



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:10 PM UTC

PDB ID : 2WXG / pdb_00002wxg
Title : The crystal structure of the murine class IA PI 3-kinase p110delta in complex with SW13.
Authors : Berndt, A.; Miller, S.; Williams, O.; Lee, D.D.; Houseman, B.T.; Pacold, J.I.; Gorrec, F.; Hon, W.-C.; Liu, Y.; Rommel, C.; Gaillard, P.; Ruckle, T.; Schwarz, M.K.; Shokat, K.M.; Shaw, J.P.; Williams, R.L.
Deposited on : 2009-11-09
Resolution : 2.00 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](#) ①) 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

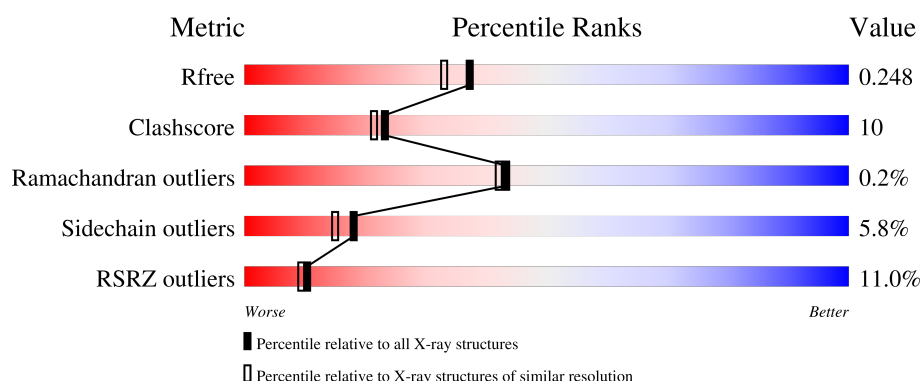
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	940	10% 72% 15% • 11%

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.

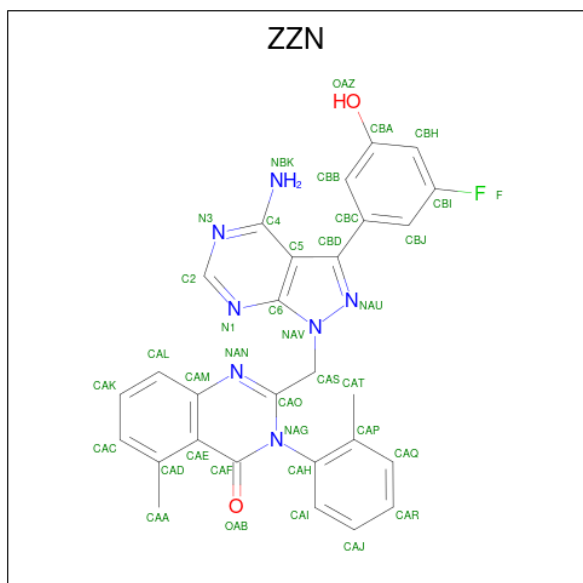
- Molecule 1 is a protein called PHOSPHATIDYLINOSITOL-4,5-BISPHOSPHATE 3-KINASE CATALYTIC SUBUNIT DELTA ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	835	Total	C	N	O	S	0	0	0
			6739	4315	1144	1226	54			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	105	GLY	-	expression tag	UNP Q3UDT3

- Molecule 2 is 2-[4-amino-3-(3-fluoro-5-hydroxyphenyl)-1H-pyrazolo[3,4-d]pyrimidin-1-yl]methyl}-5-methyl-3-(2-methylphenyl)quinazolin-4(3H)-one (CCD ID: ZZN) (formula: $C_{28}H_{22}FN_7O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			38	28	1	7	2		

