Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2024 – 01:59 pm BST

PDB ID	:	3ZW3
Title	:	Fragment based discovery of a novel and selective PI3 Kinase inhibitor
Authors	:	Brown, D.G.; Hughes, S.J.; Milan, D.S.; Kilty, I.C.; Lewthwaite, R.A.; Mathias, J.P.; O'Reilly, M.A.; Pannifer, A.; Phelan, A.; Baldock, D.A.
Deposited on	:	2011-07-28
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 ⓘ) were used in the production of this report:

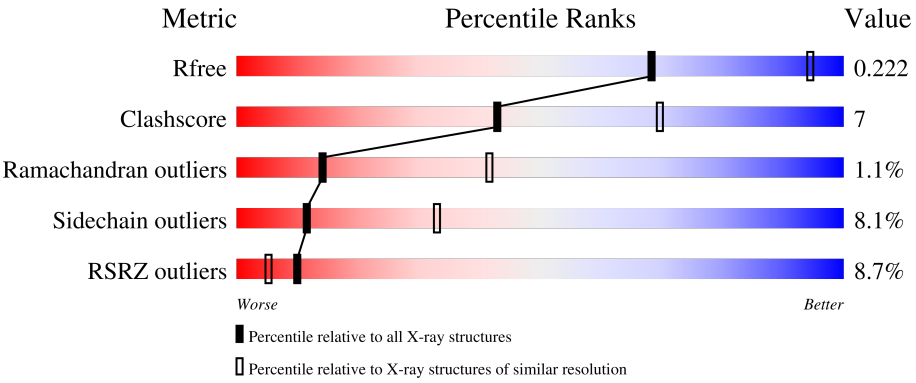
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	966	7% 70% 14% · 14%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6871 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

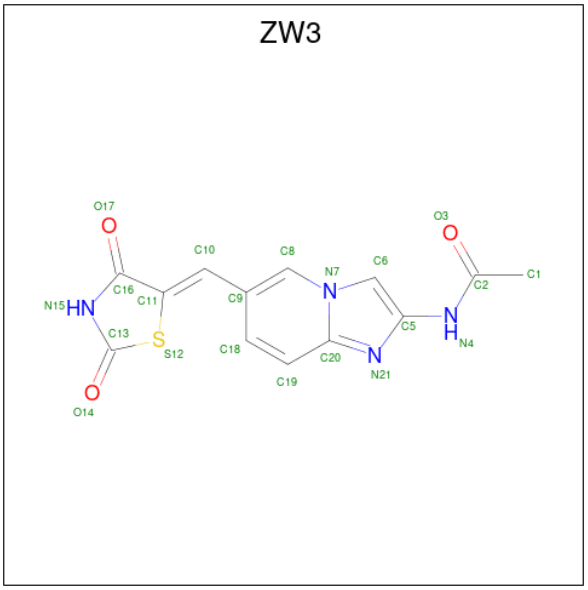
- Molecule 1 is a protein called PHOSPHATIDYLINOSITOL-4,5-BISPHOSPHATE 3-KINASE CATALYTIC SUBUNIT GAMMA ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	831	6722	4320	1145	1222	35	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	MET	-	expression tag	UNP P48736
A	1103	HIS	-	expression tag	UNP P48736
A	1104	HIS	-	expression tag	UNP P48736
A	1105	HIS	-	expression tag	UNP P48736
A	1106	HIS	-	expression tag	UNP P48736
A	1107	HIS	-	expression tag	UNP P48736
A	1108	HIS	-	expression tag	UNP P48736

- Molecule 2 is N-{6-[(Z)-(2,4-dioxo-1,3-thiazolidin-5-ylidene)methyl]imidazo[1,2-a]pyridin-2-yl}acetamide (three-letter code: ZW3) (formula: $C_{13}H_{10}N_4O_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			21	13	4	3	1		

- Molecule 3 is water.

