Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2024 – 12:17 AM EST

PDB ID	:	3OAW
Title	:	4-Methylpteridineones as Orally Active and Selective PI3K/mTOR Dual Inhibitors
Authors	:	Knighton, D.R.; Greasley, S.E.; Rodgers, C.M.-L.
Deposited on	:	2010-08-05
Resolution	:	2.75 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:

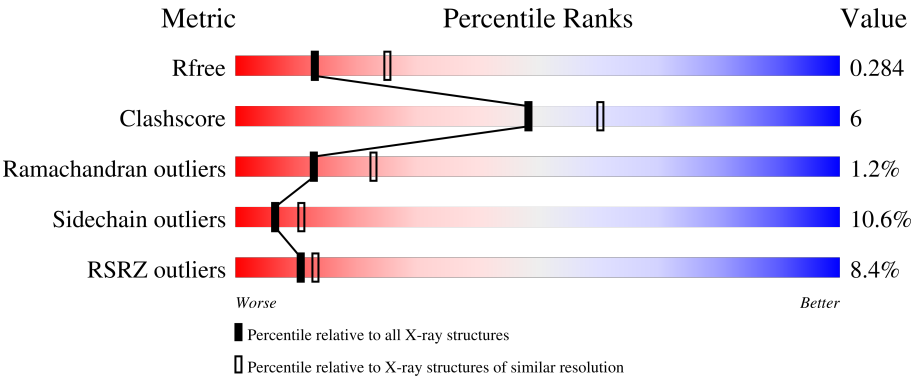
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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%, 66%, 19%, ·, 13%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6804 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.

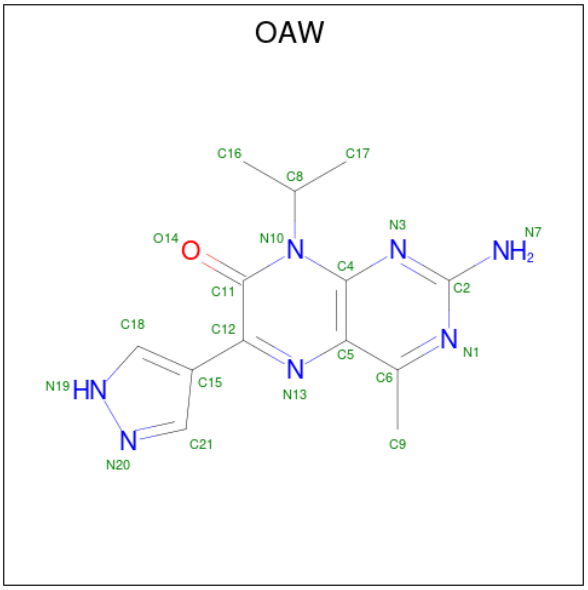
- Molecule 1 is a protein called Phosphatidylinositol-4,5-bisphosphate 3-kinase catalytic subunit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	841	6754	4344	1145	1230	35	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	MET	-	initiating methionine	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 2-amino-4-methyl-8-(1-methylethyl)-6-(1H-pyrazol-4-yl)pteridin-7(8H)-one (three-letter code: OAW) (formula: $C_{13}H_{15}N_7O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			21	13	7	1		

- Molecule 3 is water.

