



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:43 PM UTC

PDB ID : 3OAW / pdb_00003oaw
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	:	4-5-2 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

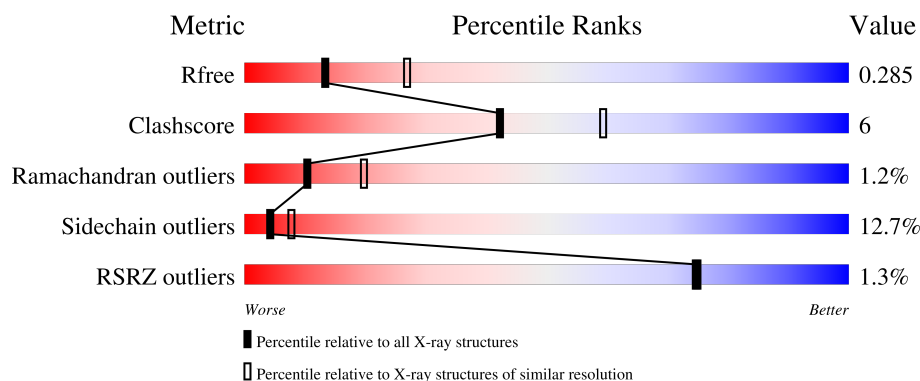
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	966	63% 20% • • 13%

2 Entry composition [i](#)

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.

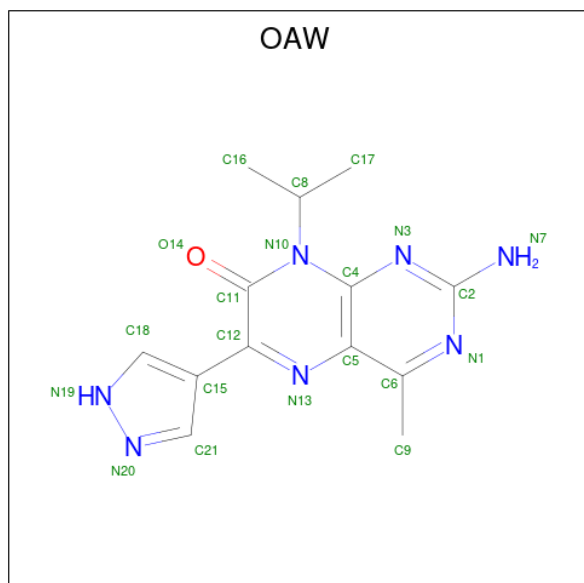
- Molecule 1 is a protein called Phosphatidylinositol-4,5-bisphosphate 3-kinase catalytic subunit gamma isoform.

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

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 (CCD ID: OAW) (formula: C₁₃H₁₅N₇O).