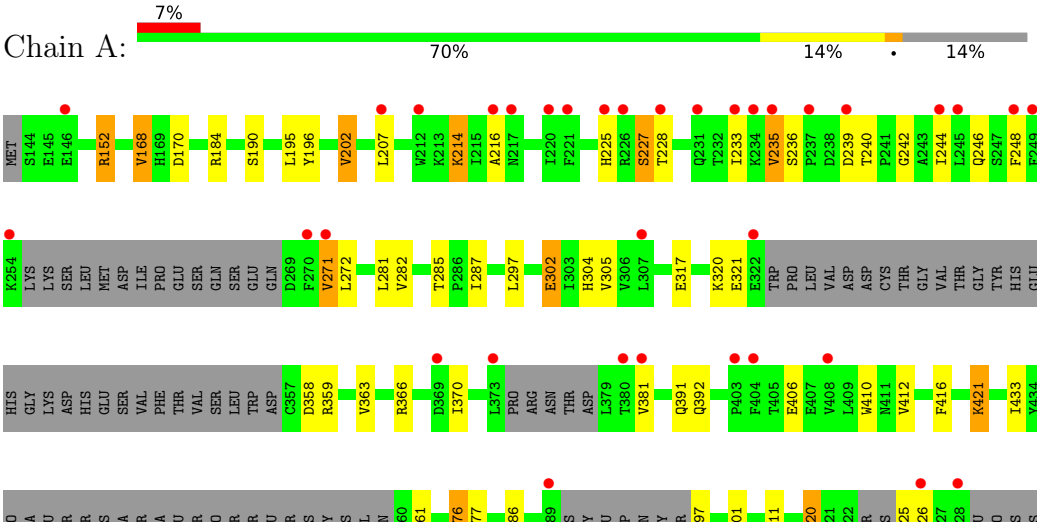
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	128	Total	O	0	0
			128	128		

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 GAMMA ISOFORM

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	142.23Å 68.52Å 107.13Å 90.00° 95.64° 90.00°	Depositor
Resolution (Å)	18.28 – 2.80 44.74 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (18.28-2.80) 99.4 (44.74-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.02 (at 2.81Å)	Xtriage
Refinement program	BUSTER 2.9.6	Depositor
R, R_{free}	0.186 , 0.211 0.201 , 0.222	Depositor DCC
R_{free} test set	1292 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	69.2	Xtriage
Anisotropy	0.359	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 80.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6871	wwPDB-VP
Average B, all atoms (Å^2)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.34% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: ZW3

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	0.50	0/6864	0.66	2/9281 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	808	LYS	N-CA-C	-7.37	91.09	111.00
1	A	1044	SER	C-N-CA	5.40	135.19	121.70

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	6722	0	6760	92	0
2	A	21	0	9	1	0
3	A	128	0	0	1	0
All	All	6871	0	6769	92	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 7.