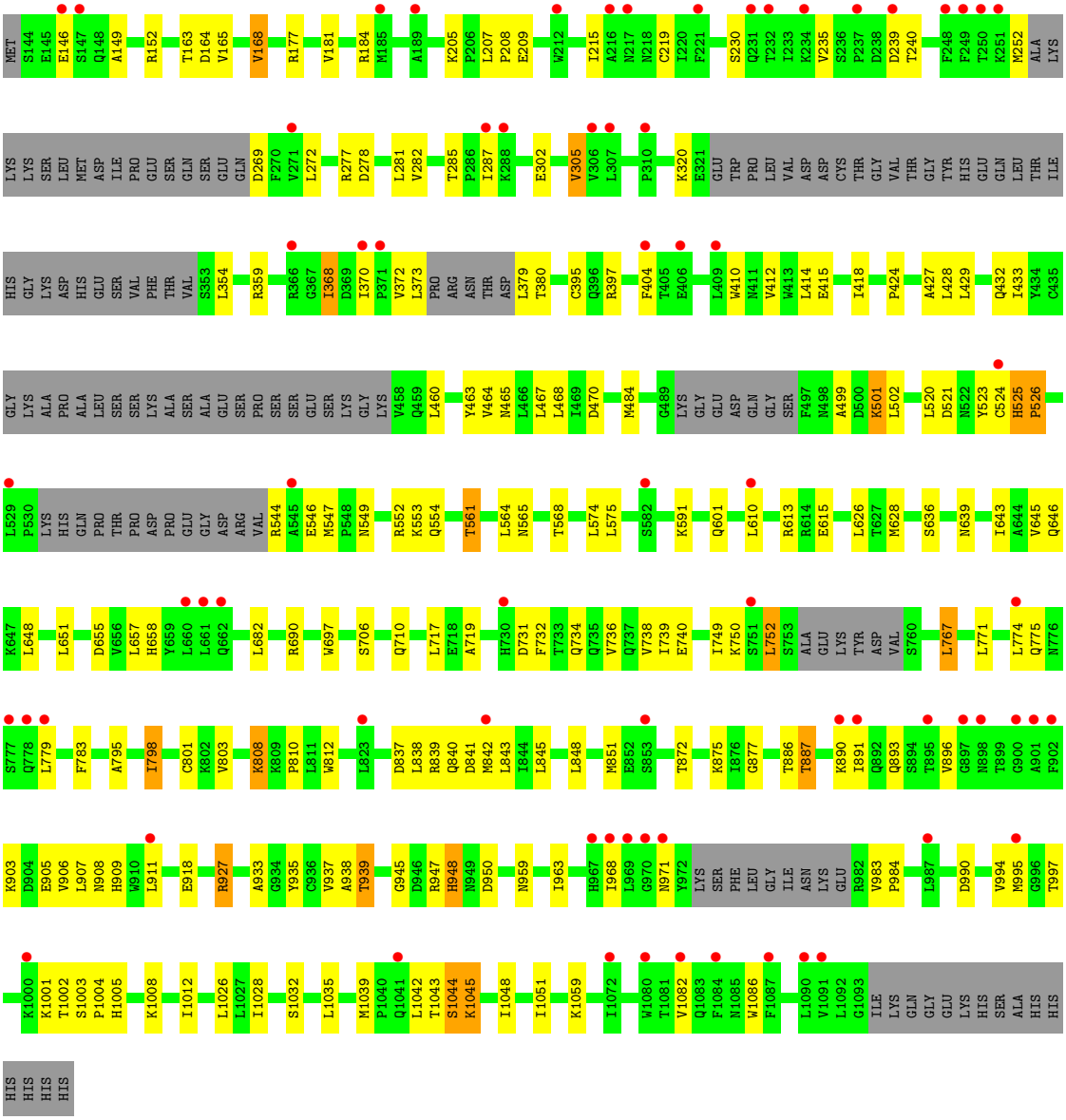
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	29	Total	O	0	0
			29	29		

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	142.75Å 67.66Å 106.03Å 90.00° 95.83° 90.00°	Depositor
Resolution (Å)	44.56 – 2.75 44.56 – 2.75	Depositor EDS
% Data completeness (in resolution range)	98.2 (44.56-2.75) 97.9 (44.56-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	1.06 (at 2.73Å)	Xtriage
Refinement program	BUSTER 2.9.5	Depositor
R, R_{free}	0.207 , 0.268 0.217 , 0.284	Depositor DCC
R_{free} test set	1309 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	76.8	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 69.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6804	wwPDB-VP
Average B, all atoms (Å^2)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.48% 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: OAW

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	0/6898	0.73	0/9340

There are no bond length outliers.

There are no bond angle outliers.

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	6754	0	6764	81	0
2	A	21	0	15	0	0
3	A	29	0	0	0	0
All	All	6804	0	6779	81	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 6.

