



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:26 PM UTC

PDB ID : 2WXM / pdb_00002wxm
Title : The crystal structure of the murine class IA PI 3-kinase p110delta in complex with DL06.
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 : 2.80 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

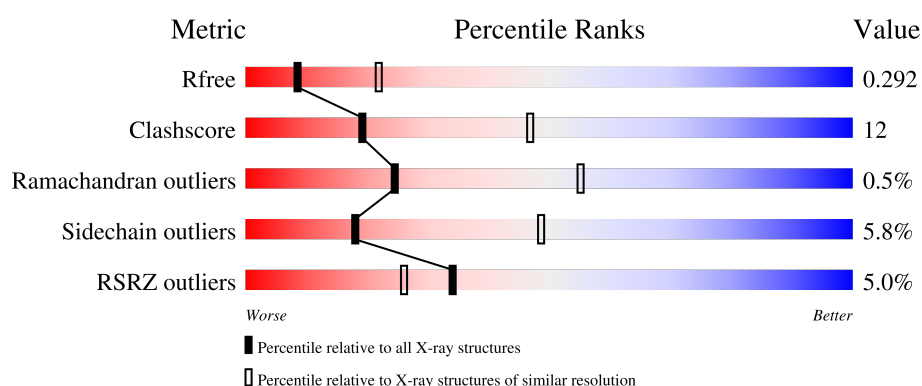
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	940	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 6654 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.

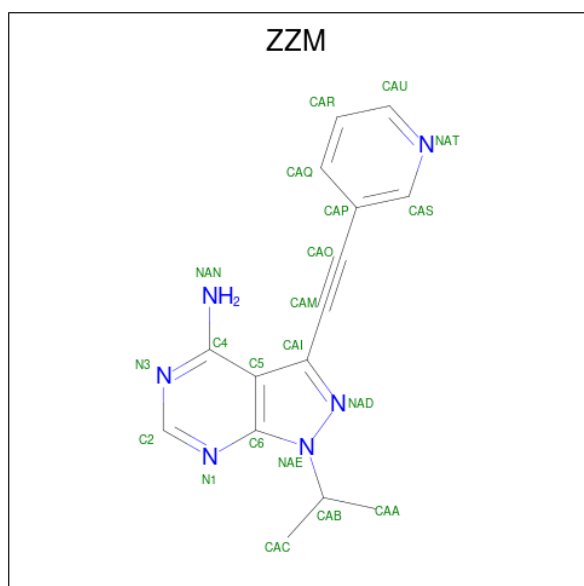
- Molecule 1 is a protein called PHOSPHATIDYLINOSITOL-4,5-BISPHOSPHATE 3-KINASE CATALYTIC SUBUNIT DELTA ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	822	Total	C	N	O	S	0	0	0
			6633	4254	1126	1199	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 1-(1-METHYLETHYL)-3-(PYRIDIN-3-YLETHYNYL)-1H-PYRAZOLO[3,4-D]PYRIMIDIN-4-AMINE (CCD ID: ZZM) (formula: C₁₅H₁₄N₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			21	15	6		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	143.28Å 64.56Å 117.44Å 90.00° 103.51° 90.00°	Depositor
Resolution (Å)	58.62 – 2.80 58.62 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.0 (58.62-2.80) 99.0 (58.62-2.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.32 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0046	Depositor
R, R_{free}	0.244 , 0.287 0.245 , 0.292	Depositor DCC
R_{free} test set	814 reflections (3.15%)	wwPDB-VP
Wilson B-factor (Å ²)	44.7	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 56.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	6654	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.20% 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: ZYM