All (92) 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:497:PHE:HA	1:A:1043:THR:HG21	1.20	1.09
1:A:152:ARG:HH11	1:A:152:ARG:HG2	1.30	0.95
1:A:225:HIS:HE1	1:A:304:HIS:HD2	1.15	0.95
1:A:939:THR:HG23	1:A:945:GLY:HA2	1.49	0.92
1:A:235:VAL:HG21	1:A:244:ILE:HG12	1.56	0.88
1:A:916:PRO:HG2	1:A:920:LYS:HD3	1.55	0.87
1:A:839:ARG:HA	1:A:842:MET:HE2	1.58	0.86
1:A:935:TYR:O	1:A:939:THR:HB	1.83	0.78
1:A:808:LYS:O	1:A:810:PRO:HD3	1.85	0.77
1:A:897:GLY:CA	1:A:898:ASN:HB3	2.16	0.75
1:A:939:THR:HG23	1:A:945:GLY:CA	2.19	0.73
1:A:497:PHE:HA	1:A:1043:THR:CG2	2.08	0.73
1:A:887:THR:HG22	1:A:890:LYS:H	1.57	0.69
1:A:558:ILE:O	1:A:561:THR:HG22	1.92	0.69
1:A:893:GLN:HA	1:A:897:GLY:O	1.93	0.69
1:A:949:ASN:H	1:A:1083:GLN:HE22	1.42	0.68
1:A:225:HIS:HE1	1:A:304:HIS:CD2	2.06	0.68
1:A:724:CYS:HB2	1:A:728:MET:HE3	1.76	0.67
1:A:525:HIS:CD2	1:A:526:PRO:HD2	2.30	0.66
1:A:214:LYS:HD3	1:A:297:LEU:O	1.97	0.64
1:A:271:VAL:CG2	1:A:282:VAL:HG11	2.28	0.62
1:A:421:LYS:NZ	1:A:525:HIS:HE1	1.99	0.60
1:A:897:GLY:HA3	1:A:898:ASN:HB3	1.81	0.60
1:A:614:ARG:HG2	1:A:617:TRP:HB3	1.84	0.60
1:A:939:THR:CG2	1:A:945:GLY:HA2	2.27	0.60
1:A:897:GLY:HA2	1:A:898:ASN:HB3	1.84	0.57
1:A:903:LYS:HB3	1:A:906:VAL:HG23	1.87	0.57
1:A:583:LEU:HD22	1:A:610:LEU:HD22	1.89	0.55
1:A:561:THR:HG21	1:A:565:ASN:HD22	1.73	0.54
1:A:851:MET:CE	1:A:938:ALA:CB	2.86	0.53
1:A:476:ARG:HB3	1:A:520:LEU:HD23	1.91	0.53
1:A:768:LYS:O	1:A:772:GLU:HG2	2.09	0.53
1:A:225:HIS:CE1	1:A:304:HIS:HD2	2.07	0.52
1:A:271:VAL:CG2	1:A:282:VAL:CG1	2.87	0.52
1:A:235:VAL:CG2	1:A:244:ILE:HG12	2.36	0.52
1:A:851:MET:HE1	1:A:938:ALA:CB	2.39	0.52
1:A:887:THR:HB	1:A:890:LYS:HD2	1.92	0.52
1:A:564:LEU:HD22	1:A:1045:LYS:HE3	1.92	0.52
1:A:152:ARG:HG2	1:A:152:ARG:NH1	2.10	0.52
1:A:905:GLU:HG3	1:A:993:PHE:CE2	2.45	0.52
1:A:168:VAL:HG13	1:A:170:ASP:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:808:LYS:O	1:A:810:PRO:CD	2.55	0.50
1:A:246:GLN:HE21	1:A:246:GLN:HA	1.76	0.50
1:A:152:ARG:HH11	1:A:152:ARG:CG	2.10	0.50
1:A:851:MET:CE	1:A:938:ALA:HB2	2.42	0.50
1:A:1040:PRO:O	1:A:1041:GLN:HB2	2.11	0.50