All (81) 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:939:THR:HG23	1:A:945:GLY:HA2	1.46	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:935:TYR:O	1:A:939:THR:HB	1.68	0.93
1:A:775:GLN:HE22	1:A:795:ALA:HB1	1.49	0.77
1:A:1035:LEU:HD23	1:A:1039:MET:HG3	1.66	0.76
1:A:657:LEU:HD11	1:A:690:ARG:HG2	1.71	0.72
1:A:808:LYS:O	1:A:810:PRO:HD3	1.91	0.70
1:A:947:ARG:NH2	1:A:963:ILE:O	2.24	0.70
1:A:397:ARG:HB3	1:A:414:LEU:HD22	1.74	0.69
1:A:564:LEU:HD11	1:A:1048:ILE:HG22	1.74	0.68
1:A:428:LEU:HD22	1:A:465:ASN:HB3	1.75	0.67
1:A:651:LEU:HD22	1:A:655:ASP:HB3	1.75	0.66
1:A:939:THR:HG23	1:A:945:GLY:CA	2.24	0.65
1:A:561:THR:HG22	1:A:591:LYS:NZ	2.16	0.60
1:A:524:CYS:N	1:A:525:HIS:HA	2.17	0.60
1:A:1003:SER:HB2	1:A:1004:PRO:HD2	1.85	0.58
1:A:905:GLU:HB3	1:A:909:HIS:CE1	2.39	0.58
1:A:424:PRO:HD2	1:A:427:ALA:HB2	1.84	0.57
1:A:939:THR:CG2	1:A:945:GLY:HA2	2.28	0.57
1:A:651:LEU:HD22	1:A:655:ASP:CB	2.34	0.57
1:A:463:TYR:CE1	1:A:501:LYS:HA	2.40	0.56
1:A:771:LEU:HA	1:A:774:LEU:HD12	1.87	0.56
1:A:1008:LYS:O	1:A:1012:ILE:HG13	2.05	0.56
1:A:561:THR:HG22	1:A:591:LYS:HZ2	1.70	0.56
1:A:851:MET:HE1	1:A:938:ALA:HB1	1.88	0.56
1:A:272:LEU:HB3	1:A:305:VAL:HG11	1.90	0.54
1:A:432:GLN:HB3	1:A:460:LEU:HD11	1.90	0.54
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.92	0.52
1:A:983:VAL:HG22	1:A:984:PRO:HD2	1.92	0.52
1:A:908:ASN:HD22	1:A:994:VAL:HA	1.74	0.52
1:A:165:VAL:HG13	1:A:168:VAL:HG12	1.92	0.52
1:A:546:GLU:HG3	1:A:547:MET:H	1.75	0.52
1:A:163:THR:HG22	1:A:177:ARG:HH12	1.75	0.51
1:A:561:THR:HG23	1:A:565:ASN:HB3	1.92	0.51
1:A:848:LEU:HA	1:A:851:MET:HE2	1.92	0.51
1:A:149:ALA:HA	1:A:152:ARG:HH11	1.75	0.51
1:A:903:LYS:HB3	1:A:906:VAL:HG23	1.93	0.51
1:A:990:ASP:O	1:A:994:VAL:HG23	2.11	0.50
1:A:546:GLU:HG3	1:A:547:MET:N	2.27	0.50
1:A:395:CYS:HB2	1:A:418:ILE:HD13	1.93	0.50
1:A:997:THR:HG23	1:A:1001:LYS:HB3	1.93	0.49
1:A:732:PHE:O	1:A:736:VAL:HG23	2.12	0.48
1:A:464:VAL:HB	1:A:484:MET:HG2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:927:ARG:HE	1:A:959:ASN:HD22	1.61	0.48
1:A:1044:SER:O	1:A:1045:LYS:HB3	2.14	0.48
1:A:207:LEU:HD22	1:A:208:PRO:HD2	1.96	0.47
1:A:432:GLN:HB3	1:A:460:LEU:CD1	2.44	0.47
1:A:887:THR:HG22	1:A:890:LYS:H	1.79	0.47
1:A:734:GLN:O	1:A:738:VAL:HG23	2.15	0.47
1:A:163:THR:O	1:A:165:VAL:HG23	2.14	0.47
1:A:281:LEU:HD23	1:A:287:ILE:HG22	1.97	0.46
1:A:410:TRP:HB3	1:A:412:VAL:HG22	1.97	0.46
1:A:368:ILE:HG21	1:A:433:ILE:HD11	1.96	0.46
1:A:524:CYS:H	1:A:525:HIS:HA	1.81	0.46
1:A:891:ILE:HG22	1:A:906:VAL:HG12	1.98	0.46
1:A:750:LYS:HE3	1:A:808:LYS:HA	1.98	0.45
1:A:933:ALA:O	1:A:937:VAL:HG23	2.17	0.45
1:A:1035:LEU:CD2	1:A:1039:MET:HG3	2.39	0.45
1:A:1028:ILE:HG12	1:A:1051:ILE:HG23	2.00	0.44
1:A:547:MET:HB3	1:A:552:ARG:NH1	2.32	0.44
1:A:499:ALA:HA	1:A:502:LEU:HD12	2.00	0.44
1:A:645:VAL:HA	1:A:648:LEU:HD12	1.99	0.44
1:A:983:VAL:HB	1:A:1082:VAL:HG21	2.00	0.44
1:A:851:MET:CE	1:A:938:ALA:HB1	2.47	0.43
1:A:184:ARG:HD3	1:A:719:ALA:O	2.18	0.43
1:A:872:THR:OG1	1:A:877:GLY:HA2	2.19	0.42
1:A:995:MET:O	1:A:1005:HIS:HB2	2.20	0.42
1:A:752:LEU:H	1:A:752:LEU:HG	1.64	0.42
1:A:181:VAL:HG22	1:A:184:ARG:HH22	1.85	0.41
1:A:525:HIS:H	1:A:526:PRO:HD2	1.85	0.41
1:A:838:LEU:O	1:A:842:MET:HG3	2.21	0.41
1:A:235:VAL:HG13	1:A:239:ASP:HB2	2.03	0.41
1:A:1045:LYS:HA	1:A:1048:ILE:HD12	2.03	0.41
1:A:706:SER:O	1:A:710:GLN:HB3	2.21	0.41
1:A:738:VAL:HG11	1:A:783:PHE:CE1	2.56	0.41
1:A:837:ASP:HB3	1:A:840:GLN:NE2	2.36	0.41
1:A:397:ARG:NE	1:A:415:GLU:O	2.55	0.40
1:A:639:ASN:O	1:A:643:ILE:HG23	2.22	0.40
1:A:697:TRP:HH2	1:A:739:ILE:HG12	1.86	0.40
1:A:948:HIS:HD2	1:A:1086:TRP:CD2	2.39	0.40
1:A:801:CYS:HA	1:A:812:TRP:O	2.20	0.40
1:A:767:LEU:HD11	1:A:803:VAL:HG23	2.03	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	823/966 (85%)	754 (92%)	59 (7%)	10 (1%)	13 23

