



# Full wwPDB X-ray Structure Validation Report ⓘ

May 12, 2020 – 11:27 pm BST

PDB ID : 3DBS  
Title : Structure of PI3K gamma in complex with GDC0941  
Authors : Wiesmann, C.; Ultsch, M.  
Deposited on : 2008-06-02  
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](mailto: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.

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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 : 2.11  
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) : 2.11

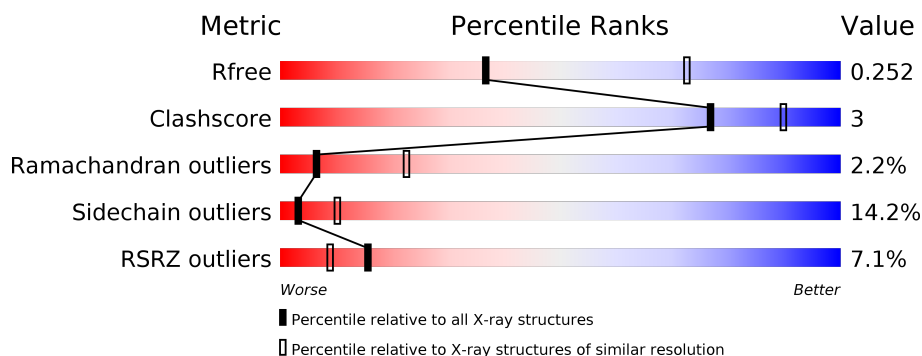
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	960	

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 6847 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.

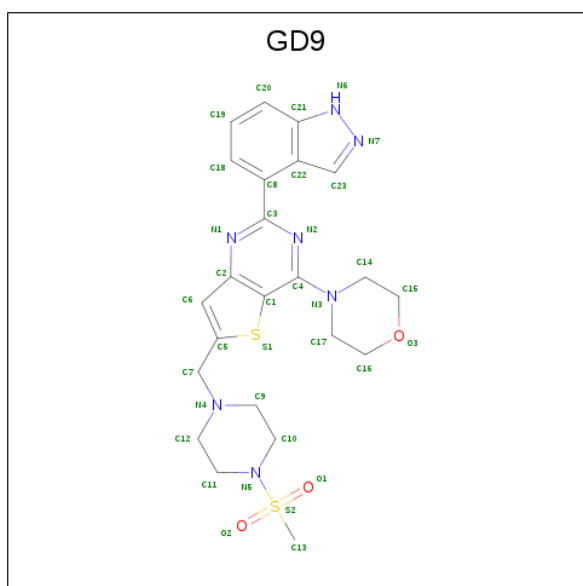
- Molecule 1 is a protein called Phosphatidylinositol-4,5-bisphosphate 3-kinase catalytic subunit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	841	Total	C	N	O	S	0	0	0
			6812	4371	1164	1242	35			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	MET	-	INITIATING METHIONINE	UNP P48736

- Molecule 2 is 2-(1H-indazol-4-yl)-6-{[4-(methylsulfonyl)piperazin-1-yl]methyl}-4-morpholin-4-yl-thieno[3,2-d]pyrimidine (three-letter code: GD9) (formula: C<sub>23</sub>H<sub>27</sub>N<sub>7</sub>O<sub>3</sub>S<sub>2</sub>).