1:A:381:VAL:CG2	1:A:433:ILE:HG23	2.42	0.49
1:A:239:ASP:O	1:A:287:ILE:HG13	2.11	0.49
1:A:593:PHE:CZ	1:A:611:LEU:HD21	2.48	0.48
1:A:651:LEU:HD22	1:A:655:ASP:HB3	1.95	0.48
1:A:317:GLU:O	1:A:726:THR:HG23	2.13	0.48
1:A:240:THR:HG22	1:A:242:GLY:H	1.79	0.48
1:A:272:LEU:HD22	1:A:305:VAL:HG11	1.96	0.48
1:A:184:ARG:HD3	1:A:719:ALA:O	2.13	0.47
1:A:271:VAL:HG22	1:A:282:VAL:CG1	2.43	0.47
1:A:202:VAL:CG2	1:A:285:THR:HG21	2.44	0.47
1:A:1002:THR:HG23	1:A:1006:PHE:HD2	1.80	0.47
1:A:391:GLN:HE21	1:A:391:GLN:HA	1.80	0.47
1:A:897:GLY:CA	1:A:898:ASN:CB	2.90	0.47
1:A:549:ASN:O	1:A:553:LYS:HG3	2.14	0.47
1:A:302:GLU:H	1:A:302:GLU:HG2	1.53	0.46
1:A:851:MET:HE1	1:A:938:ALA:HB1	1.97	0.46
1:A:196:TYR:OH	1:A:728:MET:HE2	2.16	0.46
1:A:766:GLN:HG3	3:A:2099:HOH:O	2.17	0.45
1:A:916:PRO:CG	1:A:920:LYS:HD3	2.38	0.45
1:A:302:GLU:HG3	1:A:304:HIS:CE1	2.52	0.45
1:A:410:TRP:HB3	1:A:412:VAL:HG22	1.99	0.45
1:A:302:GLU:HG3	1:A:304:HIS:HE1	1.81	0.45
1:A:317:GLU:O	1:A:726:THR:CG2	2.64	0.45
1:A:749:ILE:CD1	1:A:770:LYS:HD2	2.46	0.44
1:A:593:PHE:HZ	1:A:611:LEU:HD21	1.81	0.44
1:A:949:ASN:H	1:A:1083:GLN:NE2	2.13	0.44
1:A:739:ILE:HG13	1:A:740:GLU:N	2.32	0.43
1:A:895:THR:HA	1:A:896:VAL:HA	1.70	0.43
1:A:624:VAL:O	1:A:628:MET:HG2	2.19	0.43
1:A:735:GLN:O	1:A:739:ILE:HG23	2.18	0.43
1:A:202:VAL:HG22	1:A:285:THR:HG21	2.01	0.42
1:A:851:MET:HE3	1:A:938:ALA:CB	2.49	0.42
1:A:236:SER:O	1:A:287:ILE:HD11	2.19	0.42
1:A:851:MET:HE3	1:A:938:ALA:HB2	2.00	0.42
1:A:853:SER:O	1:A:857:THR:HG23	2.19	0.42
1:A:983:VAL:HG13	1:A:985:PHE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:749:ILE:HD12	1:A:770:LYS:HD2	2.02	0.41
1:A:363:VAL:HG23	1:A:520:LEU:CD1	2.51	0.41
1:A:406:GLU:CD	1:A:406:GLU:H	2.24	0.41
1:A:547:MET:HG2	1:A:578:PHE:CD1	2.56	0.41
1:A:227:SER:HB3	1:A:228:THR:H	1.69	0.41
1:A:743:GLN:HG2	1:A:876:ILE:HD13	2.02	0.41
1:A:833:LYS:NZ	2:A:2191:ZW3:N15	2.69	0.41
1:A:233:ILE:HD12	1:A:248:PHE:HD1	1.86	0.40
1:A:363:VAL:HG12	1:A:416:PHE:HE1	1.87	0.40
1:A:421:LYS:HZ1	1:A:525:HIS:HE1	1.67	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	811/966 (84%)	777 (96%)	25 (3%)	9 (1%)	14 41