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	0.95	5/6776 (0.1%)	1.02	10/9142 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	321	GLN	CD-NE2	8.59	1.51	1.33
1	A	479	ALA	C-O	8.10	1.39	1.23
1	A	321	GLN	CB-CG	7.03	1.73	1.52
1	A	429	LYS	CE-NZ	5.95	1.67	1.49
1	A	763	TYR	CA-C	-5.39	1.46	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	930	VAL	N-CA-C	6.75	114.43	108.63
1	A	334	ASN	N-CA-C	5.83	123.23	110.80
1	A	794	ILE	N-CA-C	-5.81	104.85	110.72
1	A	384	LEU	CA-C-N	-5.33	114.76	120.03
1	A	384	LEU	C-N-CA	-5.33	114.76	120.03
1	A	911	ASP	CB-CA-C	-5.28	103.95	112.09
1	A	444	SER	N-CA-C	5.28	117.12	108.52
1	A	911	ASP	N-CA-C	5.21	118.43	111.24
1	A	198	GLY	N-CA-C	5.16	119.37	112.77
1	A	955	ARG	N-CA-C	-5.02	105.81	111.28

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	6633	0	6615	155	0
2	A	21	0	14	3	0
All	All	6654	0	6629	155	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 12.

All (155) 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:367:SER:HB3	1:A:368:GLU:C	1.69	1.15
1:A:962:ARG:HG2	1:A:962:ARG:HH11	1.14	1.11
1:A:549:LEU:HG	1:A:564:MET:HE1	1.34	1.08
1:A:837:ILE:HD11	1:A:901:ILE:HD11	1.49	0.95
1:A:245:GLY:HA3	1:A:768:ALA:HB2	1.53	0.90
1:A:901:ILE:HD12	1:A:901:ILE:O	1.73	0.89
1:A:329:GLU:HB2	1:A:369:PRO:O	1.74	0.88
1:A:271:THR:O	1:A:273:HIS:HD2	1.58	0.86
1:A:699:VAL:HG21	1:A:715:MET:HE2	1.61	0.82
1:A:387:MET:HE3	1:A:590:CYS:HB3	1.60	0.82
1:A:837:ILE:CD1	1:A:901:ILE:HD11	2.09	0.82
1:A:549:LEU:CG	1:A:564:MET:HE1	2.09	0.81
1:A:367:SER:HB3	1:A:369:PRO:N	1.97	0.79
1:A:534:MET:HA	1:A:534:MET:HE2	1.68	0.75
1:A:752:MET:HE2	1:A:760:TRP:HE3	1.50	0.75
1:A:205:PHE:CE1	1:A:223:LYS:HG3	2.23	0.73
1:A:549:LEU:HG	1:A:564:MET:CE	2.15	0.73
1:A:752:MET:HE1	1:A:777:ILE:HG12	1.70	0.72
1:A:895:HIS:H	1:A:898:ASN:HD21	1.37	0.71
1:A:205:PHE:CZ	1:A:223:LYS:HG3	2.26	0.71
1:A:523:LEU:O	1:A:528:LYS:HE3	1.90	0.71
1:A:962:ARG:HH11	1:A:962:ARG:CG	1.98	0.71
1:A:218:ALA:O	1:A:222:ARG:HG3	1.89	0.71
1:A:387:MET:HE3	1:A:590:CYS:CB	2.21	0.70
1:A:387:MET:HE3	1:A:590:CYS:SG	2.32	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:748:GLN:NE2	1:A:762:MET:HG3	2.07	0.69
1:A:278:HIS:HD2	1:A:280:SER:OG	1.75	0.69
1:A:617:GLN:HE21	1:A:984:ALA:HA	1.58	0.69
1:A:699:VAL:HG21	1:A:715:MET:CE	2.22	0.68
1:A:110:LYS:HZ3	1:A:144:ARG:HH12	1.42	0.68
1:A:843:ASN:HB3	1:A:844:MET:HE2	1.76	0.67
1:A:715:MET:HE1	1:A:751:PHE:HB3	1.78	0.66
1:A:289:GLN:HG2	1:A:677:HIS:CD2	2.30	0.66
1:A:434:THR:HG21	1:A:477:GLU:HA	1.78	0.65
1:A:343:VAL:H	1:A:360:SER:HB2	1.61	0.65
1:A:621:TYR:CZ	1:A:983:ALA:HB2	2.33	0.64
1:A:918:ASN:HB2	1:A:988:GLU:OE1	1.98	0.64
