



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 05:56 AM UTC

PDB ID : 2WXL / pdb_00002wxl
Title : The crystal structure of the murine class IA PI 3-kinase p110delta in complex with ZSTK474.
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 : 1.99 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

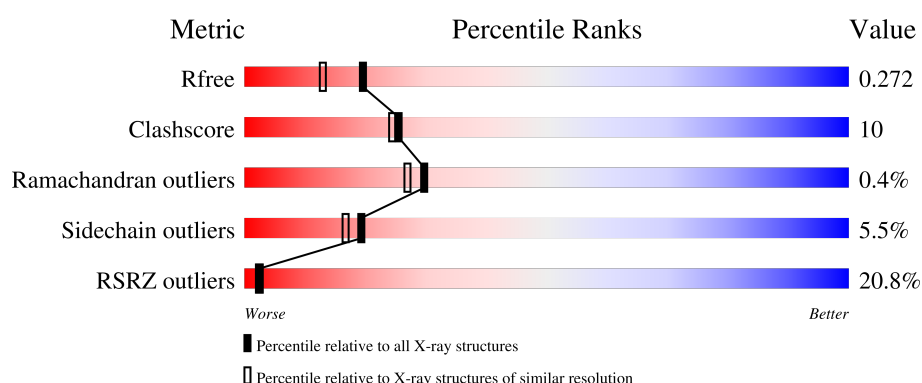
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6944 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.

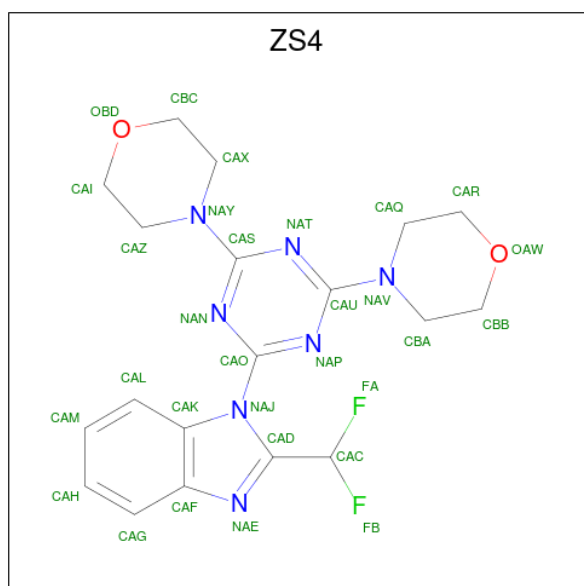
- Molecule 1 is a protein called PHOSPHATIDYLINOSITOL-4,5-BISPHOSPHATE 3-KINASE CATALYTIC SUBUNIT DELTA ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	823	6656	4268	1131	1203	54	0	2	0

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-(difluoromethyl)-1-(4,6-dimorpholin-4-yl-1,3,5-triazin-2-yl)-1H-benzimidazole (CCD ID: ZS4) (formula: C₁₉H₂₁F₂N₇O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
2	A	1	30	19	2	7	2	0	0