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	216	ALA
1	A	1044	SER
1	A	545	ALA
1	A	546	GLU
1	A	1045	LYS
1	A	895	THR
1	A	809	LYS
1	A	1089	HIS
1	A	999	GLY

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	743/864 (86%)	683 (92%)	60 (8%)	11 33

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	152	ARG
1	A	168	VAL
1	A	190	SER
1	A	195	LEU
1	A	202	VAL
1	A	207	LEU
1	A	214	LYS
1	A	227	SER
1	A	235	VAL
1	A	252	MET
1	A	271	VAL
1	A	281	LEU
1	A	302	GLU
1	A	320	LYS
1	A	321	GLU
1	A	358	ASP
1	A	359	ARG
1	A	366	ARG
1	A	370	ILE
1	A	392	GLN
1	A	421	LYS
1	A	461	LEU
1	A	476	ARG
1	A	477	ARG
1	A	486	GLN
1	A	501	LYS
1	A	511	GLU
1	A	520	LEU
1	A	574	LEU
1	A	601	GLN

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Mol	Chain	Res	Type
1	A	610	LEU
1	A	615	GLU
1	A	626	LEU
1	A	646	GLN
1	A	717	LEU
1	A	726	THR
1	A	728	MET
1	A	743	GLN
1	A	744	LYS
1	A	749	ILE
1	A	750	LYS
1	A	766	GLN
1	A	767	LEU
1	A	776	ASN
1	A	778	GLN
1	A	799	GLU
1	A	807	LYS
1	A	823	LEU
1	A	865	LEU
1	A	907	LEU
1	A	939	THR
1	A	950	ASP
1	A	957	THR
1	A	972	TYR
1	A	983	VAL
1	A	1001	LYS
1	A	1011	ASP
1	A	1039	MET
1	A	1052	ARG
1	A	1059	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	225	HIS
1	A	246	GLN
1	A	291	GLN
1	A	304	HIS
1	A	391	GLN
1	A	392	GLN
1	A	432	GLN
1	A	525	HIS

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Mol	Chain	Res	Type
1	A	565	ASN
1	A	601	GLN
1	A	639	ASN
1	A	646	GLN
1	A	743	GLN
1	A	834	HIS
1	A	840	GLN
1	A	959	ASN
1	A	1023	HIS
1	A	1083	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides 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	ZW3	A	2191	-	19,23,23	2.79	8 (42%)	21,33,33	4.63	12 (57%)

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	ZW3	A	2191	-	-	0/6/20/20	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2191	ZW3	C16-N15	-6.29	1.24	1.38
2	A	2191	ZW3	C10-C11	6.18	1.41	1.34
2	A	2191	ZW3	C13-N15	-3.89	1.31	1.36
2	A	2191	ZW3	C11-S12	3.87	1.81	1.73
2	A	2191	ZW3	C13-S12	-3.35	1.74	1.78
2	A	2191	ZW3	O17-C16	-2.95	1.18	1.23
2	A	2191	ZW3	C5-N4	-2.19	1.35	1.40
2	A	2191	ZW3	C16-C11	-2.18	1.44	1.48

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2191	ZW3	C16-N15-C13	11.36	123.99	117.79
2	A	2191	ZW3	C16-C11-S12	-10.62	101.90	109.84
2	A	2191	ZW3	C11-S12-C13	8.23	94.07	91.69
2	A	2191	ZW3	C11-C16-N15	5.82	115.08	110.22
2	A	2191	ZW3	C10-C11-C16	4.75	124.23	120.47
2	A	2191	ZW3	S12-C13-N15	-4.56	104.94	109.19
2	A	2191	ZW3	C9-C10-C11	-3.99	125.48	130.94
2	A	2191	ZW3	C10-C11-S12	3.63	133.87	129.22
2	A	2191	ZW3	C5-N4-C2	2.70	130.95	128.16
2	A	2191	ZW3	C18-C19-C20	2.46	122.74	119.76
2	A	2191	ZW3	O14-C13-S12	2.29	127.55	124.64
2	A	2191	ZW3	O17-C16-N15	-2.18	120.00	125.08

There are no chirality outliers.

There are no torsion outliers.