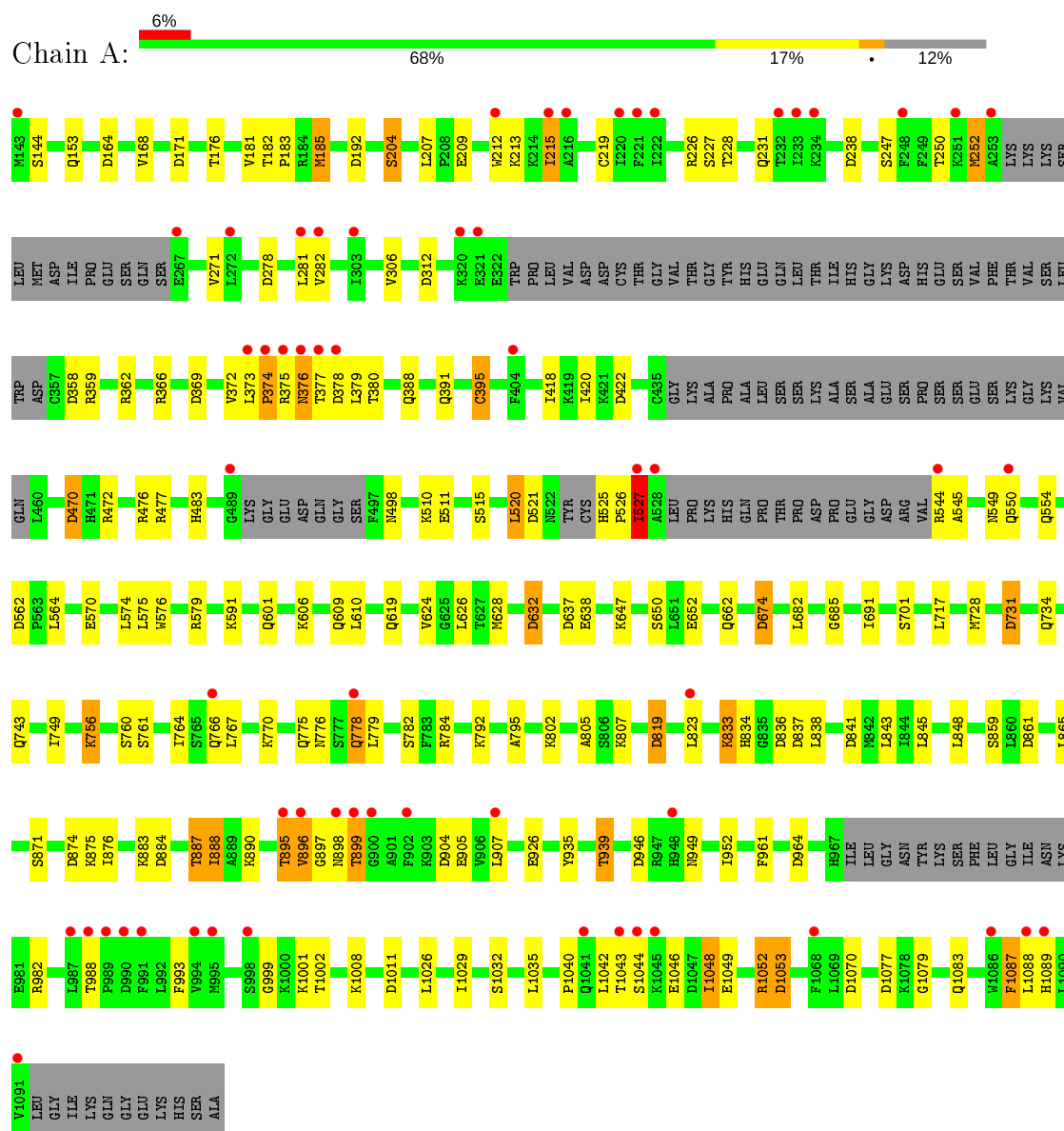


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			35	23	7	3	2		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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, $\alpha$ , $\beta$ , $\gamma$	144.28Å 67.76Å 106.97Å 90.00° 95.31° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 44.81 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.80) 99.7 (44.81-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.15 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.219 , 0.262 0.216 , 0.252	Depositor DCC
$R_{free}$ test set	1317 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	78.7	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 58.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6847	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.41% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GD9

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	0.51	1/6958 (0.0%)	0.77	28/9412 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	904	ASP	CG-OD1	7.57	1.42	1.25

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	632	ASP	CB-CG-OD2	7.32	124.89	118.30
1	A	1011	ASP	CB-CG-OD2	6.40	124.06	118.30
1	A	874	ASP	CB-CG-OD2	6.22	123.90	118.30
1	A	278	ASP	CB-CG-OD2	6.11	123.80	118.30
1	A	1070	ASP	CB-CG-OD2	6.02	123.72	118.30
1	A	378	ASP	CB-CG-OD2	6.02	123.72	118.30
1	A	837	ASP	CB-CG-OD2	6.00	123.70	118.30
1	A	521	ASP	CB-CG-OD2	5.94	123.64	118.30
1	A	192	ASP	CB-CG-OD2	5.93	123.64	118.30
1	A	238	ASP	CB-CG-OD2	5.87	123.58	118.30
1	A	358	ASP	CB-CG-OD2	5.86	123.57	118.30
1	A	637	ASP	CB-CG-OD2	5.79	123.51	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	841	ASP	CB-CG-OD2	5.70	123.43	118.30
1	A	312	ASP	CB-CG-OD2	5.66	123.39	118.30
1	A	964	ASP	CB-CG-OD2	5.63	123.37	118.30
1	A	164	ASP	CB-CG-OD2	5.62	123.36	118.30
1	A	171	ASP	CB-CG-OD2	5.59	123.33	118.30
1	A	369	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	836	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	470	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	422	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	861	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	819	ASP	CB-CG-OD2	5.18	122.97	118.30
1	A	1077	ASP	CB-CG-OD2	5.18	122.97	118.30
1	A	674	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	884	ASP	CB-CG-OD2	5.15	122.93	118.30
1	A	1053	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	562	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	756	LYS	Peptide

