)

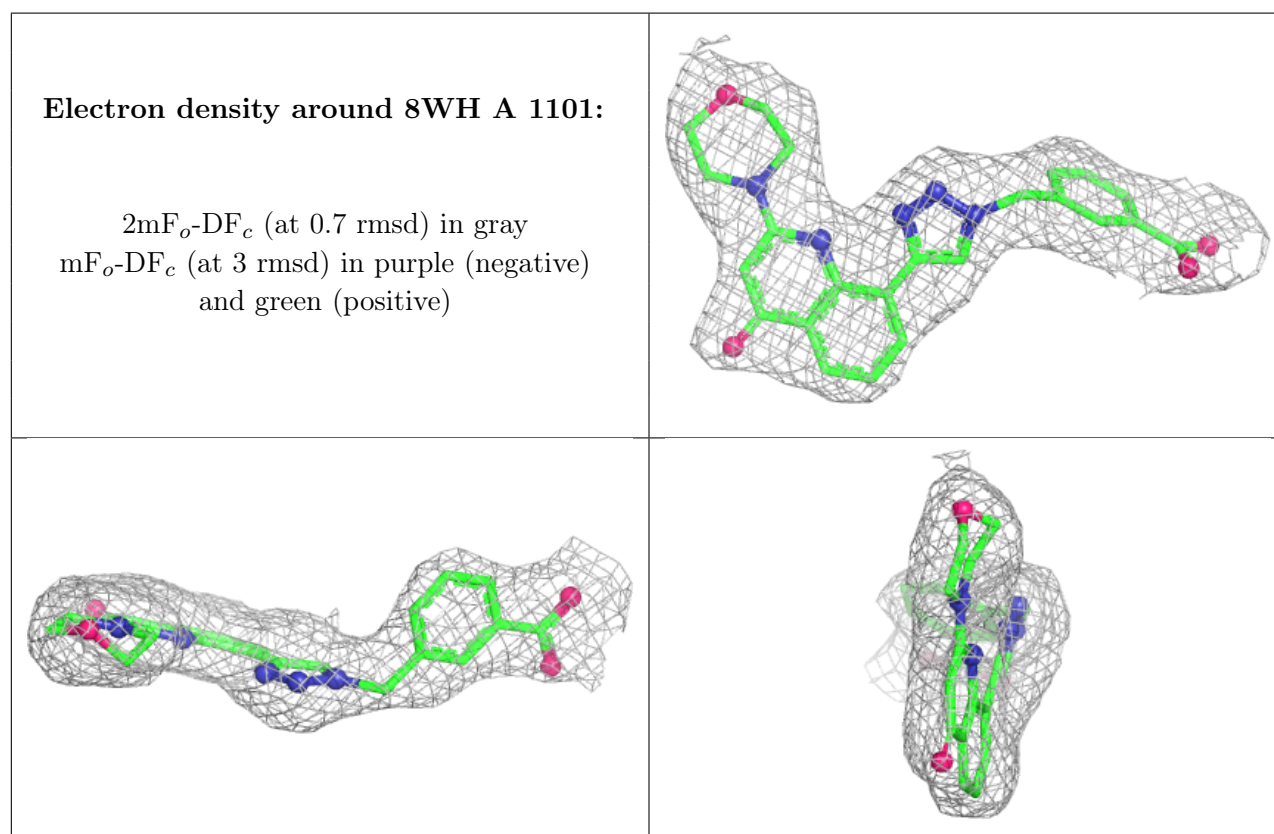
There are no oligosaccharides in this entry.

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	8WH	A	1101	32/32	0.95	0.09	26,37,50,59	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.