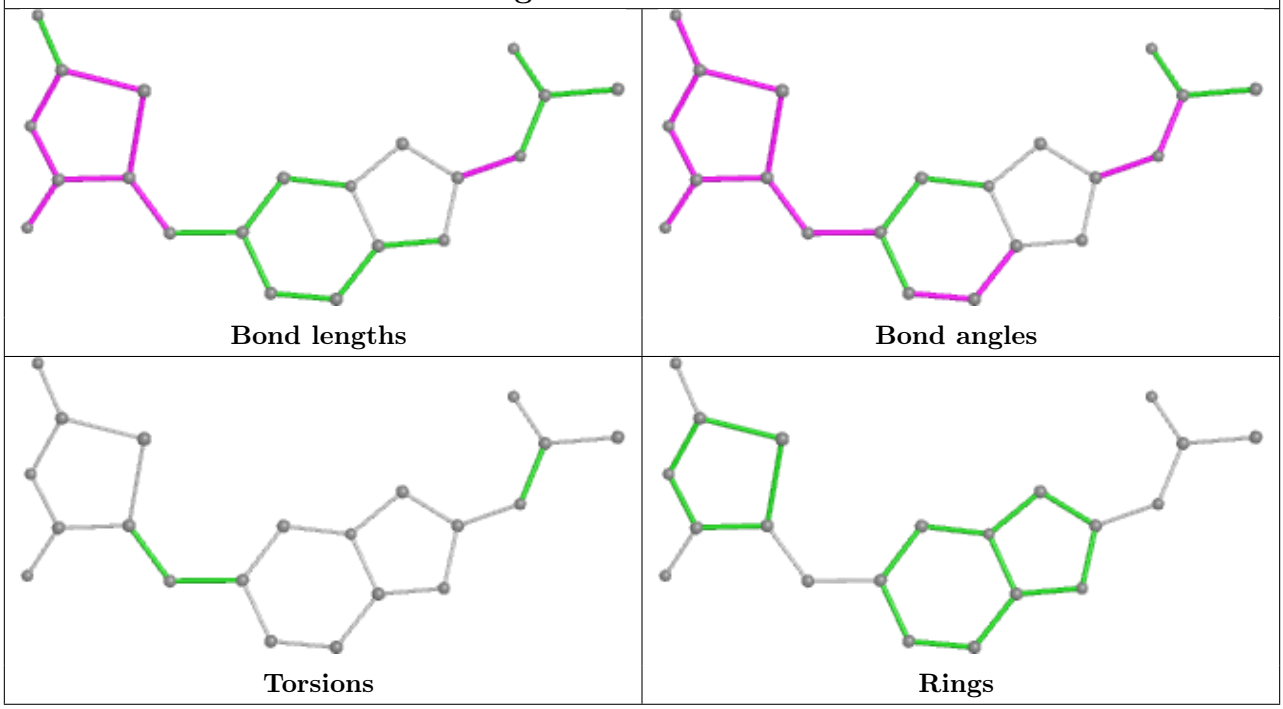
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2191	ZW3	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 then 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.

Ligand ZW3 A 2191



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, 95^{th} 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	831/966 (86%)	0.40	72 (8%) 10 5	43, 88, 149, 190	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1086	TRP	6.3
1	A	254	LYS	6.0
1	A	307	LEU	5.9
1	A	895	THR	5.9
1	A	896	VAL	5.4
1	A	253	ALA	5.3
1	A	1064	ALA	5.3
1	A	226	ARG	5.0
1	A	528	ALA	4.9
1	A	249	PHE	4.9
1	A	489	GLY	4.6
1	A	901	ALA	4.5
1	A	381	VAL	4.3
1	A	251	LYS	4.1
1	A	228	THR	4.1
1	A	373	LEU	3.9
1	A	248	PHE	3.9
1	A	237	PRO	3.7
1	A	902	PHE	3.7
1	A	900	GLY	3.7
1	A	1041	GLN	3.6
1	A	1075	CYS	3.6
1	A	217	ASN	3.5
1	A	778	GLN	3.5
1	A	972	TYR	3.5
1	A	403	PRO	3.4
1	A	322	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	779	LEU	3.3
1	A	245	LEU	3.3
1	A	270	PHE	3.3
1	A	1087	PHE	3.3
1	A	250	THR	3.3
1	A	216	ALA	3.2
1	A	776	ASN	3.2
1	A	897	GLY	3.2
1	A	1083	GLN	3.1
1	A	252	MET	3.1
1	A	526	PRO	3.1
1	A	546	GLU	2.9
1	A	220	ILE	2.9
1	A	239	ASP	2.8
1	A	1082	VAL	2.7
1	A	995	MET	2.6
1	A	404	PHE	2.6
1	A	212	TRP	2.6
1	A	244	ILE	2.6
1	A	919	GLU	2.6
1	A	774	LEU	2.6
1	A	369	ASP	2.5
1	A	899	THR	2.5
1	A	892	GLN	2.5
1	A	225	HIS	2.4
1	A	231	GLN	2.4
1	A	408	VAL	2.4
1	A	907	LEU	2.4
1	A	922	GLN	2.4
1	A	380	THR	2.4
1	A	898	ASN	2.4
1	A	271	VAL	2.3
1	A	1089	HIS	2.3
1	A	234	LYS	2.2
1	A	613	ARG	2.2
1	A	235	VAL	2.2
1	A	991	PHE	2.2
1	A	846	GLN	2.2
1	A	753	SER	2.2
1	A	146	GLU	2.1
1	A	221	PHE	2.1
1	A	1005	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	207	LEU	2.1
1	A	574	LEU	2.1
1	A	233	ILE	2.1

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 monosaccharides in this entry.