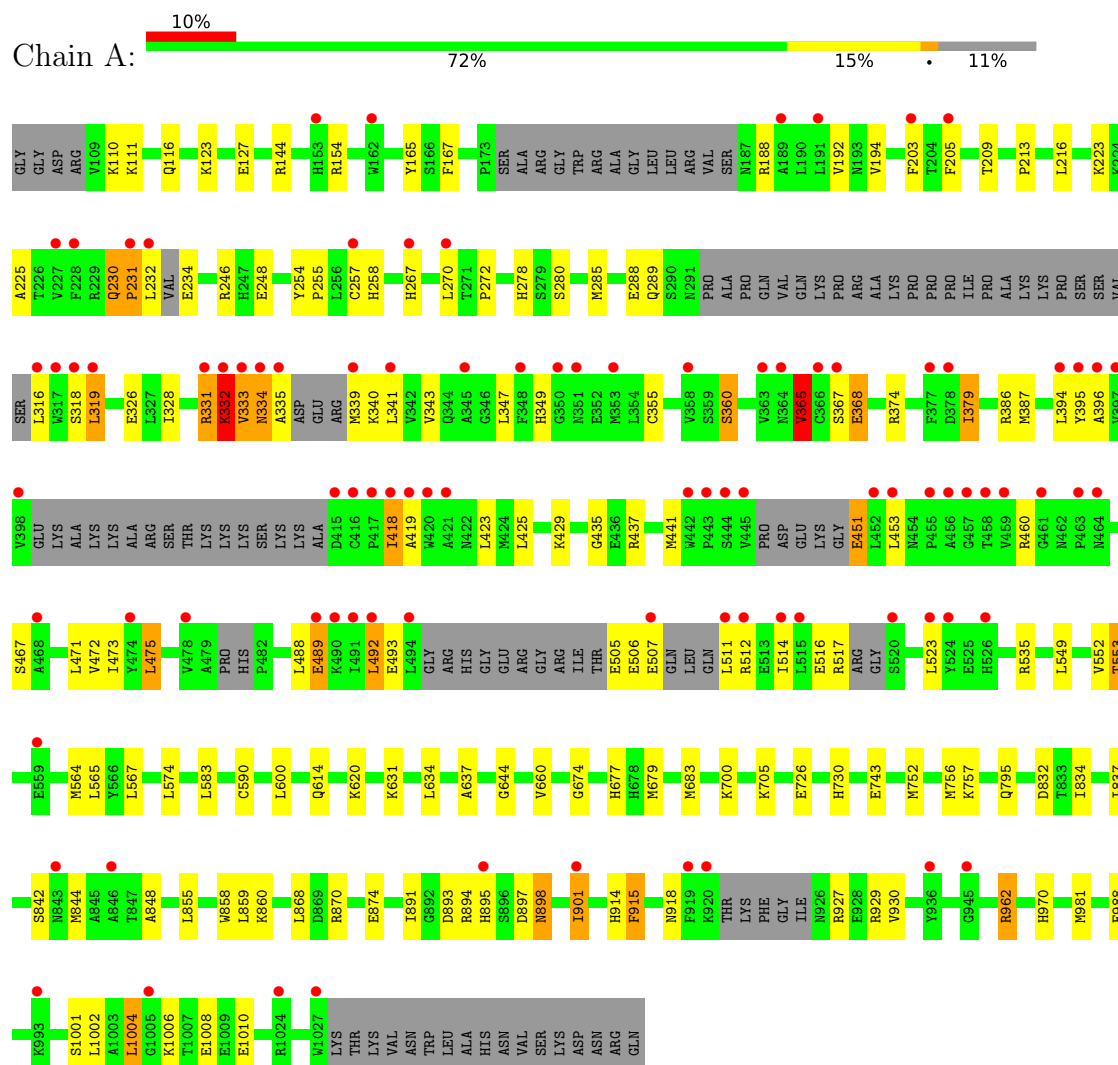
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	187	Total 187	O 187	0	0

3 Residue-property plots [i](#)

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 DELTA ISOFORM



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	141.76Å 64.67Å 116.72Å 90.00° 102.95° 90.00°	Depositor
Resolution (Å)	113.96 – 2.00 113.75 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (113.96-2.00) 99.7 (113.75-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0046	Depositor
R, R_{free}	0.206 , 0.243 0.212 , 0.248	Depositor DCC
R_{free} test set	2108 reflections (3.02%)	wwPDB-VP
Wilson B-factor (Å ²)	32.2	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6964	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% 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: ZZN

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	0.71	0/6882	0.86	5/9281 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	334	ASN	N-CA-C	7.32	117.91	108.24
1	A	230	GLN	N-CA-C	7.07	118.56	109.65
1	A	332	LYS	N-CA-C	6.62	120.33	109.94
1	A	848	ALA	N-CA-C	6.07	119.29	109.40
1	A	331	ARG	N-CA-C	5.36	118.14	109.83

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	6739	0	6704	138	0
2	A	38	0	21	1	0
3	A	187	0	0	3	0
All	All	6964	0	6725	139	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 10.

