



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 11:10 AM EDT

PDB ID : 4URK / pdb_00004urk
Title : PI3Kg in complex with AZD6482
Authors : Giordanetto, F.; Barlaam, B.; Berglund, S.; Edman, K.; Karlsson, O.; Lindberg, J.; Nylander, S.; Inghardt, T.
Deposited on : 2014-06-30
Resolution : 2.90 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

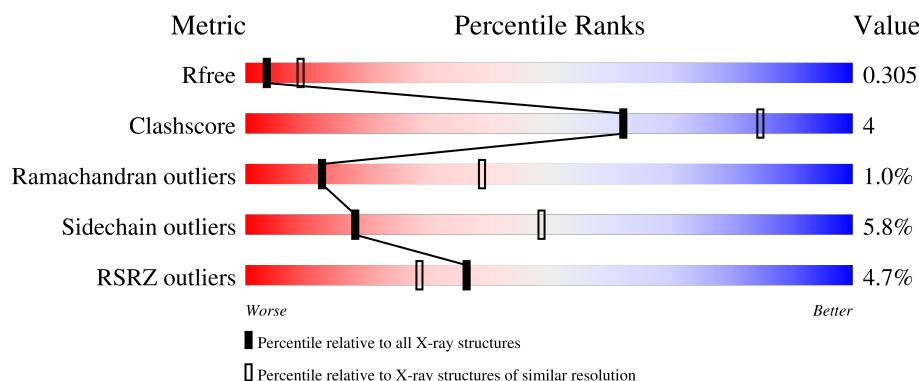
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 6823 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.

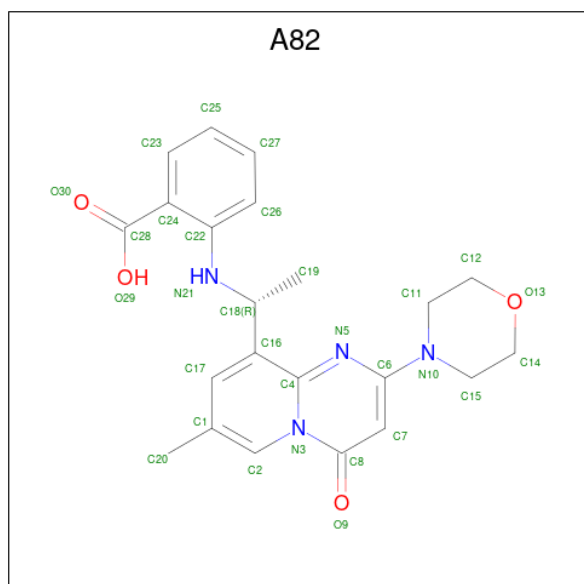
- Molecule 1 is a protein called PHOSPHATIDYLINOSITOL 4,5-BISPHOSPHATE 3-KINASE CATALYTIC SUBUNIT GAMMA ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	837	6793	4361	1159	1238	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 2-[[[(1R)-1-(7-methyl-2-morpholin-4-yl-4-oxidanylidene-pyrido[1,2-a]pyrimidin-9-yl)ethyl]amino]benzoic acid (CCD ID: A82) (formula: C₂₂H₂₄N₄O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			30	22	4	4		

WORLD WIDE
PDB
PROTEIN DATA BANK

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	143.18Å 67.52Å 106.17Å 90.00° 95.71° 90.00°	Depositor
Resolution (Å)	40.80 – 2.90 40.80 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.80-2.90) 95.8 (40.80-2.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 2.90Å)	Xtriage
Refinement program	BUSTER 2.11.1	Depositor
R, R_{free}	0.250 , 0.309 0.243 , 0.305	Depositor DCC
R_{free} test set	1111 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	61.6	Xtriage
Anisotropy	0.519	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 71.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6823	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.78% 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: A82