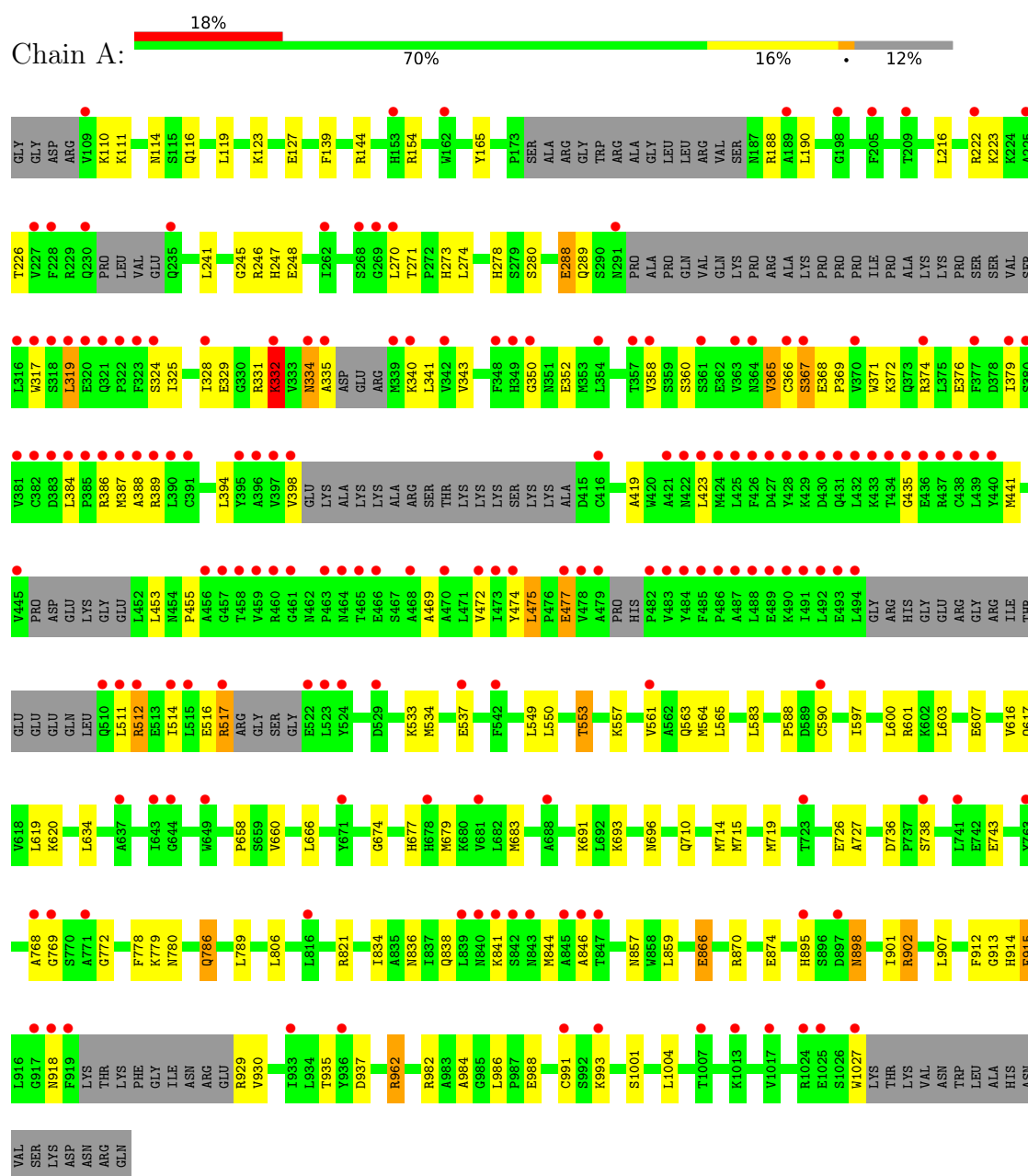
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	258	Total 258	O 258	0	0

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 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	142.54Å 64.29Å 116.72Å 90.00° 103.42° 90.00°	Depositor
Resolution (Å)	37.85 – 1.99 37.85 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.5 (37.85-1.99) 99.5 (37.85-1.99)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0046	Depositor
R, R_{free}	0.214 , 0.254 0.239 , 0.272	Depositor DCC
R_{free} test set	2115 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å ²)	28.2	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	6944	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% 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: ZS4

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	3/6805 (0.0%)	0.90	6/9180 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	379	ILE	C-O	6.22	1.31	1.23
1	A	902	ARG	CD-NE	-5.62	1.38	1.46
1	A	388	ALA	C-O	5.56	1.30	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	332	LYS	N-CA-C	7.13	117.93	107.88
1	A	736	ASP	CA-C-N	-6.19	113.43	119.87
1	A	736	ASP	C-N-CA	-6.19	113.43	119.87
1	A	334	ASN	N-CA-C	5.41	116.37	108.14
1	A	384	LEU	CA-C-N	-5.41	115.01	120.31
1	A	384	LEU	C-N-CA	-5.41	115.01	120.31