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

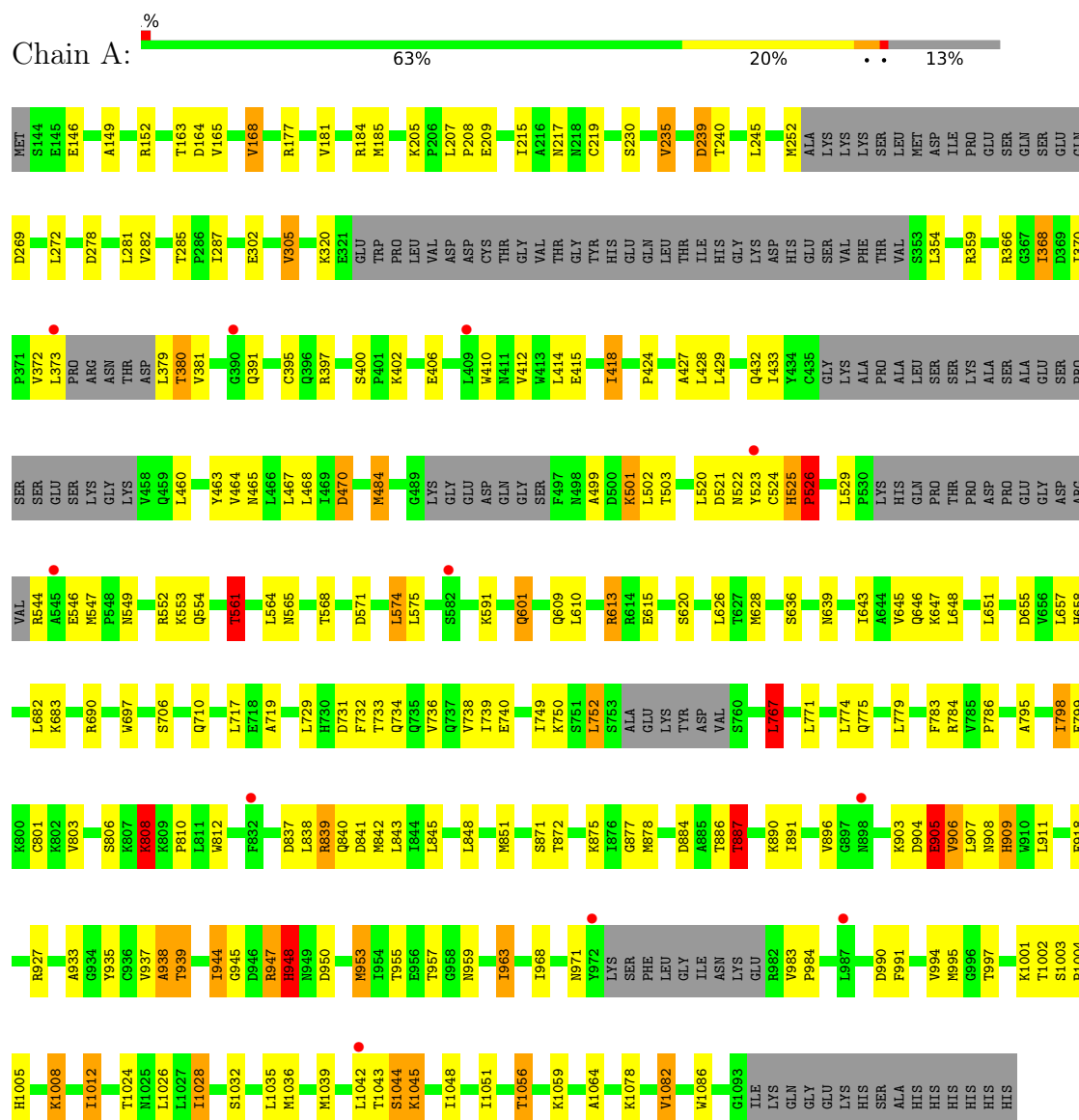
- Molecule 3 is water.

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

3 Residue-property plots

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



4 Data and refinement statistics

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) 98.1 (44.56-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 2.73Å)	Xtriage
Refinement program	BUSTER 2.9.5	Depositor
R, R_{free}	0.207 , 0.268 0.217 , 0.285	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 , 65.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	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.*

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: 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	0.85	1/6898 (0.0%)	1.43	54/9340 (0.6%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1036	MET	SD-CE	5.78	1.94	1.79

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	947	ARG	CA-C-N	8.00	133.93	122.09
1	A	947	ARG	C-N-CA	8.00	133.93	122.09
1	A	561	THR	CB-CA-C	6.61	122.34	109.33
1	A	613	ARG	CA-C-N	6.56	129.96	120.38
1	A	613	ARG	C-N-CA	6.56	129.96	120.38
1	A	484	MET	N-CA-C	6.51	120.65	110.17
1	A	991	PHE	CA-CB-CG	6.42	120.22	113.80
1	A	884	ASP	CA-CB-CG	6.31	118.91	112.60
1	A	784	ARG	CA-C-N	-6.21	118.12	122.59
1	A	784	ARG	C-N-CA	-6.21	118.12	122.59
1	A	944	ILE	CA-C-N	6.01	126.61	120.00
1	A	944	ILE	C-N-CA	6.01	126.61	120.00
1	A	601	GLN	N-CA-C	5.94	117.75	111.28
1	A	799	GLU	CA-C-N	5.91	128.68	120.29
1	A	799	GLU	C-N-CA	5.91	128.68	120.29
1	A	808	LYS	N-CA-C	-5.88	100.26	109.25
1	A	948	HIS	CA-C-N	5.83	128.36	120.38
1	A	948	HIS	C-N-CA	5.83	128.36	120.38
1	A	571	ASP	CA-CB-CG	5.79	118.39	112.60
1	A	380	THR	CB-CA-C	5.72	119.84	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	839	ARG	N-CA-C	-5.67	105.00	111.07
1	A	470	ASP	CA-CB-CG	5.64	118.24	112.60
1	A	381	VAL	N-CA-C	5.57	115.90	108.27
1	A	1056	THR	CB-CA-C	5.53	119.74	111.89
1	A	503	THR	N-CA-C	5.51	118.22	110.23
1	A	938	ALA	CA-C-N	5.50	127.64	120.28
1	A	938	ALA	C-N-CA	5.50	127.64	120.28
1	A	1008	LYS	N-CA-C	-5.35	105.34	111.07
1	A	905	GLU	CA-C-N	5.31	131.53	121.97
1	A	905	GLU	C-N-CA	5.31	131.53	121.97
1	A	909	HIS	CA-C-N	5.28	127.36	120.28
1	A	909	HIS	C-N-CA	5.28	127.36	120.28
1	A	526	PRO	N-CA-C	5.20	123.17	112.47
1	A	904	ASP	CA-CB-CG	5.11	117.71	112.60
1	A	217	ASN	CA-CB-CG	5.06	117.66	112.60
1	A	1028	ILE	CA-C-N	5.06	126.94	120.56
1	A	1028	ILE	C-N-CA	5.06	126.94	120.56
1	A	906	VAL	N-CA-C	5.06	119.87	109.34
1	A	239	ASP	N-CA-C	5.05	116.97	109.25
1	A	887	THR	CB-CA-C	5.04	118.12	109.51
1	A	522	ASN	CA-C-N	5.03	131.15	121.54
1	A	522	ASN	C-N-CA	5.03	131.15	121.54
1	A	620	SER	N-CA-C	5.03	116.78	110.24
1	A	767	LEU	CA-C-N	5.03	127.02	120.28
1	A	767	LEU	C-N-CA	5.03	127.02	120.28
1	A	1064	ALA	CA-C-N	5.02	127.01	120.28
1	A	1064	ALA	C-N-CA	5.02	127.01	120.28
1	A	609	GLN	CA-C-N	5.01	126.99	120.28
1	A	609	GLN	C-N-CA	5.01	126.99	120.28
1	A	806	SER	CA-C-N	5.01	129.16	121.19
1	A	806	SER	C-N-CA	5.01	129.16	121.19
1	A	574	LEU	CA-C-N	5.00	127.30	120.54
1	A	574	LEU	C-N-CA	5.00	127.30	120.54
1	A	245	LEU	N-CA-C	-5.00	106.87	113.12