1:A:167:PHE:HZ	1:A:285:MET:HE1	1.63	0.63
1:A:367:SER:CB	1:A:368:GLU:C	2.60	0.63
1:A:435:GLY:O	1:A:475:LEU:N	2.32	0.63
1:A:328:ILE:HB	1:A:472:VAL:HG23	1.79	0.62
1:A:334:ASN:CG	1:A:335:ALA:H	2.08	0.62
1:A:245:GLY:HA3	1:A:768:ALA:CB	2.27	0.61
1:A:368:GLU:O	1:A:368:GLU:HG3	2.01	0.61
1:A:387:MET:CE	1:A:590:CYS:SG	2.89	0.60
1:A:208:SER:OG	1:A:210:LYS:HG2	2.02	0.60
1:A:334:ASN:ND2	1:A:335:ALA:H	2.00	0.60
1:A:435:GLY:HA2	1:A:475:LEU:O	2.01	0.60
1:A:962:ARG:HG2	1:A:962:ARG:NH1	1.94	0.60
1:A:984:ALA:HB3	1:A:986:LEU:HD13	1.85	0.58
1:A:271:THR:O	1:A:273:HIS:CD2	2.50	0.57
1:A:858:TRP:CZ3	1:A:901:ILE:HD13	2.39	0.57
1:A:1023:LEU:O	1:A:1026:SER:HB3	2.05	0.56
1:A:679:MET:O	1:A:683:MET:HG3	2.05	0.56
1:A:617:GLN:HE22	1:A:620:LYS:NZ	2.04	0.55
1:A:752:MET:HE2	1:A:760:TRP:CE3	2.39	0.55
1:A:779:LYS:NZ	2:A:1500:ZYM:NAT	2.52	0.55
1:A:842:SER:O	1:A:844:MET:HE2	2.07	0.55
1:A:291:ASN:ND2	1:A:676:THR:H	2.04	0.54
1:A:335:ALA:C	1:A:339:MET:HB2	2.33	0.54
1:A:512:ARG:NH1	1:A:534:MET:HB3	2.24	0.53
1:A:617:GLN:NE2	1:A:984:ALA:HA	2.23	0.53
1:A:110:LYS:NZ	1:A:144:ARG:HH12	2.06	0.53
1:A:911:ASP:OD1	2:A:1500:ZYM:CAS	2.57	0.53
1:A:383:ASP:OD2	1:A:557:LYS:HA	2.08	0.52
1:A:167:PHE:CZ	1:A:285:MET:HE1	2.43	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:915:PHE:CD2	1:A:915:PHE:C	2.88	0.52
1:A:914:HIS:CD2	1:A:918:ASN:O	2.63	0.52
1:A:205:PHE:CE1	1:A:219:CYS:HB3	2.45	0.52
1:A:895:HIS:H	1:A:898:ASN:ND2	2.06	0.52
1:A:146:PHE:CE1	1:A:631:LYS:HD2	2.45	0.51
1:A:194:VAL:HG21	1:A:216:LEU:HD21	1.91	0.51
1:A:255:PRO:HG2	1:A:258:HIS:CD2	2.46	0.51
1:A:431:GLN:HB2	1:A:484:TYR:CE1	2.46	0.50
1:A:637:ALA:HB1	1:A:644:GLY:HA2	1.91	0.50
1:A:512:ARG:HH11	1:A:534:MET:HB3	1.77	0.50
1:A:364:ASN:C	1:A:366:CYS:H	2.20	0.50
1:A:786:GLN:HG2	1:A:913:GLY:HA2	1.94	0.50
1:A:911:ASP:OD1	2:A:1500:ZMZ:NAT	2.45	0.49
1:A:332:LYS:HZ3	1:A:341:LEU:HD21	1.78	0.49
1:A:367:SER:HB3	1:A:368:GLU:CA	2.39	0.49
1:A:620:LYS:HE2	1:A:660:VAL:HG11	1.94	0.49
1:A:335:ALA:O	1:A:339:MET:HB2	2.12	0.49
1:A:917:GLY:O	1:A:919:PHE:N	2.45	0.49
1:A:146:PHE:CZ	1:A:631:LYS:HD2	2.48	0.48
1:A:246:ARG:NH1	1:A:248:GLU:OE1	2.46	0.48
1:A:291:ASN:HD21	1:A:676:THR:H	1.61	0.48
1:A:962:ARG:CG	1:A:962:ARG:NH1	2.66	0.48
1:A:553:THR:CG2	1:A:564:MET:HE3	2.43	0.48
1:A:154:ARG:HD2	1:A:165:TYR:CE2	2.49	0.48
1:A:344:GLN:NE2	1:A:453:LEU:HD13	2.29	0.47
1:A:355:CYS:HB2	1:A:378:ASP:HB3	1.96	0.47
1:A:332:LYS:NZ	1:A:341:LEU:HD21	2.30	0.47
1:A:368:GLU:N	1:A:369:PRO:CD	2.78	0.47
1:A:734:PRO:O	1:A:816:LEU:HD22	2.14	0.47
1:A:742:GLU:HG3	1:A:765:SER:HB2	1.97	0.47
1:A:870:ARG:NH2	1:A:874:GLU:OE2	2.46	0.47