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	6656	0	6642	127	0
2	A	30	0	21	1	0
3	A	258	0	0	12	0
All	All	6944	0	6663	128	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 (128) 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	1.70	1.16
1:A:386:ARG:HG3	1:A:387:MET:HE2	1.35	1.08
1:A:962[A]:ARG:HH11	1:A:962[A]:ARG:HG2	1.19	1.07
1:A:549:LEU:HG	1:A:564:MET:HE1	1.07	1.05
1:A:962[A]:ARG:HG2	1:A:962[A]:ARG:NH1	1.74	0.98
1:A:962[A]:ARG:HH11	1:A:962[A]:ARG:CG	1.75	0.98
1:A:110:LYS:HE3	1:A:114:ASN:HD21	1.38	0.87
1:A:836:ASN:CG	3:A:2208:HOH:O	2.17	0.86
1:A:902:ARG:HD3	3:A:2201:HOH:O	1.76	0.85
1:A:328:ILE:O	1:A:371:TRP:O	1.92	0.85
1:A:549:LEU:CG	1:A:564:MET:HE1	2.02	0.82
1:A:549:LEU:HG	1:A:564:MET:CE	2.02	0.81
1:A:246:ARG:NH1	1:A:248:GLU:OE1	2.15	0.80
1:A:387:MET:HE3	1:A:590:CYS:SG	2.27	0.75
1:A:110:LYS:NZ	1:A:144:ARG:HH12	1.88	0.72
1:A:929:ARG:HH22	1:A:1001:SER:HB3	1.56	0.71
1:A:512:ARG:HH11	1:A:512:ARG:HG3	1.54	0.70
1:A:617:GLN:HE21	1:A:984:ALA:HA	1.56	0.70
1:A:821:ARG:HD2	3:A:2193:HOH:O	1.91	0.70
1:A:394:LEU:CD2	1:A:441:MET:HE1	2.22	0.69
1:A:332:LYS:HZ3	1:A:341:LEU:HD11	1.56	0.69
1:A:902:ARG:CD	3:A:2201:HOH:O	2.34	0.69
1:A:534:MET:HA	1:A:534:MET:HE2	1.74	0.69
1:A:512:ARG:O	1:A:516:GLU:HB2	1.97	0.65
1:A:394:LEU:HD22	1:A:441:MET:HE1	1.78	0.64
1:A:278:HIS:HD2	1:A:280:SER:OG	1.80	0.63
1:A:841:LYS:HD3	1:A:844:MET:HE3	1.80	0.63
1:A:768:ALA:HB3	1:A:772:GLY:HA3	1.78	0.63
1:A:553:THR:HG22	1:A:564:MET:HE2	1.79	0.63
1:A:806:LEU:HD13	1:A:962[B]:ARG:HD2	1.82	0.62
1:A:222:ARG:O	1:A:226:THR:HG23	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:SER:HB3	1:A:368:GLU:O	2.00	0.61
1:A:367:SER:HB3	1:A:368:GLU:CA	2.29	0.61
1:A:553:THR:CG2	1:A:564:MET:HE2	2.31	0.61
1:A:620:LYS:HE2	1:A:660:VAL:HG11	1.82	0.60
1:A:245:GLY:HA3	1:A:768:ALA:HB2	1.84	0.60
1:A:123:LYS:NZ	1:A:127:GLU:OE1	2.36	0.59
1:A:836:ASN:HB2	3:A:2208:HOH:O	2.02	0.58
1:A:836:ASN:CB	3:A:2208:HOH:O	2.50	0.58
1:A:895:HIS:H	1:A:898:ASN:HD21	1.51	0.58
1:A:915:PHE:C	1:A:915:PHE:CD1	2.79	0.57
1:A:435:GLY:HA2	1:A:475:LEU:O	2.05	0.56
1:A:332:LYS:HZ2	1:A:341:LEU:HD21	1.71	0.56
1:A:328:ILE:HB	1:A:472:VAL:HG23	1.88	0.55
1:A:110:LYS:HZ3	1:A:144:ARG:HH12	1.54	0.55
1:A:419:ALA:HB3	1:A:441:MET:HE3	1.87	0.55
1:A:870:ARG:NH2	1:A:874:GLU:OE2	2.40	0.55
1:A:512:ARG:NH1	1:A:534:MET:HG3	2.22	0.55
1:A:319:LEU:N	1:A:319:LEU:HD23	2.22	0.54
1:A:154:ARG:HG2	1:A:154:ARG:HH11	1.72	0.54
1:A:324:SER:HB3	1:A:376:GLU:HG3	1.90	0.54
1:A:841:LYS:HB2	1:A:844:MET:HG3	1.89	0.53
1:A:915:PHE:C	1:A:915:PHE:HD1	2.16	0.53
1:A:154:ARG:HD2	1:A:165:TYR:CE2	2.43	0.53
1:A:779:LYS:HG2	3:A:2166:HOH:O	2.08	0.52
1:A:389:ARG:NH1	1:A:455:PRO:O	2.40	0.52
1:A:553:THR:CG2	1:A:564:MET:CE	2.88	0.52
1:A:216:LEU:HD22	1:A:241:LEU:HD11	1.92	0.51
1:A:110:LYS:HE3	1:A:114:ASN:ND2	2.19	0.51
1:A:329:GLU:HB2	1:A:369:PRO:O	2.11	0.51
1:A:617:GLN:NE2	1:A:984:ALA:HA	2.23	0.51
1:A:371:TRP:O	1:A:372:LYS:HG3	2.10	0.50
1:A:914:HIS:HB3	1:A:918:ASN:O	2.12	0.50