All (139) 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:549:LEU:HG	1:A:564:MET:HE1	1.15	1.08
1:A:837:ILE:HD11	1:A:901:ILE:HD11	1.37	1.07
1:A:837:ILE:CD1	1:A:901:ILE:HD11	1.83	1.06
1:A:386:ARG:HG3	1:A:387:MET:HE2	1.45	0.98
1:A:419:ALA:HB3	1:A:441:MET:HE3	1.46	0.97
1:A:553:THR:CG2	1:A:564:MET:HE3	2.00	0.92
1:A:387:MET:HE3	1:A:590:CYS:SG	2.11	0.89
1:A:549:LEU:CG	1:A:564:MET:HE1	2.05	0.85
1:A:365:VAL:CG1	1:A:365:VAL:O	2.25	0.84
1:A:435:GLY:HA2	1:A:475:LEU:O	1.78	0.82
1:A:553:THR:HG21	1:A:564:MET:HE3	1.59	0.82
1:A:962:ARG:HG2	1:A:962:ARG:HH11	1.47	0.80
1:A:553:THR:CG2	1:A:564:MET:CE	2.61	0.78
1:A:553:THR:HG21	1:A:564:MET:CE	2.15	0.77
1:A:918:ASN:ND2	1:A:927:ARG:HG2	1.99	0.77
1:A:837:ILE:HD12	1:A:901:ILE:HD11	1.65	0.76
1:A:225:ALA:HB1	1:A:230:GLN:HB3	1.68	0.75
1:A:343:VAL:H	1:A:360:SER:HB2	1.54	0.71
1:A:419:ALA:CB	1:A:441:MET:HE3	2.20	0.71
1:A:837:ILE:CD1	1:A:901:ILE:CD1	2.68	0.70
1:A:549:LEU:HG	1:A:564:MET:CE	2.09	0.70
1:A:553:THR:HG22	1:A:564:MET:HE3	1.75	0.68
1:A:365:VAL:O	1:A:365:VAL:HG12	1.95	0.67
1:A:110:LYS:HE2	1:A:144:ARG:HH12	1.59	0.66
1:A:246:ARG:NH1	1:A:248:GLU:OE2	2.29	0.66
1:A:901:ILE:H	1:A:901:ILE:HD13	1.59	0.66
1:A:231:PRO:HB2	1:A:232:LEU:HA	1.78	0.66
1:A:553:THR:HG22	1:A:564:MET:CE	2.26	0.65
1:A:365:VAL:O	1:A:365:VAL:HG13	1.97	0.64
1:A:419:ALA:HB3	1:A:441:MET:CE	2.23	0.63
1:A:929:ARG:HH22	1:A:1001:SER:HB3	1.63	0.63
1:A:225:ALA:HB1	1:A:230:GLN:CB	2.28	0.63
1:A:837:ILE:HD12	1:A:901:ILE:CD1	2.28	0.63
1:A:116:GLN:HB2	1:A:683:MET:SD	2.39	0.62
1:A:347:LEU:HD12	1:A:379:ILE:HD11	1.82	0.62
1:A:110:LYS:HE2	1:A:144:ARG:HH22	1.65	0.61
1:A:355:CYS:SG	1:A:379:ILE:HD12	2.41	0.61
1:A:334:ASN:ND2	1:A:335:ALA:H	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:PRO:CB	1:A:232:LEU:HA	2.32	0.60
1:A:194:VAL:HG21	1:A:216:LEU:HD21	1.84	0.60
1:A:332:LYS:HG2	1:A:394:LEU:HD21	1.84	0.59
1:A:331:ARG:HB3	1:A:368:GLU:HG2	1.84	0.59
1:A:331:ARG:HA	1:A:367:SER:O	2.02	0.59
1:A:895:HIS:HB2	1:A:897:ASP:OD1	2.03	0.59
1:A:192:VAL:HG22	1:A:272:PRO:HG2	1.84	0.58
1:A:205:PHE:CE1	1:A:223:LYS:HG3	2.39	0.58
1:A:451:GLU:O	1:A:451:GLU:HG3	2.03	0.57
1:A:832:ASP:O	1:A:901:ILE:HD13	2.04	0.57
1:A:395:TYR:HA	1:A:418:ILE:HG22	1.86	0.57
1:A:918:ASN:ND2	1:A:927:ARG:CG	2.66	0.56
1:A:232:LEU:O	1:A:234:GLU:N	2.38	0.56
1:A:267:HIS:HE1	1:A:870:ARG:HH21	1.54	0.56
1:A:387:MET:HE3	1:A:590:CYS:CB	2.35	0.56
1:A:437:ARG:HB2	1:A:473:ILE:HD11	1.88	0.56
1:A:387:MET:HE3	1:A:590:CYS:HB3	1.88	0.56
1:A:332:LYS:HD2	1:A:341:LEU:HD11	1.89	0.55
1:A:318:SER:HB2	1:A:319:LEU:HD12	1.89	0.55
1:A:394:LEU:HD23	1:A:418:ILE:HD12	1.89	0.55
1:A:893:ASP:OD1	1:A:895:HIS:HE1	1.90	0.55
1:A:918:ASN:HD22	1:A:927:ARG:HG2	1.71	0.54
1:A:583:LEU:HD11	1:A:600:LEU:HD11	1.87	0.54
1:A:929:ARG:HH22	1:A:1001:SER:CB	2.20	0.54
1:A:123:LYS:NZ	1:A:127:GLU:OE1	2.41	0.53
1:A:394:LEU:CD2	1:A:441:MET:HE1	2.38	0.53
1:A:231:PRO:HB2	1:A:232:LEU:CA	2.40	0.52
1:A:386:ARG:CG	1:A:387:MET:HE2	2.31	0.52
1:A:918:ASN:HD21	1:A:927:ARG:HG2	1.75	0.52
1:A:319:LEU:HD12	1:A:319:LEU:N	2.25	0.51
1:A:679:MET:O	1:A:683:MET:HG3	2.11	0.51
1:A:637:ALA:HB1	1:A:644:GLY:HA2	1.92	0.51
1:A:511:LEU:HA	1:A:514:ILE:HD12	1.92	0.51
1:A:278:HIS:HD2	1:A:280:SER:OG	1.94	0.51