1:A:323:PHE:HD2	1:A:377:PHE:CD2	2.33	0.46
1:A:843:ASN:O	1:A:843:ASN:ND2	2.48	0.46
1:A:256:LEU:O	1:A:262:ILE:HB	2.14	0.46
1:A:532:TRP:CZ3	1:A:553:THR:HB	2.49	0.46
1:A:617:GLN:HE22	1:A:620:LYS:HZ1	1.63	0.46
1:A:247:HIS:HB2	1:A:738:SER:HA	1.96	0.46
1:A:437:ARG:O	1:A:472:VAL:HA	2.16	0.46
1:A:617:GLN:HE21	1:A:984:ALA:CA	2.27	0.46
1:A:693:LYS:HE2	1:A:780:ASN:ND2	2.30	0.46
1:A:894:ARG:HD3	1:A:909:HIS:ND1	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:GLU:O	1:A:437:ARG:HD2	2.16	0.46
1:A:842:SER:O	1:A:844:MET:CE	2.64	0.46
1:A:327:LEU:O	1:A:372:LYS:N	2.49	0.45
1:A:525:GLU:HA	1:A:528:LYS:HD2	1.97	0.45
1:A:189:ALA:HA	1:A:207:VAL:O	2.17	0.45
1:A:700:LYS:HE3	1:A:756:MET:O	2.17	0.45
1:A:759:LEU:O	1:A:777:ILE:HA	2.17	0.45
1:A:330:GLY:O	1:A:368:GLU:HA	2.16	0.45
1:A:955:ARG:NH2	1:A:959:TYR:OH	2.49	0.45
1:A:1002:LEU:O	1:A:1003:ALA:C	2.61	0.44
1:A:242:GLN:HB2	1:A:249:TYR:CE2	2.52	0.44
1:A:419:ALA:HB1	1:A:441:MET:HB3	2.00	0.44
1:A:523:LEU:HG	1:A:528:LYS:HG3	1.98	0.44
1:A:485:PHE:HA	1:A:486:PRO:HD3	1.86	0.44
1:A:901:ILE:HD12	1:A:901:ILE:C	2.39	0.44
1:A:278:HIS:CD2	1:A:280:SER:H	2.36	0.44
1:A:553:THR:HG22	1:A:564:MET:HE3	1.99	0.43
1:A:188:ARG:HD2	1:A:189:ALA:O	2.18	0.43
1:A:929:ARG:HH22	1:A:1001:SER:HB3	1.82	0.43
1:A:225:ALA:O	1:A:230:GLN:N	2.52	0.43
1:A:699:VAL:CG2	1:A:715:MET:CE	2.93	0.43
1:A:750:THR:OG1	1:A:751:PHE:N	2.51	0.43
1:A:319:LEU:H	1:A:319:LEU:HG	1.49	0.42
1:A:365:VAL:CG1	1:A:365:VAL:O	2.67	0.42
1:A:713:GLU:O	1:A:717:MET:HG3	2.20	0.42
1:A:349:HIS:HB2	1:A:354:LEU:HD11	2.00	0.42
1:A:138:ASP:O	1:A:139:PHE:C	2.62	0.42
1:A:527:GLU:O	1:A:531:VAL:HG23	2.20	0.42
1:A:834:ILE:HD11	1:A:901:ILE:HG23	2.02	0.42
1:A:352:GLU:OE1	1:A:352:GLU:HA	2.19	0.42
1:A:583:LEU:HD11	1:A:600:LEU:HD11	2.02	0.42
1:A:929:ARG:HH22	1:A:1001:SER:CB	2.32	0.42
1:A:1006:LYS:HB3	1:A:1010:GLU:HB2	2.01	0.41
1:A:154:ARG:HG2	1:A:154:ARG:HH11	1.85	0.41
1:A:323:PHE:CD2	1:A:377:PHE:CD2	3.08	0.41
1:A:698:PHE:CZ	1:A:714:MET:HB3	2.55	0.41
1:A:237:GLU:OE1	1:A:237:GLU:N	2.50	0.41
1:A:356:LYS:H	1:A:356:LYS:HG2	1.66	0.41
1:A:454:ASN:ND2	1:A:457:GLY:HA3	2.35	0.41
1:A:910:ILE:HD13	1:A:910:ILE:HG21	1.87	0.41
1:A:171:LEU:O	1:A:260:GLN:NE2	2.40	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:GLU:HG3	1:A:490:LYS:N	2.36	0.41
1:A:832:ASP:CG	1:A:836:ASN:HD22	2.29	0.41
1:A:579:ALA:HB1	1:A:600:LEU:HG	2.03	0.40
1:A:188:ARG:HD2	1:A:189:ALA:N	2.37	0.40
1:A:137:ASN:O	1:A:141:THR:HG23	2.21	0.40
1:A:316:LEU:HD12	1:A:317:TRP:N	2.36	0.40
1:A:325:ILE:O	1:A:325:ILE:HG13	2.21	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	800/940 (85%)	761 (95%)	35 (4%)	4 (0%)	24 55