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	523	TYR
1	A	526	PRO
1	A	615	GLU
1	A	164	ASP
1	A	798	ILE
1	A	1044	SER
1	A	1045	LYS
1	A	521	ASP
1	A	525	HIS
1	A	896	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	743/864 (86%)	664 (89%)	79 (11%)	6 11

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	GLU

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Mol	Chain	Res	Type
1	A	168	VAL
1	A	205	LYS
1	A	209	GLU
1	A	215	ILE
1	A	219	CYS
1	A	230	SER
1	A	240	THR
1	A	252	MET
1	A	269	ASP
1	A	277	ARG
1	A	278	ASP
1	A	282	VAL
1	A	285	THR
1	A	302	GLU
1	A	305	VAL
1	A	320	LYS
1	A	354	LEU
1	A	359	ARG
1	A	368	ILE
1	A	370	ILE
1	A	372	VAL
1	A	373	LEU
1	A	379	LEU
1	A	380	THR
1	A	404	PHE
1	A	467	LEU
1	A	470	ASP
1	A	501	LYS
1	A	520	LEU
1	A	544	ARG
1	A	549	ASN
1	A	553	LYS
1	A	554	GLN
1	A	561	THR
1	A	568	THR
1	A	574	LEU
1	A	575	LEU
1	A	601	GLN
1	A	610	LEU
1	A	613	ARG
1	A	626	LEU
1	A	628	MET