1:A:533:LYS:HG3	1:A:534:MET:HE3	1.94	0.50
1:A:786:GLN:HE22	1:A:988:GLU:HB2	1.77	0.50
1:A:907:LEU:C	1:A:907:LEU:HD23	2.38	0.49
1:A:154:ARG:NH2	1:A:674:GLY:O	2.46	0.49
1:A:929:ARG:HH22	1:A:1001:SER:CB	2.22	0.49
1:A:838:GLN:NE2	1:A:937:ASP:OD2	2.45	0.49
1:A:394:LEU:HD23	1:A:441:MET:HE1	1.94	0.49
1:A:895:HIS:H	1:A:898:ASN:ND2	2.11	0.49
1:A:343:VAL:H	1:A:360:SER:HB3	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:ASN:CG	1:A:335:ALA:H	2.21	0.48
1:A:241:LEU:HD13	1:A:274:LEU:HD13	1.95	0.48
1:A:366:CYS:O	1:A:367:SER:HB2	2.13	0.48
1:A:334:ASN:CG	1:A:335:ALA:N	2.72	0.48
1:A:516:GLU:C	1:A:517:ARG:HG2	2.39	0.47
1:A:982:ARG:NH2	1:A:991:CYS:HA	2.29	0.47
1:A:715:MET:O	1:A:719:MET:HG3	2.15	0.47
1:A:617:GLN:HE21	1:A:984:ALA:CA	2.27	0.47
1:A:693:LYS:HE2	1:A:780:ASN:ND2	2.29	0.47
1:A:588:PRO:HD2	3:A:2077:HOH:O	2.14	0.47
1:A:597:ILE:HG22	1:A:601:ARG:NH2	2.30	0.47
1:A:332:LYS:NZ	1:A:341:LEU:HD11	2.29	0.46
1:A:247:HIS:O	1:A:738:SER:HB2	2.15	0.46
1:A:561:VAL:O	1:A:565:LEU:HD13	2.15	0.46
1:A:154:ARG:HD2	1:A:165:TYR:CZ	2.51	0.46
1:A:913:GLY:N	3:A:2232:HOH:O	2.49	0.46
1:A:289:GLN:HG2	1:A:677:HIS:CD2	2.51	0.45
1:A:328:ILE:HD11	1:A:474:TYR:HB2	1.97	0.45
1:A:691:LYS:HG3	1:A:727:ALA:CB	2.47	0.44
2:A:1500:ZS4:CAC	2:A:1500:ZS4:NAN	2.80	0.44
1:A:512:ARG:HG3	1:A:512:ARG:NH1	2.29	0.44
1:A:583:LEU:HD11	1:A:600:LEU:HD11	2.00	0.44
1:A:334:ASN:HD22	1:A:365:VAL:HG22	1.83	0.44
1:A:834:ILE:O	1:A:838:GLN:HG3	2.18	0.44
1:A:859:LEU:HD21	1:A:901:ILE:HD11	1.98	0.44
1:A:350:GLY:HA3	1:A:588:PRO:HG3	2.00	0.43
1:A:603:LEU:HD22	1:A:607:GLU:HB3	2.00	0.43
1:A:477:GLU:H	1:A:477:GLU:HG2	1.53	0.43
1:A:553:THR:HG22	1:A:564:MET:CE	2.46	0.43
1:A:537:GLU:HG3	3:A:2067:HOH:O	2.19	0.43
1:A:902:ARG:HD2	3:A:2201:HOH:O	2.11	0.43
1:A:419:ALA:HB3	1:A:441:MET:CE	2.48	0.43
1:A:912:PHE:HA	3:A:2232:HOH:O	2.18	0.43
1:A:982:ARG:HH21	1:A:991:CYS:HA	1.83	0.43
1:A:343:VAL:H	1:A:360:SER:CB	2.32	0.42
1:A:898:ASN:HD22	1:A:898:ASN:C	2.26	0.42
1:A:119:LEU:HD23	1:A:683:MET:HE3	2.01	0.42
1:A:139:PHE:CE2	1:A:666:LEU:HB3	2.54	0.42
1:A:866:GLU:H	1:A:866:GLU:HG2	1.36	0.42
1:A:419:ALA:CB	1:A:441:MET:HE3	2.49	0.42
1:A:693:LYS:HE2	1:A:780:ASN:HD21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:846:ALA:HA	1:A:857:ASN:HB3	2.01	0.42
1:A:679:MET:O	1:A:683:MET:HG3	2.20	0.42
1:A:331:ARG:O	1:A:469:ALA:HA	2.19	0.41
1:A:789:LEU:HD23	1:A:915:PHE:CE2	2.56	0.41
1:A:288:GLU:HG2	1:A:289:GLN:HG3	2.02	0.41
1:A:325:ILE:HG22	1:A:475:LEU:HD12	2.03	0.41
1:A:216:LEU:C	1:A:216:LEU:HD23	2.46	0.40
1:A:271:THR:O	1:A:273:HIS:HD2	2.03	0.40
1:A:616:VAL:O	1:A:619:LEU:HB2	2.21	0.40
1:A:696:ASN:HD22	1:A:778:PHE:HD2	1.69	0.40
1:A:710:GLN:O	1:A:714:MET:HG2	2.21	0.40
1:A:550:LEU:HA	1:A:564:MET:HE3	2.04	0.40
1:A:116:GLN:HB3	1:A:683:MET:SD	2.62	0.40
1:A:332:LYS:NZ	1:A:334:ASN:HB3	2.36	0.40
1:A:367:SER:HB3	1:A:369:PRO:N	2.30	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	803/940 (85%)	777 (97%)	23 (3%)	3 (0%)	30 27