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	755	LYS
1	A	918	ASN
1	A	365	VAL
1	A	478	VAL

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	728/827 (88%)	686 (94%)	42 (6%)	18	49

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	LYS
1	A	132	ARG
1	A	203	PHE
1	A	229	ARG
1	A	263	CYS
1	A	291	ASN
1	A	316	LEU
1	A	317	TRP
1	A	319	LEU
1	A	328	ILE
1	A	332	LYS
1	A	333	VAL
1	A	339	MET
1	A	340	LYS
1	A	352	GLU
1	A	365	VAL
1	A	366	CYS
1	A	367	SER
1	A	394	LEU
1	A	398	VAL
1	A	423	LEU
1	A	467	SER
1	A	517	ARG
1	A	523	LEU
1	A	530	LEU
1	A	553	THR
1	A	631	LYS
1	A	705	LYS
1	A	726	GLU
1	A	743	GLU
1	A	753	ASP
1	A	755	LYS
1	A	759	LEU
1	A	804	GLU
1	A	855	LEU
1	A	898	ASN
1	A	912	PHE
1	A	915	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	962	ARG
1	A	990	SER
1	A	1004	LEU
1	A	1009	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	GLN
1	A	273	HIS
1	A	278	HIS
1	A	291	ASN
1	A	334	ASN
1	A	344	GLN
1	A	536	HIS
1	A	617	GLN
1	A	696	ASN
1	A	704	GLN
1	A	748	GLN
1	A	780	ASN
1	A	836	ASN
1	A	843	ASN
1	A	895	HIS
1	A	898	ASN
1	A	914	HIS
1	A	918	ASN
1	A	1014	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

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	ZZM	A	1500	-	21,23,23	1.89	1 (4%)	31,32,32	3.25	11 (35%)

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	ZZM	A	1500	-	-	2/7/9/9	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1500	ZZM	NAE-NAD	-7.44	1.24	1.38