6.4 Ligands (i)

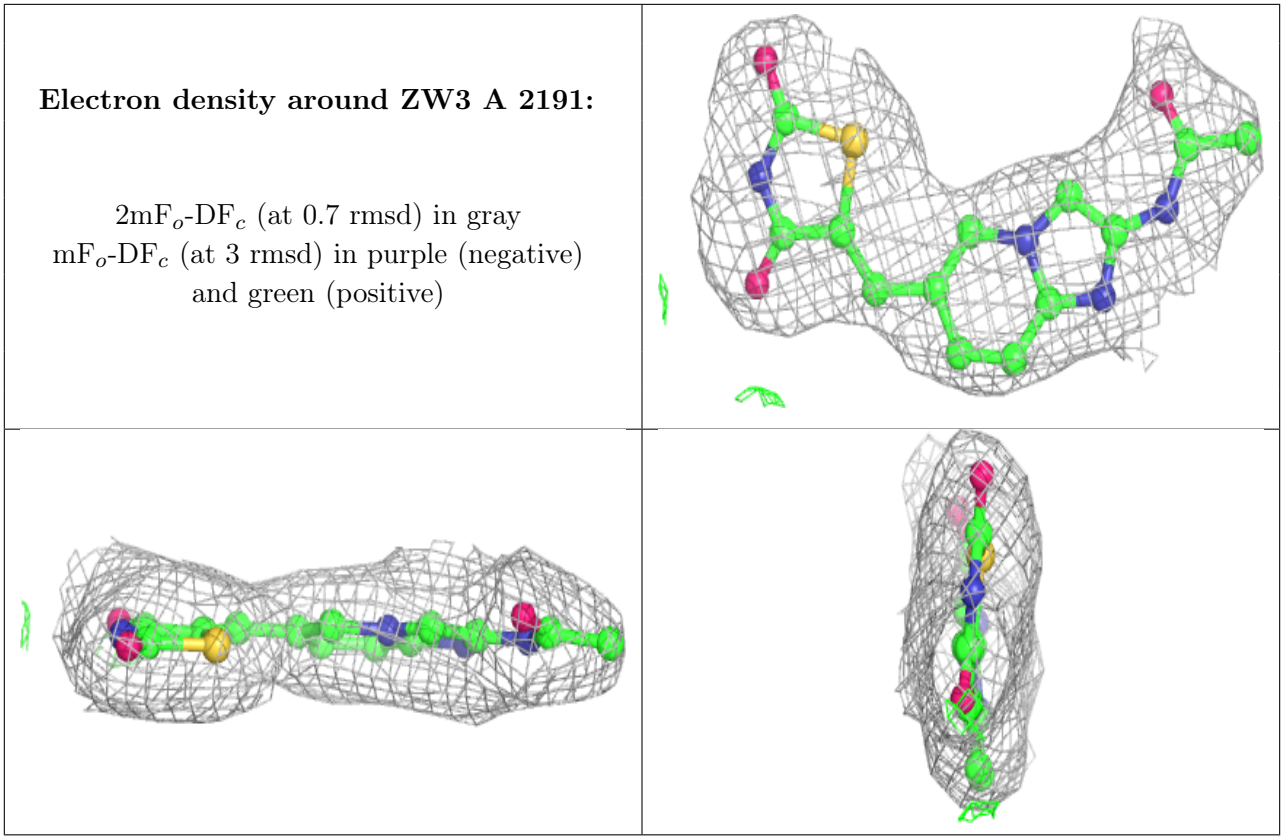
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZW3	A	2191	21/21	0.98	0.15	58,63,65,67	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 ZW3 A 2191:

$2mF_o$-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.