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	367	SER
1	A	365	VAL
1	A	769	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	731/827 (88%)	690 (94%)	41 (6%)	19	16

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	LYS
1	A	188	ARG
1	A	190	LEU
1	A	223	LYS
1	A	270	LEU
1	A	288	GLU
1	A	317	TRP
1	A	319	LEU
1	A	332	LYS
1	A	340	LYS
1	A	352	GLU
1	A	358	VAL
1	A	374	ARG
1	A	398	VAL
1	A	423	LEU
1	A	453	LEU
1	A	475	LEU
1	A	477	GLU
1	A	511	LEU
1	A	512	ARG
1	A	514	ILE
1	A	517	ARG
1	A	553	THR
1	A	557	LYS
1	A	563	GLN
1	A	634	LEU
1	A	658	PRO
1	A	726	GLU
1	A	743	GLU
1	A	786	GLN

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Mol	Chain	Res	Type
1	A	866	GLU
1	A	898	ASN
1	A	915	PHE
1	A	930	VAL
1	A	935	THR
1	A	962[A]	ARG
1	A	962[B]	ARG
1	A	986	LEU
1	A	993	LYS
1	A	1004	LEU
1	A	1027	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	GLN
1	A	156	GLN
1	A	193	ASN
1	A	247	HIS
1	A	258	HIS
1	A	273	HIS
1	A	278	HIS
1	A	334	ASN
1	A	344	GLN
1	A	351	ASN
1	A	422	ASN
1	A	431	GLN
1	A	536	HIS
1	A	563	GLN
1	A	610	GLN
1	A	617	GLN
1	A	696	ASN
1	A	721	GLN
1	A	780	ASN
1	A	786	GLN
1	A	792	GLN
1	A	838	GLN
1	A	898	ASN
1	A	906	GLN
1	A	918	ASN
1	A	948	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

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	ZS4	A	1500	-	33,34,34	1.84	5 (15%)	40,48,48	2.13	13 (32%)

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	ZS4	A	1500	-	-	1/14/32/32	0/5/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1500	ZS4	CAO-NAJ	-6.49	1.32	1.41
2	A	1500	ZS4	CAK-NAJ	-5.09	1.32	1.40
2	A	1500	ZS4	CAF-NAE	-3.68	1.32	1.39
2	A	1500	ZS4	CAD-NAJ	-3.46	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1500	ZS4	CAU-NAV	2.21	1.40	1.35

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1500	ZS4	CAO-NAP-CAU	4.71	121.27	113.63
2	A	1500	ZS4	CBC-OBD-CAI	4.65	124.92	109.88
2	A	1500	ZS4	CAK-NAJ-CAD	4.16	107.71	106.44
2	A	1500	ZS4	CAX-NAY-CAZ	4.02	120.61	111.57
2	A	1500	ZS4	NAT-CAU-NAP	-3.76	119.58	126.27
2	A	1500	ZS4	NAN-CAO-NAP	-3.62	119.83	126.27
2	A	1500	ZS4	CAS-NAT-CAU	3.39	119.14	113.63
2	A	1500	ZS4	CAO-NAN-CAS	3.22	118.86	113.63
2	A	1500	ZS4	NAP-CAU-NAV	2.96	121.33	117.12
2	A	1500	ZS4	NAN-CAS-NAT	-2.81	121.27	126.27
2	A	1500	ZS4	CBA-NAV-CAQ	2.40	116.98	111.57
2	A	1500	ZS4	OBD-CAI-CAZ	2.19	116.48	111.77
2	A	1500	ZS4	NAN-CAS-NAY	2.12	120.14	117.12