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	0.79	0/6938	1.39	21/9384 (0.2%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	776	ASN	N-CA-C	7.69	119.45	111.14
1	A	470	ASP	CA-CB-CG	6.34	118.94	112.60
1	A	503	THR	N-CA-C	6.32	119.52	110.10
1	A	632	ASP	CA-CB-CG	5.87	118.47	112.60
1	A	632	ASP	CA-C-N	5.86	128.72	120.28
1	A	632	ASP	C-N-CA	5.86	128.72	120.28
1	A	1043	THR	N-CA-C	5.81	117.86	108.34
1	A	181	VAL	CA-C-N	5.75	126.21	119.83
1	A	181	VAL	C-N-CA	5.75	126.21	119.83
1	A	692	GLY	CA-C-N	5.57	127.68	120.44
1	A	692	GLY	C-N-CA	5.57	127.68	120.44
1	A	547	MET	N-CA-C	5.55	122.08	109.81
1	A	369	ASP	CA-CB-CG	5.43	118.03	112.60
1	A	553	LYS	CA-C-N	5.24	127.25	120.44
1	A	553	LYS	C-N-CA	5.24	127.25	120.44
1	A	833	LYS	N-CA-C	5.11	116.72	108.34
1	A	544	ARG	CA-C-N	5.09	128.08	120.90
1	A	544	ARG	C-N-CA	5.09	128.08	120.90
1	A	569	ALA	CA-C-N	5.08	127.04	120.44
1	A	569	ALA	C-N-CA	5.08	127.04	120.44
1	A	1056	THR	CB-CA-C	5.02	119.81	112.09

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	6793	0	6841	56	0
2	A	30	0	23	2	0
All	All	6823	0	6864	56	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 4.

All (56) 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:1014:VAL:HG11	1:A:1065:LYS:HG3	1.76	0.67
1:A:804:MET:HE3	1:A:806:SER:HB2	1.77	0.65
1:A:786:PRO:HD2	1:A:878:MET:HE1	1.77	0.65
1:A:706:SER:O	1:A:710:GLN:HB3	1.98	0.63
1:A:576:TRP:O	1:A:579:ARG:HG3	2.00	0.62
1:A:1013:CYS:HB3	1:A:1068:PHE:HE2	1.65	0.62
1:A:735:GLN:O	1:A:739:ILE:HG12	2.00	0.61
1:A:804:MET:HB2	1:A:810:PRO:HD2	1.83	0.61
1:A:579:ARG:HB3	1:A:610:LEU:HD21	1.84	0.60
1:A:839:ARG:HA	1:A:842:MET:HE2	1.85	0.58
1:A:880:GLU:O	2:A:2092:A82:H122	2.04	0.57
1:A:739:ILE:HG21	1:A:872:THR:HG21	1.87	0.56
1:A:146:GLU:HB3	1:A:319:ARG:HH22	1.71	0.55
1:A:833:LYS:HE3	1:A:836:ASP:HB2	1.89	0.55
1:A:640:VAL:O	1:A:643:ILE:HG12	2.07	0.54
1:A:368:ILE:HG21	1:A:433:ILE:HD11	1.90	0.54
1:A:410:TRP:HB3	1:A:412:VAL:HG22	1.90	0.54
1:A:775:GLN:HE21	1:A:798:ILE:HD11	1.72	0.53
1:A:238:ASP:HA	1:A:286:PRO:HB3	1.92	0.52
1:A:750:LYS:HE2	1:A:834:HIS:HD2	1.75	0.52
1:A:558:ILE:HG21	1:A:575:LEU:HD21	1.91	0.52
1:A:1035:LEU:HD23	1:A:1039:MET:HG3	1.92	0.52
1:A:497:PHE:O	1:A:1043:THR:HB	2.12	0.50
1:A:881:ILE:HA	2:A:2092:A82:H142	1.94	0.49
1:A:804:MET:CB	1:A:810:PRO:HD2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1039:MET:HB3	1:A:1042:LEU:HD23	1.96	0.48
1:A:435:CYS:HB3	1:A:461:LEU:HD11	1.96	0.47
1:A:893:GLN:HG2	1:A:898:ASN:H	1.79	0.47
1:A:613:ARG:O	1:A:615:GLU:N	2.47	0.46
1:A:989:PRO:HA	1:A:992:LEU:HB2	1.97	0.46
1:A:1083:GLN:HA	1:A:1086:TRP:HD1	1.81	0.46
1:A:741:MET:HA	1:A:744:LYS:HE3	1.99	0.45
1:A:831:ILE:HB	1:A:879:ILE:HB	1.99	0.44
1:A:471:HIS:H	1:A:471:HIS:CD2	2.34	0.44
1:A:1013:CYS:HB3	1:A:1068:PHE:CE2	2.50	0.43
1:A:807:LYS:HE3	1:A:808:LYS:HE3	1.99	0.43
1:A:632:ASP:HB3	1:A:1033:MET:HE3	2.01	0.43
1:A:613:ARG:C	1:A:615:GLU:H	2.27	0.43
1:A:586:PRO:O	1:A:626:LEU:HD21	2.19	0.43
1:A:855:TRP:HB3	1:A:860:LEU:HB2	2.01	0.42
1:A:198:MET:HG2	1:A:280:TYR:CG	2.55	0.42
1:A:564:LEU:HD11	1:A:1048:ILE:HG22	2.02	0.42
1:A:802:LYS:HG2	1:A:812:TRP:HB3	2.01	0.42
1:A:834:HIS:HA	1:A:875:LYS:O	2.20	0.42
1:A:1083:GLN:HA	1:A:1086:TRP:CD1	2.55	0.42
1:A:221:PHE:CE1	1:A:234:LYS:HG2	2.55	0.42
1:A:998:SER:H	1:A:1001:LYS:HD2	1.85	0.42
1:A:847:ILE:HG21	1:A:942:LEU:HD21	2.02	0.41
1:A:925:VAL:O	1:A:929:VAL:HG23	2.20	0.41
1:A:939:THR:HB	1:A:945:GLY:HA2	2.01	0.41
1:A:939:THR:HG21	1:A:962:HIS:CE1	2.55	0.41
1:A:761:SER:HA	1:A:764:ILE:HD12	2.02	0.41
1:A:390:GLY:C	1:A:392:GLN:H	2.29	0.41
1:A:843:LEU:HD13	1:A:1034:MET:HG3	2.02	0.40
1:A:885:ALA:HB2	1:A:955:THR:HG22	2.03	0.40
1:A:968:ILE:HD12	1:A:969:LEU:HG	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%)	761 (92%)	54 (7%)	8 (1%)	12	39