1:A:379:ILE:HD13	1:A:379:ILE:N	2.27	0.50
1:A:901:ILE:CD1	1:A:901:ILE:H	2.24	0.50
1:A:901:ILE:CD1	1:A:901:ILE:N	2.75	0.49
1:A:154:ARG:HD2	1:A:165:TYR:CE2	2.48	0.49
1:A:347:LEU:CD1	1:A:379:ILE:HD11	2.43	0.49
1:A:962:ARG:HH11	1:A:962:ARG:CG	2.23	0.49
2:A:1500:ZZN:OAB	2:A:1500:ZZN:HAA1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1006:LYS:HD2	1:A:1010:GLU:HB3	1.94	0.48
1:A:918:ASN:HD22	1:A:927:ARG:CG	2.26	0.48
1:A:858:TRP:CZ3	1:A:901:ILE:HG12	2.49	0.48
1:A:752:MET:O	1:A:757:LYS:HA	2.14	0.48
1:A:231:PRO:HD2	1:A:232:LEU:HD12	1.95	0.48
1:A:213:PRO:HD3	1:A:254:TYR:O	2.14	0.47
1:A:255:PRO:HG2	1:A:258:HIS:CD2	2.50	0.47
1:A:326:GLU:HB2	1:A:374:ARG:NH1	2.30	0.47
1:A:583:LEU:HD11	1:A:600:LEU:CD1	2.45	0.47
1:A:870:ARG:NH2	1:A:874:GLU:OE2	2.47	0.47
1:A:110:LYS:CE	1:A:144:ARG:HH12	2.27	0.47
1:A:894:ARG:HA	1:A:898:ASN:HD21	1.80	0.47
1:A:167:PHE:HZ	1:A:285:MET:HE1	1.79	0.46
1:A:154:ARG:NH2	1:A:674:GLY:O	2.49	0.46
1:A:512:ARG:HH21	1:A:516:GLU:CD	2.24	0.46
1:A:553:THR:CG2	1:A:564:MET:HE2	2.42	0.46
1:A:387:MET:CE	1:A:590:CYS:SG	2.95	0.45
1:A:860:LYS:HG2	1:A:868:LEU:HD22	1.96	0.45
1:A:915:PHE:CD2	1:A:915:PHE:C	2.93	0.45
1:A:394:LEU:HD23	1:A:441:MET:HE1	1.97	0.45
1:A:891:ILE:HD13	1:A:915:PHE:HB3	1.99	0.45
1:A:288:GLU:HG2	1:A:289:GLN:HG3	1.99	0.45
1:A:842:SER:O	1:A:844:MET:HG2	2.17	0.45
1:A:488:LEU:HG	1:A:492:LEU:HD22	1.98	0.44
1:A:110:LYS:HE2	1:A:144:ARG:NH2	2.32	0.44
1:A:355:CYS:HB3	1:A:379:ILE:HG23	1.98	0.44
1:A:289:GLN:HG2	1:A:677:HIS:CD2	2.53	0.44
1:A:1002:LEU:HB3	1:A:1004:LEU:HD23	1.99	0.44
1:A:203:PHE:HB2	1:A:205:PHE:CE2	2.53	0.44
1:A:267:HIS:CE1	1:A:870:ARG:HH21	2.33	0.44
1:A:110:LYS:HE2	1:A:144:ARG:NH1	2.28	0.43
1:A:343:VAL:H	1:A:360:SER:CB	2.26	0.43
1:A:970:HIS:HD2	3:A:2050:HOH:O	2.01	0.43
1:A:460:ARG:NH2	3:A:2043:HOH:O	2.50	0.43
1:A:231:PRO:CD	1:A:232:LEU:HA	2.49	0.43
1:A:893:ASP:OD1	1:A:895:HIS:CE1	2.71	0.43
1:A:328:ILE:HD12	1:A:472:VAL:HG12	2.00	0.42
1:A:332:LYS:HE3	1:A:333:VAL:N	2.33	0.42
1:A:834:ILE:HD11	1:A:901:ILE:HG23	2.01	0.42
1:A:915:PHE:C	1:A:915:PHE:HD2	2.27	0.42
1:A:700:LYS:HE2	1:A:756:MET:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:LEU:N	1:A:319:LEU:CD1	2.82	0.42
1:A:535:ARG:HG3	1:A:567:LEU:HD11	2.02	0.42
1:A:340:LYS:O	1:A:396:ALA:HA	2.20	0.42
1:A:154:ARG:HG2	1:A:154:ARG:HH11	1.83	0.42
1:A:347:LEU:HD12	1:A:379:ILE:CD1	2.47	0.42
1:A:209:THR:HB	1:A:257:CYS:HB3	2.02	0.41
1:A:549:LEU:O	1:A:552:VAL:HG22	2.21	0.41
1:A:512:ARG:O	1:A:516:GLU:HB2	2.21	0.41
1:A:914:HIS:HD2	1:A:988:GLU:OE2	2.03	0.41
1:A:418:ILE:C	1:A:418:ILE:HD13	2.46	0.41
1:A:489:GLU:O	1:A:493:GLU:HG3	2.21	0.41
1:A:349:HIS:HE1	3:A:2056:HOH:O	2.03	0.41
1:A:614:GLN:HG3	1:A:981:MET:HG2	2.02	0.40
1:A:730:HIS:HE1	1:A:743:GLU:OE2	2.03	0.40
1:A:205:PHE:CZ	1:A:223:LYS:HG3	2.57	0.40
1:A:335:ALA:HB3	1:A:339:MET:HE3	2.03	0.40
1:A:425:LEU:HD23	1:A:425:LEU:HA	1.93	0.40
1:A:620:LYS:HE2	1:A:660:VAL:HG11	2.03	0.40
1:A:278:HIS:CD2	1:A:280:SER:H	2.39	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	811/940 (86%)	785 (97%)	24 (3%)	2 (0%)	43 42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	365	VAL
1	A	231	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	740/827 (90%)	697 (94%)	43 (6%)	18	15