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1500	ZS4	FA-CAC-CAD-NAJ

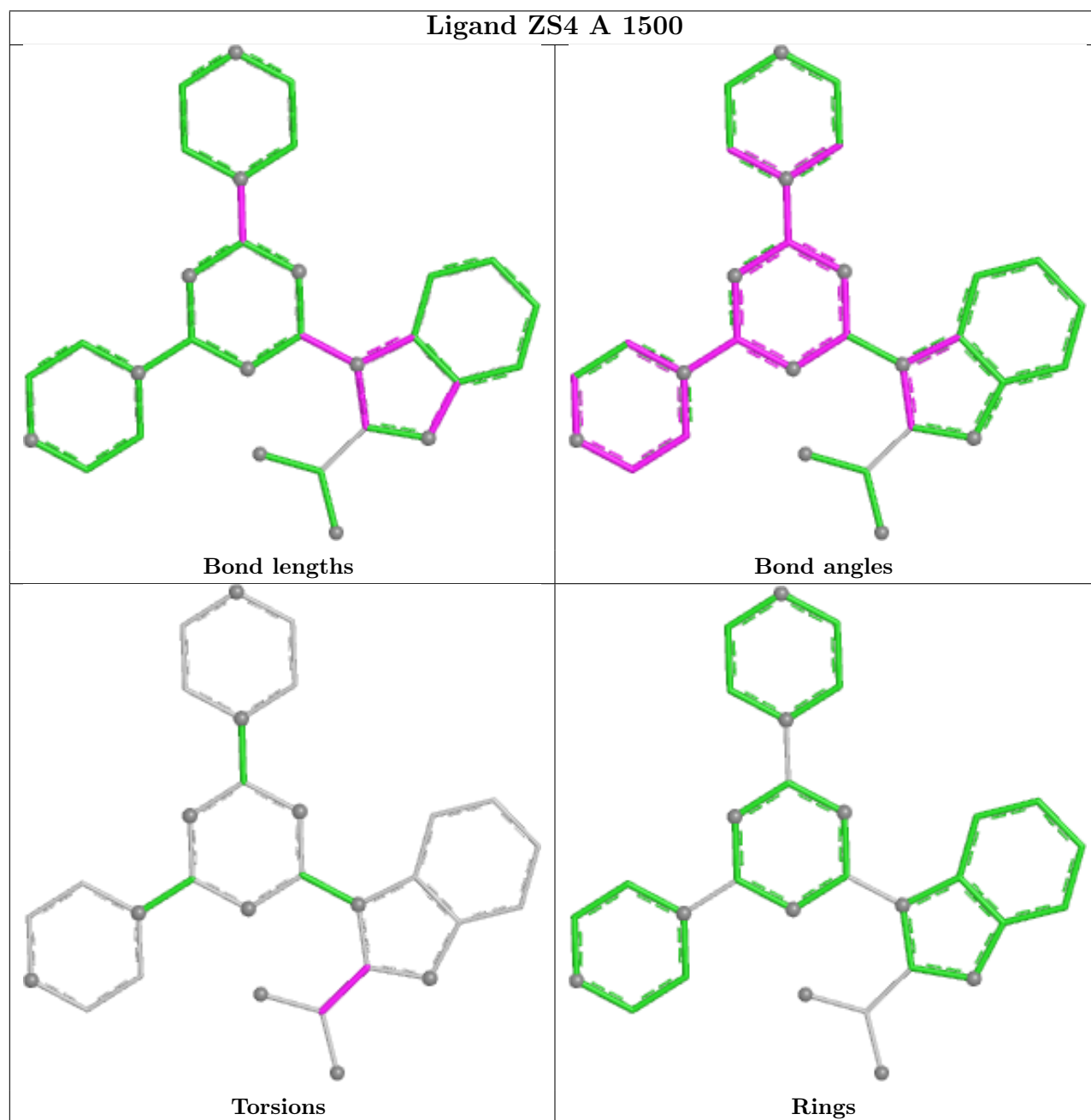
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1500	ZS4	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	823/940 (87%)	1.26	171 (20%) 2 2	2, 14, 28, 49	2 (0%)