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	614	ARG
1	A	755	GLU
1	A	190	SER
1	A	649	GLU
1	A	896	VAL
1	A	964	ASP
1	A	1079	GLY
1	A	723	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	754/864 (87%)	710 (94%)	44 (6%)	18	49

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	231	GLN
1	A	271	VAL
1	A	299	ASN
1	A	302	GLU
1	A	307	LEU
1	A	368	ILE
1	A	369	ASP
1	A	379	LEU
1	A	381	VAL
1	A	391	GLN
1	A	411	ASN

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Mol	Chain	Res	Type
1	A	420	ILE
1	A	464	VAL
1	A	475	LEU
1	A	476	ARG
1	A	486	GLN
1	A	518	ILE
1	A	547	MET
1	A	555	LEU
1	A	575	LEU
1	A	610	LEU
1	A	629	GLN
1	A	658	HIS
1	A	700	ARG
1	A	710	GLN
1	A	726	THR
1	A	731	ASP
1	A	749	ILE
1	A	755	GLU
1	A	763	VAL
1	A	764	ILE
1	A	767	LEU
1	A	770	LYS
1	A	853	SER
1	A	896	VAL
1	A	899	THR
1	A	904	ASP
1	A	944	ILE
1	A	954	ILE
1	A	968	ILE
1	A	980	LYS
1	A	1043	THR
1	A	1051	ILE
1	A	1057	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	389	HIS
1	A	522	ASN
1	A	550	GLN
1	A	629	GLN
1	A	734	GLN

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Mol	Chain	Res	Type
1	A	773	ASN
1	A	775	GLN
1	A	834	HIS
1	A	846	GLN
1	A	898	ASN
1	A	909	HIS
1	A	962	HIS
1	A	967	HIS
1	A	1007	GLN
1	A	1010	GLN

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	A82	A	2092	-	32,33,33	0.93	1 (3%)	37,47,47	1.61	7 (18%)

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	A82	A	2092	-	-	7/13/24/24	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2092	A82	O29-C28	2.02	1.36	1.30

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2092	A82	O9-C8-N3	4.55	126.97	118.34
2	A	2092	A82	O9-C8-C7	-3.18	117.76	125.61
2	A	2092	A82	C8-C7-C6	-2.97	119.47	121.49
2	A	2092	A82	C2-C1-C17	2.45	120.47	118.25
2	A	2092	A82	C23-C24-C22	2.35	121.46	118.81
2	A	2092	A82	O29-C28-C24	-2.33	108.64	115.28
2	A	2092	A82	O13-C14-C15	-2.13	107.18	111.77

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2092	A82	C22-C24-C28-O29
2	A	2092	A82	C22-C24-C28-O30
2	A	2092	A82	C26-C22-N21-C18
2	A	2092	A82	C19-C18-N21-C22
2	A	2092	A82	C23-C24-C28-O29
2	A	2092	A82	C23-C24-C28-O30
2	A	2092	A82	C24-C22-N21-C18