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	LYS
1	A	188	ARG
1	A	270	LEU
1	A	316	LEU
1	A	319	LEU
1	A	332	LYS
1	A	333	VAL
1	A	360	SER
1	A	365	VAL
1	A	368	GLU
1	A	379	ILE
1	A	418	ILE
1	A	423	LEU
1	A	429	LYS
1	A	451	GLU
1	A	453	LEU
1	A	467	SER
1	A	471	LEU
1	A	475	LEU
1	A	489	GLU
1	A	492	LEU
1	A	505	GLU
1	A	506	GLU
1	A	507	GLU
1	A	517	ARG
1	A	523	LEU
1	A	553	THR
1	A	565	LEU
1	A	574	LEU
1	A	631	LYS

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Mol	Chain	Res	Type
1	A	634	LEU
1	A	705	LYS
1	A	726	GLU
1	A	795	GLN
1	A	855	LEU
1	A	859	LEU
1	A	898	ASN
1	A	901	ILE
1	A	915	PHE
1	A	930	VAL
1	A	962	ARG
1	A	1004	LEU
1	A	1008	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	193	ASN
1	A	247	HIS
1	A	267	HIS
1	A	273	HIS
1	A	278	HIS
1	A	291	ASN
1	A	334	ASN
1	A	344	GLN
1	A	349	HIS
1	A	351	ASN
1	A	364	ASN
1	A	539	GLN
1	A	617	GLN
1	A	677	HIS
1	A	721	GLN
1	A	830	HIS
1	A	895	HIS
1	A	898	ASN
1	A	906	GLN
1	A	914	HIS
1	A	918	ASN
1	A	926	ASN
1	A	948	ASN
1	A	970	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	ZZN	A	1500	-	43,43,43	2.21	6 (13%)	58,64,64	2.59	23 (39%)