All (171) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	291	ASN	18.2
1	A	479	ALA	11.5
1	A	494	LEU	11.1
1	A	482	PRO	10.3
1	A	428	TYR	9.8
1	A	318	SER	9.3
1	A	316	LEU	9.2
1	A	487	ALA	8.0
1	A	485	PHE	7.2
1	A	384	LEU	7.0
1	A	491	ILE	7.0
1	A	386	ARG	6.7
1	A	486	PRO	6.6
1	A	484	TYR	6.6
1	A	478	VAL	6.5
1	A	379	ILE	6.3
1	A	459	VAL	6.1
1	A	430	ASP	6.0
1	A	477	GLU	5.8
1	A	492	LEU	5.8
1	A	387	MET	5.8
1	A	490	LYS	5.6
1	A	846	ALA	5.6
1	A	395	TYR	5.6
1	A	317	TRP	5.5
1	A	463	PRO	5.5
1	A	366	CYS	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	349	HIS	5.5
1	A	458	THR	5.5
1	A	514	ILE	5.3
1	A	434	THR	5.3
1	A	461	GLY	5.2
1	A	429	LYS	5.2
1	A	388	ALA	5.2
1	A	426	PHE	5.2
1	A	385	PRO	5.1
1	A	381	VAL	5.1
1	A	489	GLU	4.8
1	A	319	LEU	4.8
1	A	847	THR	4.8
1	A	1027	TRP	4.7
1	A	435	GLY	4.6
1	A	424	MET	4.6
1	A	456	ALA	4.5
1	A	919	PHE	4.5
1	A	334	ASN	4.4
1	A	427	ASP	4.4
1	A	445	VAL	4.4
1	A	398	VAL	4.3
1	A	322	PRO	4.3
1	A	382	CYS	4.3
1	A	460	ARG	4.3
1	A	348	PHE	4.2
1	A	367	SER	4.2
1	A	396	ALA	4.2
1	A	488	LEU	4.2
1	A	431	GLN	4.1
1	A	425	LEU	4.1
1	A	323	PHE	4.0
1	A	422	ASN	3.9
1	A	335	ALA	3.9
1	A	771	ALA	3.9
1	A	342	VAL	3.9
1	A	483	VAL	3.8
1	A	380	SER	3.8
1	A	440	TYR	3.8
1	A	269	GLY	3.7
1	A	228	PHE	3.7
1	A	230	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	320	GLU	3.6
1	A	432	LEU	3.6
1	A	391	CYS	3.6
1	A	472	VAL	3.6
1	A	473	ILE	3.5
1	A	468	ALA	3.5
1	A	511	LEU	3.5
1	A	510	GLN	3.5
1	A	225	ALA	3.5
1	A	205	PHE	3.4
1	A	457	GLY	3.4
1	A	512	ARG	3.3
1	A	474	TYR	3.3
1	A	841	LYS	3.3
1	A	437	ARG	3.3
1	A	936	TYR	3.2
1	A	364	ASN	3.2
1	A	370	VAL	3.2
1	A	839	LEU	3.2
1	A	493	GLU	3.1
1	A	1017	VAL	3.1
1	A	324	SER	3.1
1	A	515	LEU	3.0
1	A	189	ALA	3.0
1	A	328	ILE	3.0
1	A	433	LYS	3.0
1	A	198	GLY	3.0
1	A	439	LEU	2.9
1	A	768	ALA	2.9
1	A	361	SER	2.9
1	A	522	GLU	2.9
1	A	738	SER	2.8
1	A	416	CYS	2.8
1	A	390	LEU	2.8
1	A	840	ASN	2.8
1	A	1024	ARG	2.8
1	A	438	CYS	2.7
1	A	991	CYS	2.7
1	A	357	THR	2.7
1	A	681	VAL	2.7
1	A	358	VAL	2.6
1	A	389	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	897	ASP	2.6
1	A	109	VAL	2.6
1	A	845	ALA	2.6
1	A	350	GLY	2.6
1	A	363	VAL	2.6
1	A	842	SER	2.6
1	A	678	HIS	2.5
1	A	235	GLN	2.5
1	A	321	GLN	2.5
1	A	377	PHE	2.5
1	A	993	LYS	2.5
1	A	383	ASP	2.5
1	A	423	LEU	2.5
1	A	464	ASN	2.5
1	A	637	ALA	2.5
1	A	397	VAL	2.5
1	A	1007	THR	2.4
1	A	1013	LYS	2.4
1	A	561	VAL	2.4
1	A	529	ASP	2.4
1	A	517	ARG	2.4
1	A	436	GLU	2.4
1	A	162	TRP	2.4
1	A	470	ALA	2.3
1	A	769	GLY	2.3
1	A	649	TRP	2.3
1	A	723	THR	2.3
1	A	153	HIS	2.3
1	A	270	LEU	2.3
1	A	741	LEU	2.3
1	A	688	ALA	2.3
1	A	466	GLU	2.3
1	A	1025	GLU	2.2
1	A	268	SER	2.2
1	A	227	VAL	2.2
1	A	340	LYS	2.2
1	A	354	LEU	2.2
1	A	644	GLY	2.2
1	A	542	PHE	2.2
1	A	523	LEU	2.2
1	A	763	TYR	2.2
1	A	222	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	843	ASN	2.2
1	A	332	LYS	2.2
1	A	339	MET	2.1
1	A	537	GLU	2.1
1	A	816	LEU	2.1
1	A	643	ILE	2.1
1	A	671	TYR	2.1
1	A	209	THR	2.1
1	A	374	ARG	2.1
1	A	918	ASN	2.1
1	A	262	ILE	2.1
1	A	933	ILE	2.1
1	A	917	GLY	2.1
1	A	524	TYR	2.0
1	A	465	THR	2.0
1	A	895	HIS	2.0
1	A	590	CYS	2.0
1	A	421	ALA	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](#)