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Mol	Chain	Res	Type
1	A	636	SER
1	A	646	GLN
1	A	658	HIS
1	A	682	LEU
1	A	717	LEU
1	A	731	ASP
1	A	740	GLU
1	A	749	ILE
1	A	752	LEU
1	A	767	LEU
1	A	779	LEU
1	A	798	ILE
1	A	808	LYS
1	A	839	ARG
1	A	841	ASP
1	A	843	LEU
1	A	845	LEU
1	A	875	LYS
1	A	886	THR
1	A	887	THR
1	A	893	GLN
1	A	907	LEU
1	A	911	LEU
1	A	918	GLU
1	A	927	ARG
1	A	939	THR
1	A	948	HIS
1	A	950	ASP
1	A	968	ILE
1	A	971	ASN
1	A	1002	THR
1	A	1026	LEU
1	A	1032	SER
1	A	1042	LEU
1	A	1043	THR
1	A	1059	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	GLN
1	A	291	GLN

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Mol	Chain	Res	Type
1	A	392	GLN
1	A	498	ASN
1	A	565	ASN
1	A	639	ASN
1	A	769	GLN
1	A	775	GLN
1	A	776	ASN
1	A	834	HIS
1	A	840	GLN
1	A	908	ASN
1	A	909	HIS
1	A	951	ASN
1	A	959	ASN
1	A	1083	GLN
1	A	1085	ASN

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	OAW	A	1	-	20,23,23	1.02	1 (5%)	19,34,34	2.61	10 (52%)

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	OAW	A	1	-	-	0/4/8/8	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	OAW	C2-N7	2.39	1.38	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1	OAW	C2-N1-C6	5.74	121.47	116.79
2	A	1	OAW	C8-N10-C11	5.17	124.20	117.71
2	A	1	OAW	C4-C5-C6	4.05	117.76	114.58
2	A	1	OAW	C2-N3-C4	2.89	121.87	113.89
2	A	1	OAW	N3-C2-N1	-2.70	121.19	125.42
2	A	1	OAW	O14-C11-C12	-2.51	119.51	124.92
2	A	1	OAW	C16-C8-N10	2.46	114.73	111.16
2	A	1	OAW	C5-N13-C12	2.21	121.63	117.82
2	A	1	OAW	C9-C6-C5	-2.20	120.95	123.05
2	A	1	OAW	C9-C6-N1	2.19	119.87	116.49

There are no chirality outliers.

There are no torsion outliers.