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	ZZN	A	1500	-	-	0/10/12/12	0/6/6/6

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1500	ZZN	CAS-CAO	8.47	1.57	1.49
2	A	1500	ZZN	NAV-NAU	-6.08	1.25	1.36
2	A	1500	ZZN	CBC-CBD	-5.52	1.41	1.49
2	A	1500	ZZN	C6-NAV	-4.34	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1500	ZZN	CAO-NAN	3.08	1.35	1.29
2	A	1500	ZZN	CAE-CAF	-2.86	1.41	1.47

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1500	ZZN	C5-CBD-NAU	-5.98	106.08	110.19
2	A	1500	ZZN	CAP-CAH-NAG	5.65	125.81	118.69
2	A	1500	ZZN	CAS-NAV-C6	-5.60	124.26	127.81
2	A	1500	ZZN	N3-C2-N1	-5.51	120.24	128.58
2	A	1500	ZZN	CAO-CAS-NAV	-5.36	104.70	112.14
2	A	1500	ZZN	CBD-NAU-NAV	5.07	110.76	106.02
2	A	1500	ZZN	CAE-CAF-NAG	4.91	120.60	115.14
2	A	1500	ZZN	C5-C6-N1	-4.50	122.19	126.97
2	A	1500	ZZN	CAS-NAV-NAU	4.17	123.32	120.01
2	A	1500	ZZN	CBB-CBC-CBD	3.95	126.60	120.34
2	A	1500	ZZN	N1-C6-NAV	3.89	131.41	125.34
2	A	1500	ZZN	C2-N3-C4	3.15	123.90	118.73
2	A	1500	ZZN	CBJ-CBC-CBD	-2.98	115.61	120.34
2	A	1500	ZZN	C2-N1-C6	2.96	119.07	111.83
2	A	1500	ZZN	CBC-CBJ-CBI	2.85	121.41	118.48
2	A	1500	ZZN	CAQ-CAP-CAH	2.51	120.55	117.42
2	A	1500	ZZN	CBH-CBI-CBJ	-2.44	120.54	123.50
2	A	1500	ZZN	OAB-CAF-NAG	-2.40	117.19	120.38
2	A	1500	ZZN	CAM-NAN-CAO	2.39	123.06	117.26
2	A	1500	ZZN	C6-NAV-NAU	2.36	112.38	111.05
2	A	1500	ZZN	CAI-CAH-NAG	-2.35	113.94	118.61
2	A	1500	ZZN	F-CBI-CBJ	2.10	121.26	118.28
2	A	1500	ZZN	C5-CBD-CBC	2.03	133.69	131.28

There are no chirality outliers.

There are no torsion outliers.