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	86	0
2	A	21	0	15	1	0
3	A	29	0	0	0	0
All	All	6804	0	6779	86	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 (86) 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
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:851:MET:HE1	1:A:938:ALA:HB1	1.71	0.71
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:786:PRO:HD2	1:A:878:MET:HE1	1.92	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: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
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:842:MET:HE2	1:A:871:SER:HB2	1.96	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: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:181:VAL:HG12	1:A:185:MET:HE2	2.01	0.42
1:A:848:LEU:HA	1:A:851:MET:HE2	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:955:THR:C	1:A:957:THR:H	2.28	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:729:LEU:O	1:A:733:THR:OG1	2.37	0.40
1:A:397:ARG:NE	1:A:415:GLU:O	2.55	0.40
1:A:953:MET:HE3	2:A:1:OAW:H16B	2.03	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 ⓘ

5.3.1 Protein backbone ⓘ

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%)	10	20

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

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Mol	Chain	Res	Type
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 ⓘ

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%)	649 (87%)	94 (13%)	4 8

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	GLU
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	235	VAL
1	A	240	THR
1	A	252	MET
1	A	269	ASP
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	366	ARG

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Mol	Chain	Res	Type
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	391	GLN
1	A	400	SER
1	A	402	LYS
1	A	406	GLU
1	A	418	ILE
1	A	467	LEU
1	A	470	ASP
1	A	501	LYS
1	A	520	LEU
1	A	529	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
1	A	636	SER
1	A	646	GLN
1	A	647	LYS
1	A	658	HIS
1	A	682	LEU
1	A	683	LYS
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

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Mol	Chain	Res	Type
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	905	GLU
1	A	907	LEU
1	A	911	LEU
1	A	918	GLU
1	A	939	THR
1	A	944	ILE
1	A	948	HIS
1	A	950	ASP
1	A	953	MET
1	A	963	ILE
1	A	968	ILE
1	A	971	ASN
1	A	1002	THR
1	A	1012	ILE
1	A	1024	THR
1	A	1026	LEU
1	A	1032	SER
1	A	1042	LEU
1	A	1043	THR
1	A	1056	THR
1	A	1059	LYS
1	A	1078	LYS
1	A	1082	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	218	ASN
1	A	291	GLN
1	A	295	HIS
1	A	389	HIS
1	A	392	GLN
1	A	565	ASN

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Mol	Chain	Res	Type
1	A	711	GLN
1	A	743	GLN
1	A	766	GLN
1	A	769	GLN
1	A	775	GLN
1	A	834	HIS
1	A	840	GLN
1	A	893	GLN
1	A	908	ASN
1	A	909	HIS
1	A	949	ASN
1	A	959	ASN
1	A	971	ASN
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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OAW	A	1	-	23,23,23	1.14	2 (8%)	23,34,34	2.56	11 (47%)