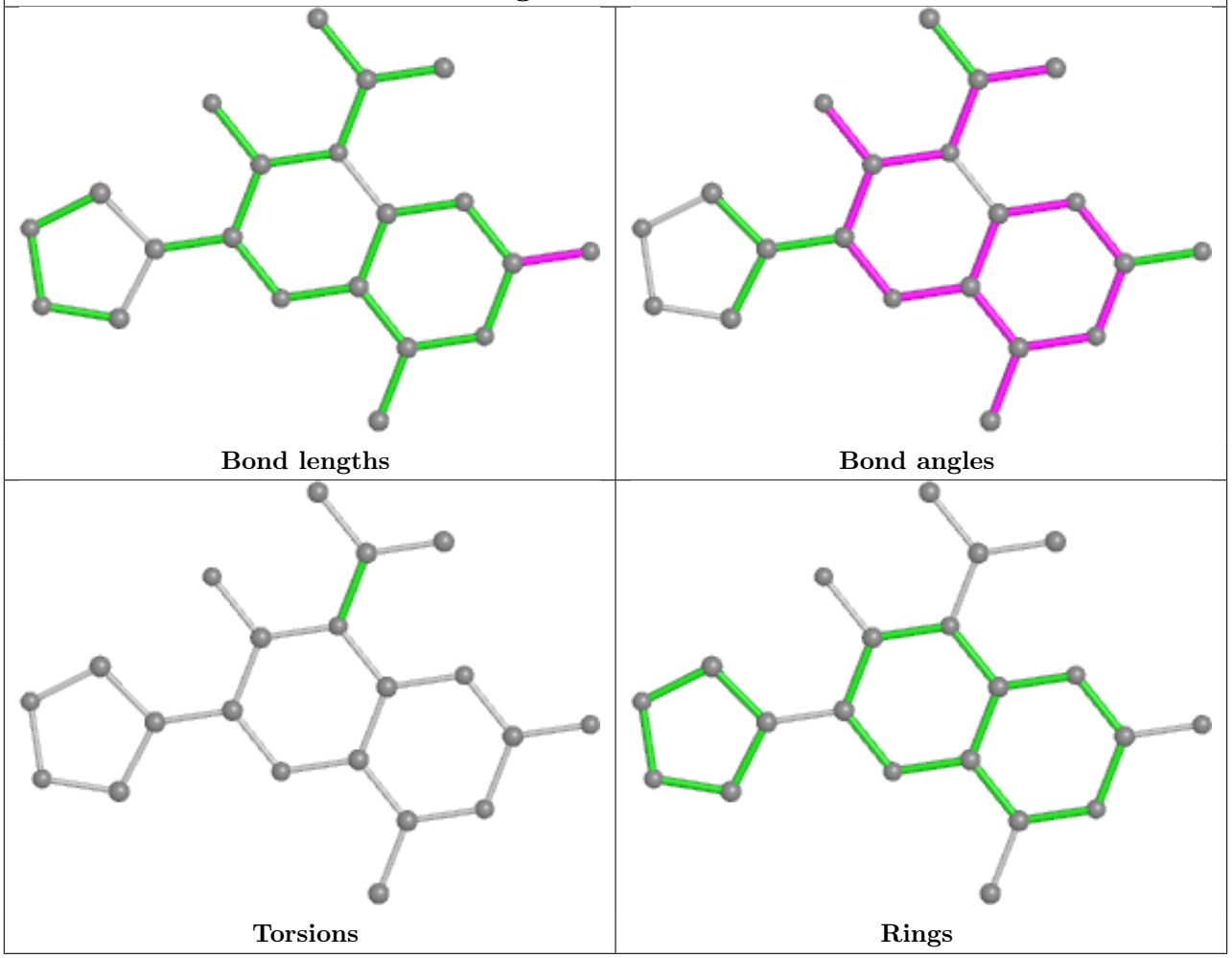
There are no ring outliers.

No monomer is involved in short contacts.

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 OAW A 1



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	841/966 (87%)	0.60	71 (8%)	11	13	44, 84, 127, 154	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	249	PHE	4.5
1	A	216	ALA	4.4
1	A	1041	GLN	4.3
1	A	987	LEU	4.2
1	A	231	GLN	4.1
1	A	251	LYS	4.0
1	A	404	PHE	4.0
1	A	902	PHE	3.9
1	A	971	ASN	3.9
1	A	234	LYS	3.9
1	A	890	LYS	3.8
1	A	370	ILE	3.8
1	A	306	VAL	3.7
1	A	898	ASN	3.7
1	A	239	ASP	3.7
1	A	307	LEU	3.5
1	A	409	LEU	3.5
1	A	287	ILE	3.4
1	A	900	GLY	3.4
1	A	237	PRO	3.2
1	A	524	CYS	3.2
1	A	779	LEU	3.1
1	A	891	ILE	3.0
1	A	582	SER	2.9
1	A	271	VAL	2.9
1	A	250	THR	2.9
1	A	995	MET	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	1087	PHE	2.8
1	A	147	SER	2.8
1	A	777	SER	2.8
1	A	911	LEU	2.8
1	A	310	PRO	2.7
1	A	895	THR	2.7
1	A	545	ALA	2.7
1	A	1084	PHE	2.7
1	A	212	TRP	2.6
1	A	406	GLU	2.5
1	A	778	GLN	2.5
1	A	146	GLU	2.5
1	A	529	LEU	2.5
1	A	968	ILE	2.5
1	A	221	PHE	2.5
1	A	970	GLY	2.5
1	A	1072	ILE	2.5
1	A	288	LYS	2.5
1	A	1091	VAL	2.5
1	A	897	GLY	2.4
1	A	774	LEU	2.4
1	A	232	THR	2.3
1	A	730	HIS	2.3
1	A	610	LEU	2.3
1	A	371	PRO	2.3
1	A	842	MET	2.3
1	A	217	ASN	2.2
1	A	1080	TRP	2.2
1	A	901	ALA	2.2
1	A	1000	LYS	2.2
1	A	823	LEU	2.2
1	A	185	MET	2.2
1	A	248	PHE	2.2
1	A	967	HIS	2.2
1	A	853	SER	2.2
1	A	660	LEU	2.1
1	A	1082	VAL	2.1
1	A	751	SER	2.1
1	A	661	LEU	2.1
1	A	366	ARG	2.1
1	A	189	ALA	2.0
1	A	662	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	969	LEU	2.0
1	A	1090	LEU	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 monosaccharides in this entry.