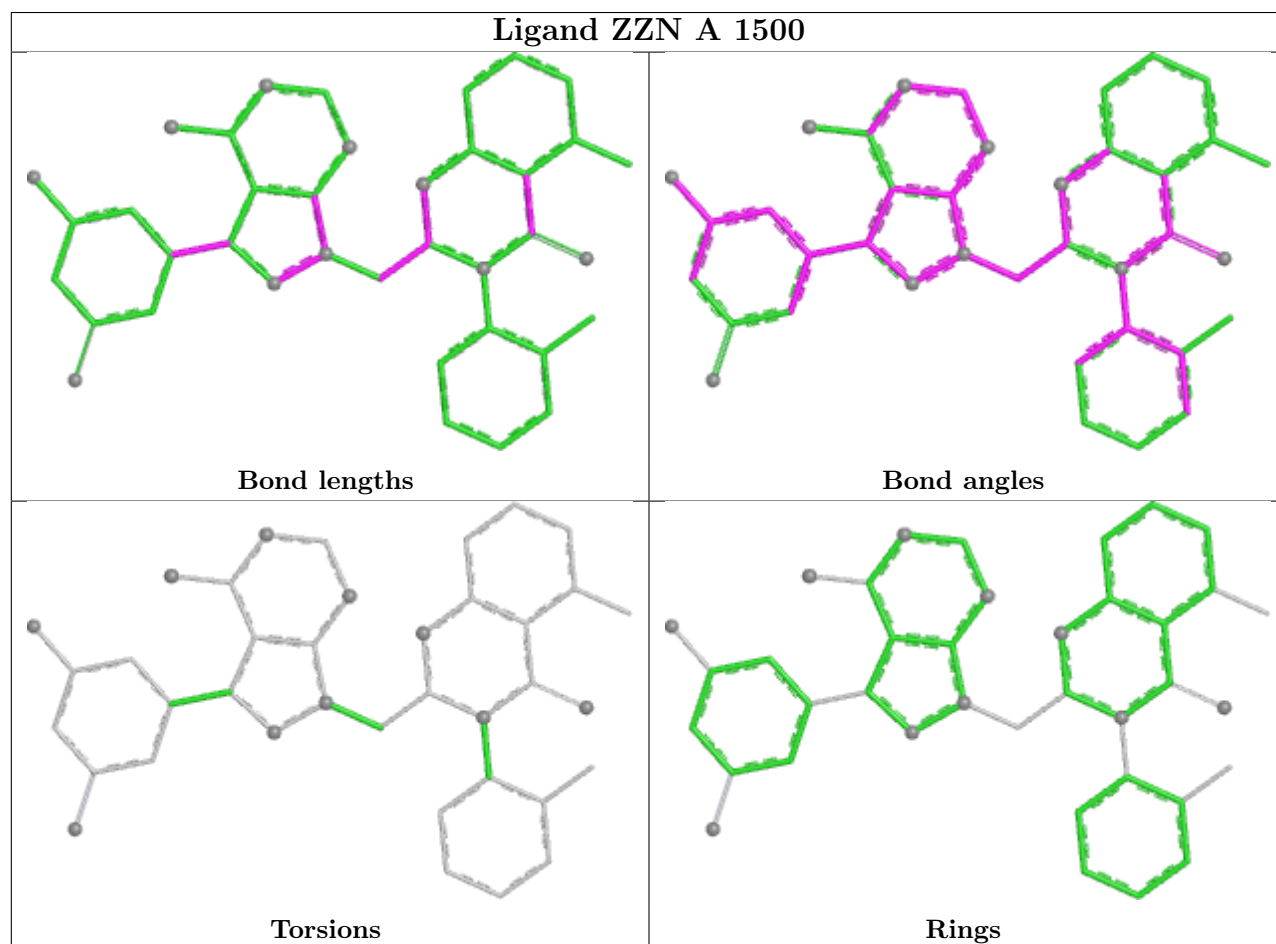
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1500	ZZN	1	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 ⓘ

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	835/940 (88%)	0.53	92 (11%) 10 9	9, 22, 42, 65	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	335	ALA	9.1
1	A	332	LYS	5.7
1	A	1027	TRP	5.5
1	A	333	VAL	5.4
1	A	511	LEU	5.2
1	A	398	VAL	5.2
1	A	445	VAL	5.1
1	A	317	TRP	5.0
1	A	232	LEU	4.8
1	A	270	LEU	4.3
1	A	316	LEU	4.2
1	A	936	TYR	3.9
1	A	334	ASN	3.7
1	A	507	GLU	3.7
1	A	418	ILE	3.7
1	A	363	VAL	3.6
1	A	919	PHE	3.6
1	A	514	ILE	3.6
1	A	358	VAL	3.4
1	A	846	ALA	3.4
1	A	228	PHE	3.4
1	A	442	TRP	3.4
1	A	318	SER	3.4
1	A	367	SER	3.3
1	A	341	LEU	3.3
1	A	415	ASP	3.3
1	A	512	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	515	LEU	3.2
1	A	339	MET	3.2
1	A	443	PRO	2.9
1	A	257	CYS	2.9
1	A	901	ILE	2.9
1	A	524	TYR	2.9
1	A	395	TYR	2.8
1	A	348	PHE	2.8
1	A	397	VAL	2.8
1	A	452	LEU	2.7
1	A	520	SER	2.7
1	A	350	GLY	2.7
1	A	459	VAL	2.7
1	A	526	HIS	2.7
1	A	523	LEU	2.6
1	A	420	TRP	2.6
1	A	455	PRO	2.6
1	A	331	ARG	2.6
1	A	153	HIS	2.6
1	A	463	PRO	2.6
1	A	444	SER	2.6
1	A	417	PRO	2.6
1	A	231	PRO	2.5
1	A	559	GLU	2.5
1	A	461	GLY	2.5
1	A	458	THR	2.4
1	A	378	ASP	2.4
1	A	345	ALA	2.4
1	A	453	LEU	2.4
1	A	419	ALA	2.3
1	A	377	PHE	2.3
1	A	464	ASN	2.3
1	A	366	CYS	2.3
1	A	478	VAL	2.3
1	A	191	LEU	2.3
1	A	843	ASN	2.2
1	A	319	LEU	2.2
1	A	492	LEU	2.2
1	A	474	TYR	2.2
1	A	205	PHE	2.2
1	A	490	LYS	2.2
1	A	457	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	945	GLY	2.2
1	A	203	PHE	2.2
1	A	489	GLU	2.2
1	A	189	ALA	2.2
1	A	416	CYS	2.2
1	A	494	LEU	2.2
1	A	351	ASN	2.2
1	A	1005	GLY	2.1
1	A	456	ALA	2.1
1	A	468	ALA	2.1
1	A	394	LEU	2.1
1	A	227	VAL	2.1
1	A	1024	ARG	2.1
1	A	993	LYS	2.1
1	A	353	MET	2.1
1	A	491	ILE	2.1
1	A	364	ASN	2.1
1	A	920	LYS	2.1
1	A	396	ALA	2.1
1	A	421	ALA	2.1
1	A	267	HIS	2.0
1	A	162	TRP	2.0
1	A	895	HIS	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](#)