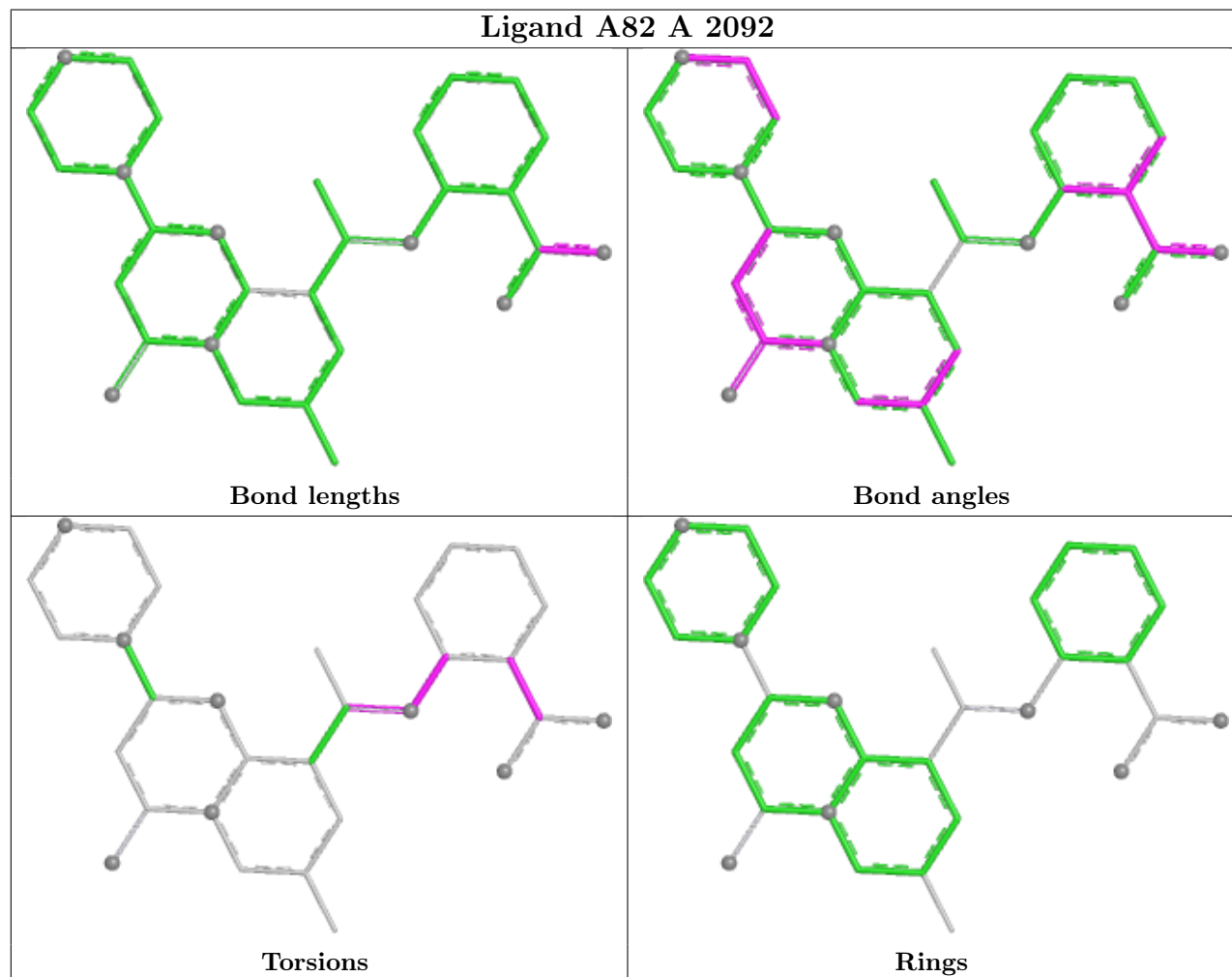
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2092	A82	2	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	837/966 (86%)	0.51	39 (4%) 36 28	23, 66, 116, 141	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	987	LEU	5.3
1	A	901	ALA	4.0
1	A	988	THR	3.5
1	A	779	LEU	3.4
1	A	379	LEU	3.1
1	A	248	PHE	3.0
1	A	1087	PHE	2.9
1	A	1084	PHE	2.8
1	A	1091	VAL	2.8
1	A	986	VAL	2.8
1	A	895	THR	2.7
1	A	1056	THR	2.7
1	A	907	LEU	2.7
1	A	992	LEU	2.6
1	A	1064	ALA	2.6
1	A	995	MET	2.6
1	A	991	PHE	2.6
1	A	1083	GLN	2.5
1	A	891	ILE	2.5
1	A	823	LEU	2.5
1	A	404	PHE	2.5
1	A	1075	CYS	2.4
1	A	990	ASP	2.3
1	A	380	THR	2.3
1	A	892	GLN	2.2
1	A	929	VAL	2.2
1	A	1002	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	249	PHE	2.2
1	A	1069	LEU	2.1
1	A	374	PRO	2.1
1	A	288	LYS	2.1
1	A	900	GLY	2.1
1	A	1086	TRP	2.1
1	A	1079	GLY	2.1
1	A	1090	LEU	2.1
1	A	275	CYS	2.0
1	A	1005	HIS	2.0
1	A	522	ASN	2.0
1	A	911	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](#)