6.4 Ligands (i)

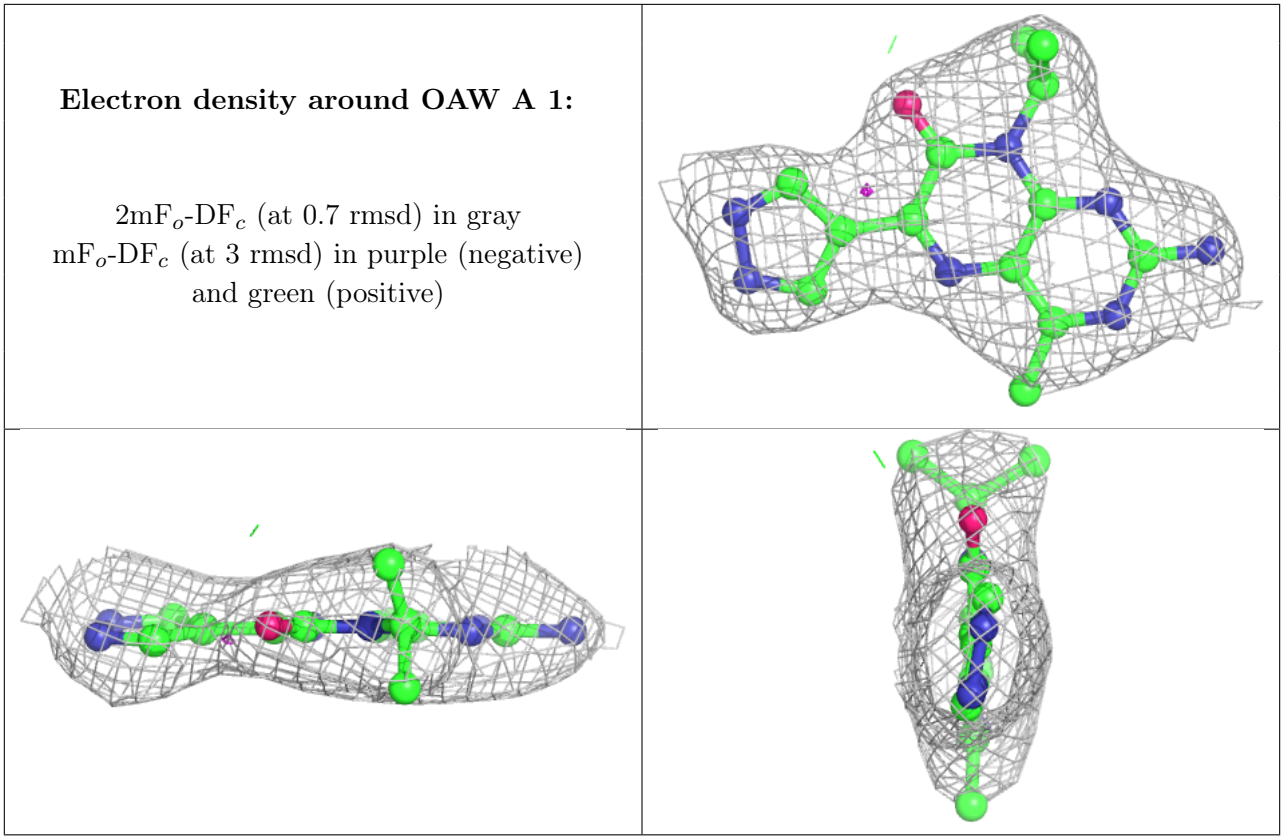
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	OAW	A	1	21/21	0.97	0.16	61,67,70,70	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 OAW A 1:

$2mF_o$-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.