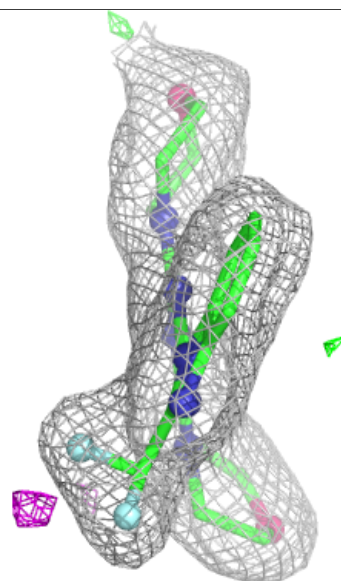
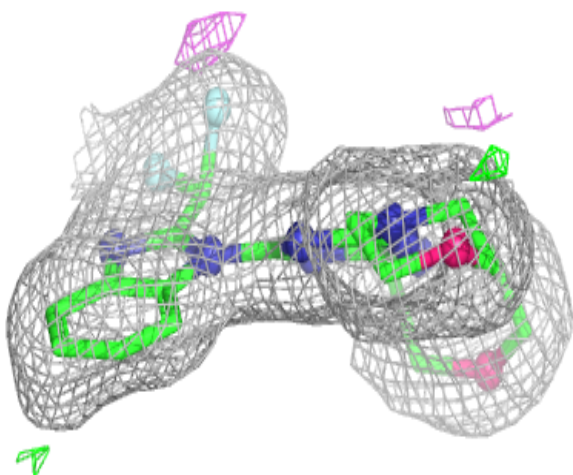
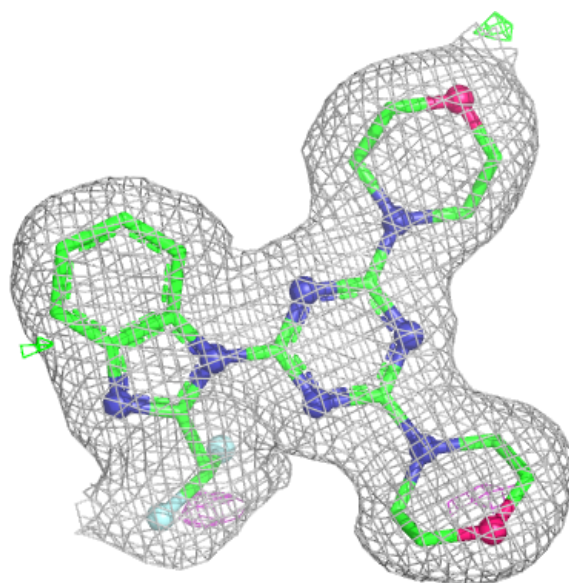
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	ZS4	A	1500	30/30	0.94	0.08	19,26,34,40	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 ZS4 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 ⓘ

There are no such residues in this entry.