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1500	ZZM	C5-C6-N1	-9.41	116.98	126.97
2	A	1500	ZZM	CAI-NAD-NAE	7.40	110.87	103.81
2	A	1500	ZZM	N1-C6-NAE	7.36	135.64	126.05
2	A	1500	ZZM	N3-C2-N1	-5.02	120.99	128.58
2	A	1500	ZZM	C4-C5-C6	5.01	119.49	115.74
2	A	1500	ZZM	C2-N1-C6	4.65	123.19	111.83
2	A	1500	ZZM	CAA-CAB-NAE	3.29	115.79	109.98
2	A	1500	ZZM	CAU-NAT-CAS	2.44	121.13	116.85
2	A	1500	ZZM	C5-CAI-NAD	-2.35	108.59	110.19
2	A	1500	ZZM	C6-NAE-NAD	-2.32	109.42	110.90
2	A	1500	ZZM	C4-C5-CAI	-2.22	136.82	139.12

There are no chirality outliers.

All (2) torsion outliers are listed below:

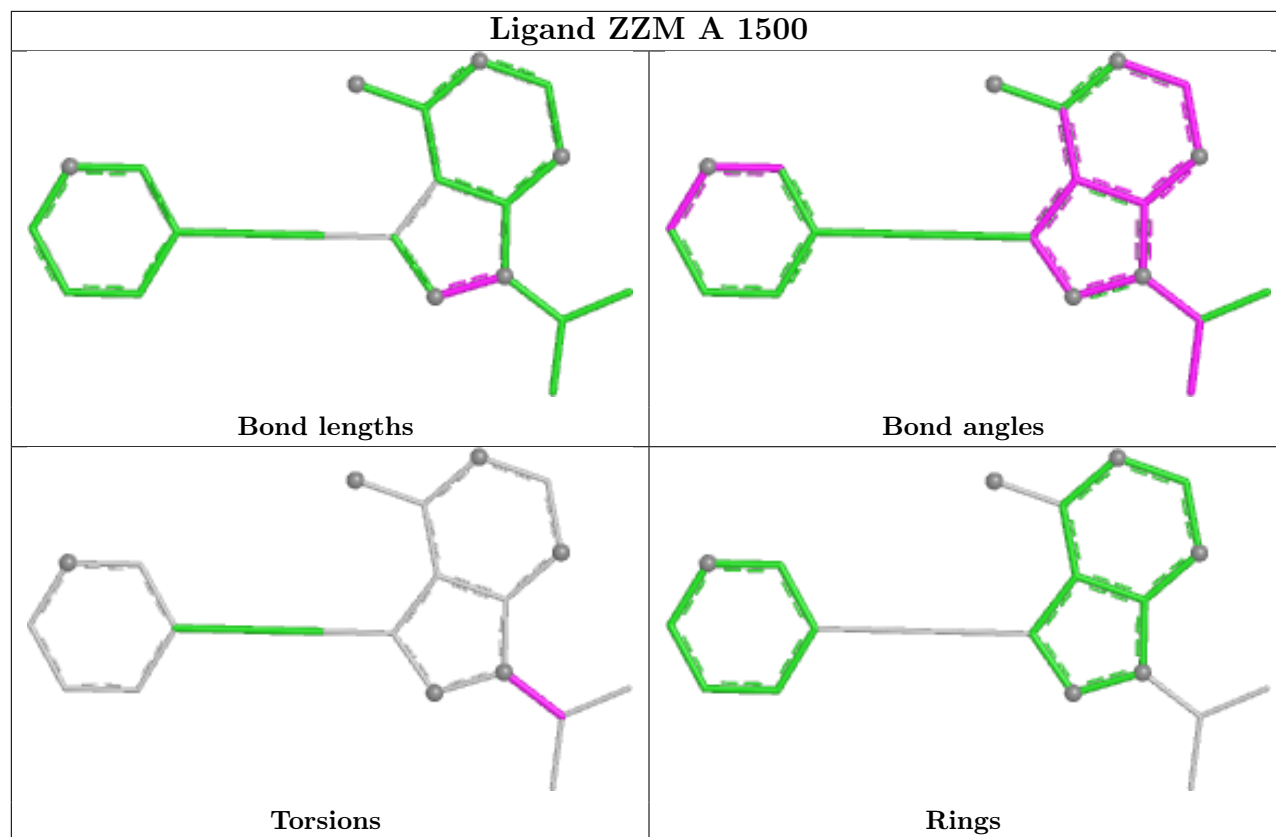
Mol	Chain	Res	Type	Atoms
2	A	1500	ZZM	CAA-CAB-NAE-NAD
2	A	1500	ZZM	CAA-CAB-NAE-C6