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	-	-	0/6/8/8	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	OAW	C2-N7	2.40	1.38	1.33
2	A	1	OAW	N19-N20	2.32	1.40	1.35

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	OAW	C2-N1-C6	5.74	121.47	116.79
2	A	1	OAW	C8-N10-C11	5.21	124.20	117.75
2	A	1	OAW	C4-C5-C6	3.94	117.76	114.61
2	A	1	OAW	C11-C12-N13	-3.61	119.40	124.24
2	A	1	OAW	C2-N3-C4	3.12	121.87	113.51
2	A	1	OAW	N3-C2-N1	-2.80	121.19	125.48
2	A	1	OAW	C16-C8-N10	2.57	114.73	111.11
2	A	1	OAW	C9-C6-N1	2.15	119.87	116.53
2	A	1	OAW	C5-N13-C12	2.11	121.63	118.10
2	A	1	OAW	C9-C6-C5	-2.11	120.95	123.12
2	A	1	OAW	C17-C8-N10	2.09	114.05	111.11

There are no chirality outliers.

There are no torsion outliers.

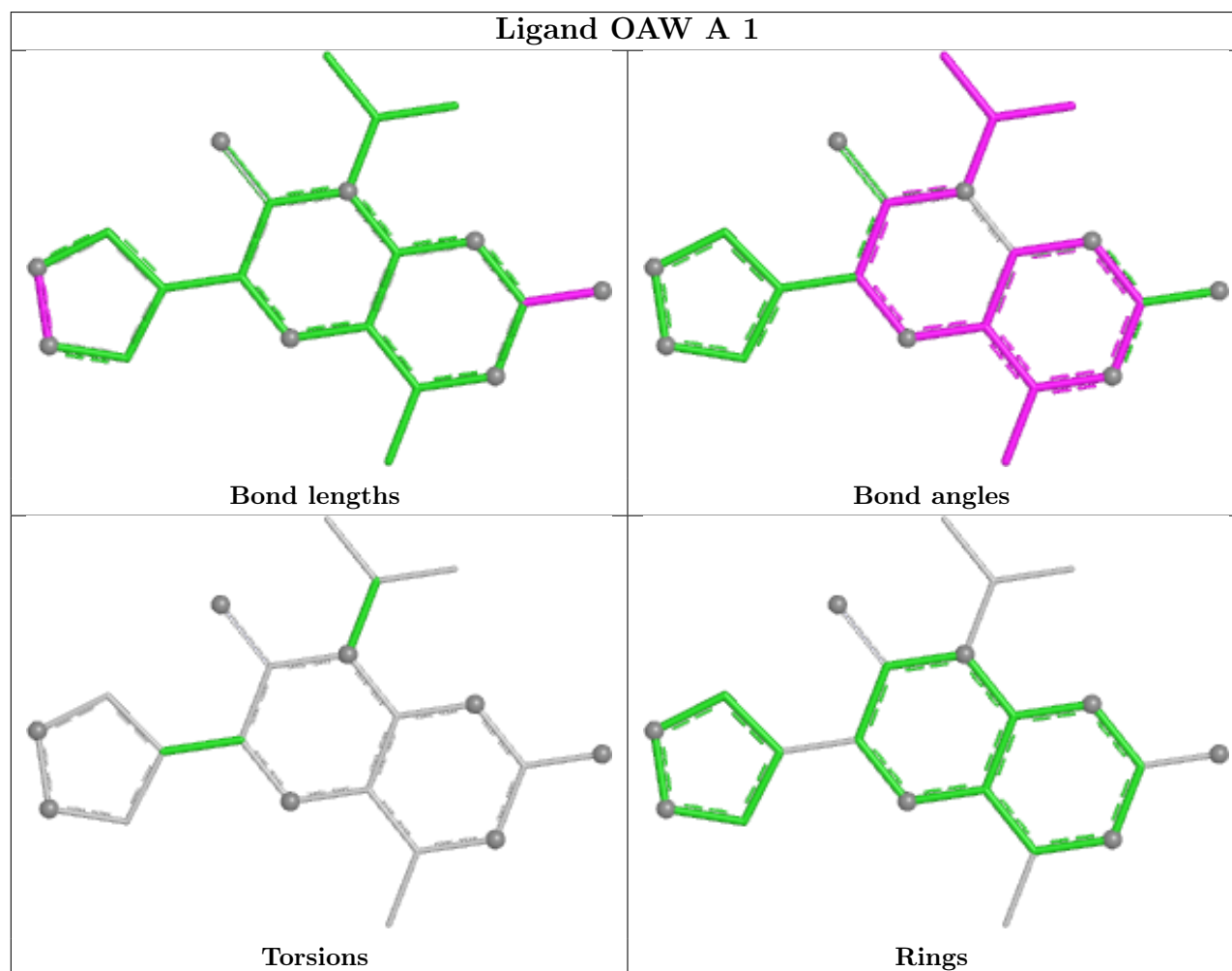
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	OAW	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	841/966 (87%)	0.19	11 (1%) 75 75	44, 84, 127, 154	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	972	TYR	3.7
1	A	523	TYR	3.3
1	A	390	GLY	2.9
1	A	987	LEU	2.8
1	A	582	SER	2.8
1	A	545	ALA	2.6
1	A	1042	LEU	2.5
1	A	409	LEU	2.2
1	A	373	LEU	2.1
1	A	832	PHE	2.1
1	A	898	ASN	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 oligosaccharides in this entry.