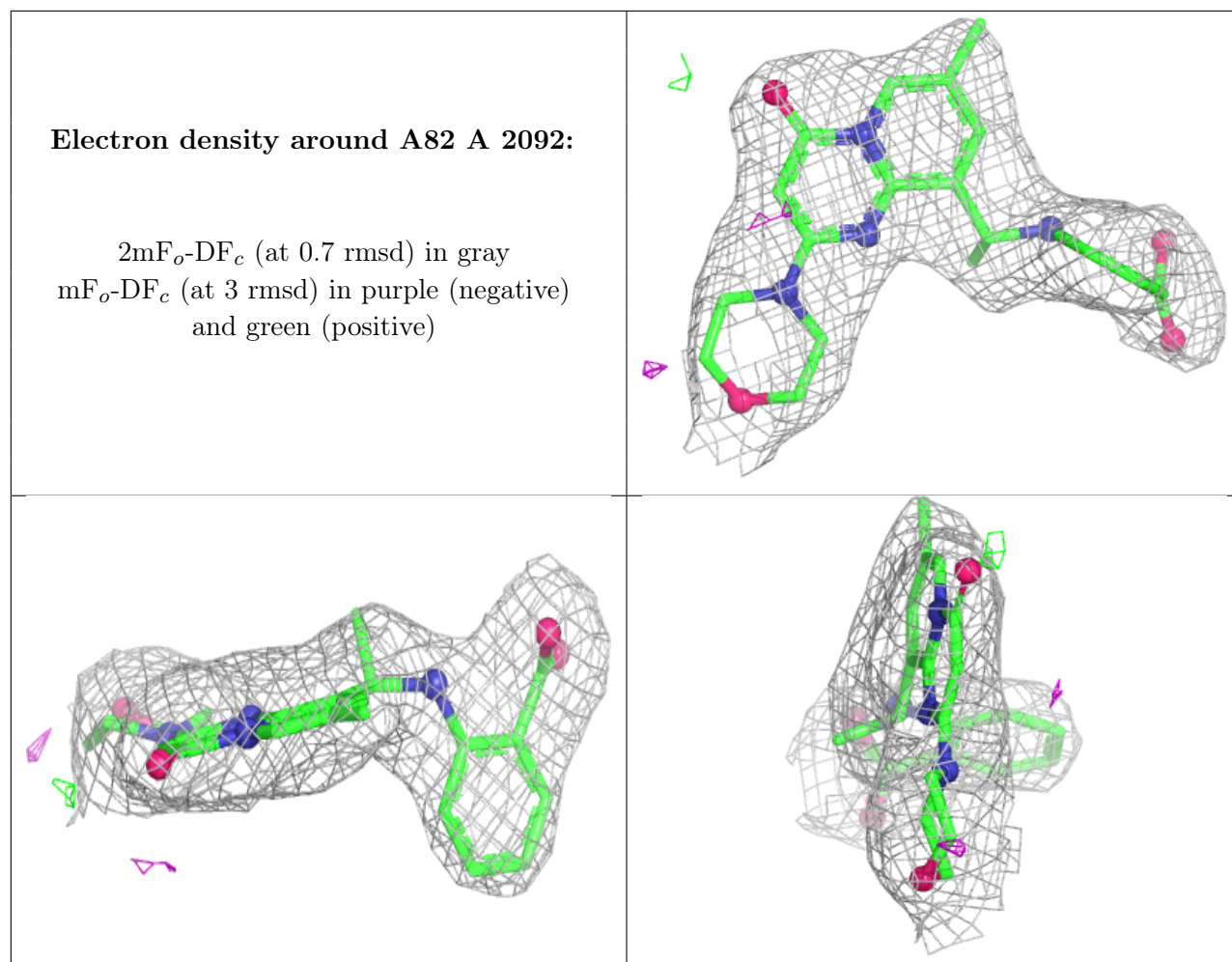
There are no oligosaccharides in this entry.

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	A82	A	2092	30/30	0.93	0.11	64,66,69,69	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 [i](#)

There are no such residues in this entry.