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1500	ZZM	3	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	822/940 (87%)	0.38	41 (4%) 34 26	9, 19, 33, 51	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	479	ALA	6.9
1	A	334	ASN	4.7
1	A	494	LEU	4.7
1	A	428	TYR	4.2
1	A	846	ALA	4.2
1	A	317	TRP	4.1
1	A	335	ALA	4.0
1	A	486	PRO	4.0
1	A	482	PRO	4.0
1	A	341	LEU	3.5
1	A	484	TYR	3.1
1	A	319	LEU	3.1
1	A	386	ARG	3.0
1	A	318	SER	3.0
1	A	485	PHE	2.7
1	A	429	LYS	2.6
1	A	388	ALA	2.6
1	A	511	LEU	2.5
1	A	770	SER	2.5
1	A	478	VAL	2.4
1	A	842	SER	2.4
1	A	366	CYS	2.4
1	A	430	ASP	2.4
1	A	427	ASP	2.4
1	A	487	ALA	2.3
1	A	322	PRO	2.2
1	A	387	MET	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	490	LYS	2.2
1	A	374	ARG	2.2
1	A	838	GLN	2.2
1	A	342	VAL	2.2
1	A	382	CYS	2.2
1	A	379	ILE	2.2
1	A	381	VAL	2.2
1	A	769	GLY	2.2
1	A	323	PHE	2.1
1	A	349	HIS	2.1
1	A	173	PRO	2.1
1	A	459	VAL	2.0
1	A	919	PHE	2.0
1	A	371	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](#)

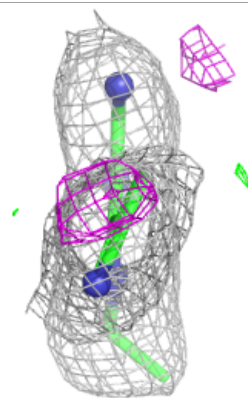
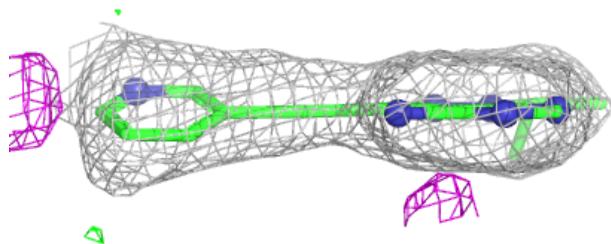
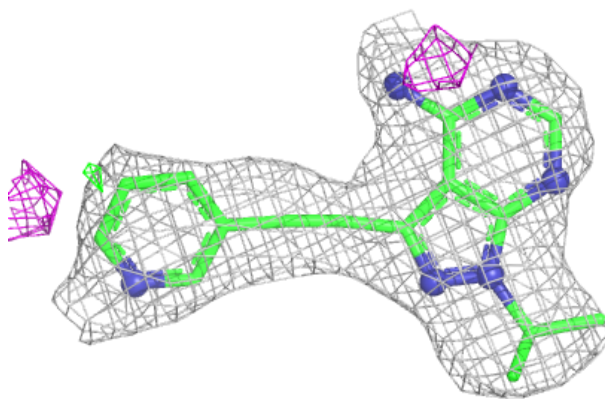
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	ZZM	A	1500	21/21	0.93	0.09	25,30,33,33	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.

Electron density around ZZM A 1500:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.