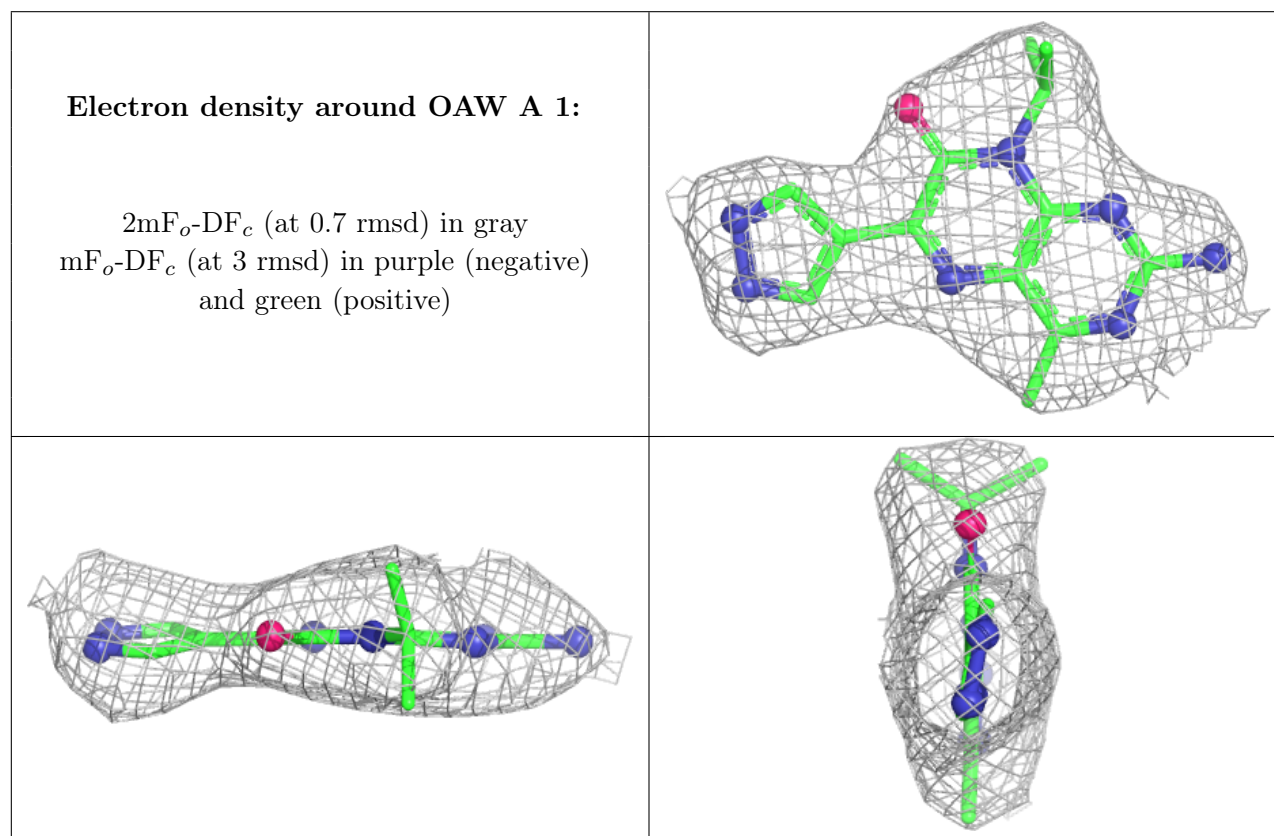
6.4 Ligands [i](#)

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(Å ²)	Q<0.9
2	OAW	A	1	21/21	0.96	0.08	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.