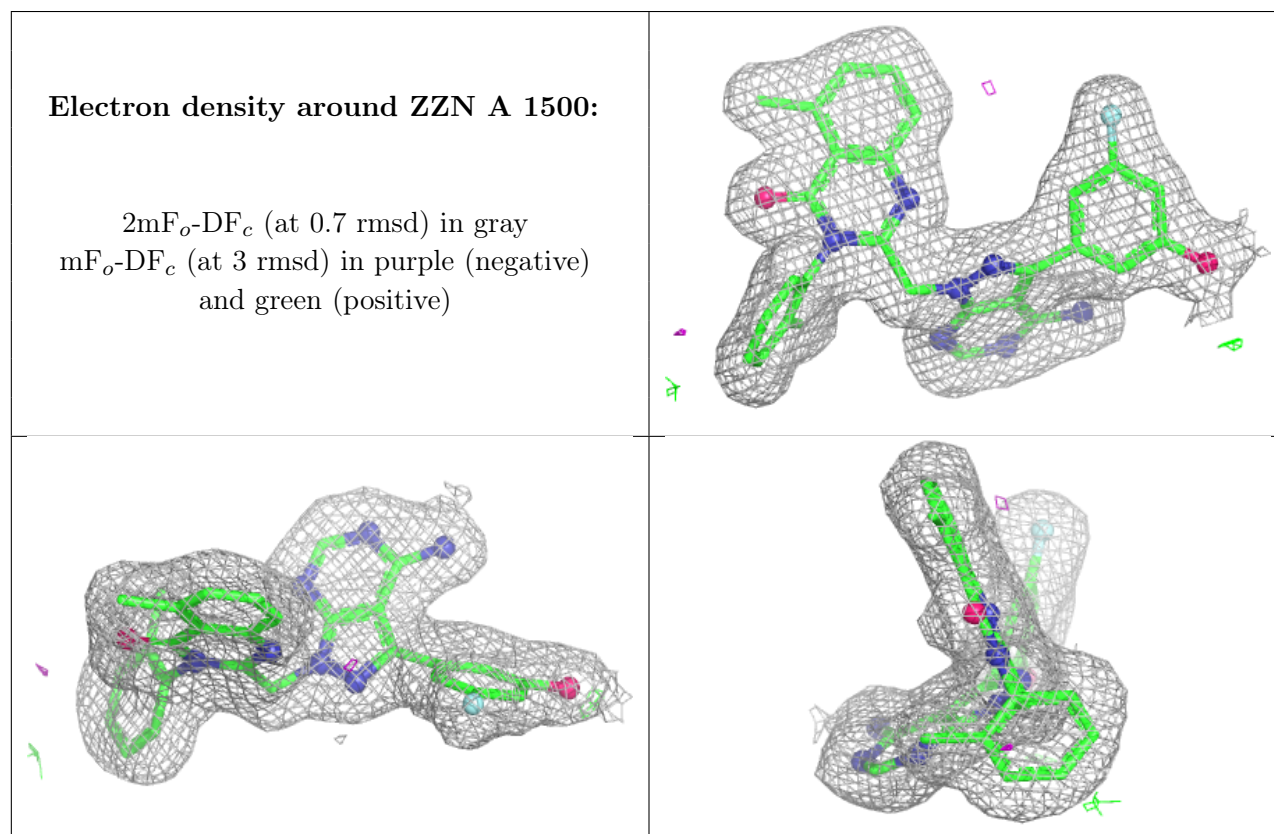
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZZN	A	1500	38/38	0.96	0.06	18,23,29,30	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 ⓘ

There are no such residues in this entry.