## 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	6812	0	6843	40	0
2	A	35	0	27	2	0
All	All	6847	0	6870	41	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 3.

All (41) 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:802:LYS:NZ	2:A:1:GD9:O1	2.14	0.80
1:A:576:TRP:O	1:A:579:ARG:HD3	1.96	0.66
1:A:743:GLN:HE21	1:A:876:ILE:HG12	1.61	0.66
1:A:606:LYS:HA	1:A:609:GLN:HE21	1.63	0.64
1:A:731:ASP:OD2	1:A:784:ARG:NE	2.35	0.60
1:A:527:ILE:HG23	1:A:601:GLN:HE22	1.70	0.57
1:A:905:GLU:HA	1:A:993:PHE:CD2	2.41	0.55
1:A:734:GLN:HA	1:A:734:GLN:HE21	1.72	0.54
1:A:204:SER:OG	1:A:652:GLU:OE2	2.18	0.53
1:A:576:TRP:O	1:A:579:ARG:CD	2.57	0.52
1:A:182:THR:HB	1:A:183:PRO:HD3	1.92	0.52
1:A:834:HIS:HB2	1:A:876:ILE:HD12	1.92	0.51
1:A:624:VAL:O	1:A:628:MET:HG2	2.11	0.50
1:A:743:GLN:NE2	1:A:876:ILE:HG23	2.26	0.50
1:A:935:TYR:O	1:A:939:THR:HB	2.10	0.50
1:A:209:GLU:HB2	1:A:859:SER:HB3	1.92	0.50
1:A:181:VAL:O	1:A:185:MET:HG3	2.11	0.50
1:A:743:GLN:HE22	1:A:876:ILE:HG23	1.77	0.48
1:A:807:LYS:O	1:A:833:LYS:NZ	2.37	0.48
1:A:895:THR:O	1:A:897:GLY:N	2.45	0.48
1:A:176:THR:HG23	1:A:674:ASP:HB2	1.96	0.48
1:A:1035:LEU:HD12	1:A:1048:ILE:HD13	1.95	0.48
1:A:373:LEU:N	1:A:374:PRO:CD	2.77	0.47
1:A:498:ASN:C	1:A:498:ASN:OD1	2.53	0.47
1:A:743:GLN:NE2	1:A:876:ILE:HG12	2.28	0.46
1:A:775:GLN:HE22	1:A:795:ALA:HB1	1.80	0.46
1:A:395:CYS:SG	1:A:418:ILE:HG12	2.56	0.45
1:A:564:LEU:HB2	1:A:1052:ARG:HD2	1.98	0.45
1:A:359:ARG:O	1:A:420:ILE:HG12	2.16	0.45
1:A:888:ILE:HD13	1:A:952:ILE:HG22	1.99	0.44
1:A:632:ASP:C	1:A:632:ASP:OD1	2.56	0.44
1:A:476:ARG:HG2	1:A:520:LEU:HD23	2.00	0.43
1:A:734:GLN:NE2	1:A:734:GLN:HA	2.34	0.43
1:A:212:TRP:CE3	1:A:215:ILE:HD12	2.54	0.42
1:A:685:GLY:HA2	1:A:691:ILE:HG22	2.02	0.42
2:A:1:GD9:S1	2:A:1:GD9:H17A	2.60	0.42
1:A:895:THR:O	1:A:896:VAL:C	2.58	0.41
1:A:887:THR:HG22	1:A:890:LYS:H	1.85	0.41
1:A:949:ASN:H	1:A:1083:GLN:HE22	1.66	0.41
1:A:935:TYR:CE1	1:A:961:PHE:HA	2.56	0.41
1:A:483:HIS:CD2	1:A:510:LYS:HE3	2.57	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	825/960 (86%)	757 (92%)	50 (6%)	18 (2%)	6	22

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	776	ASN
1	A	896	VAL
1	A	898	ASN
1	A	805	ALA
1	A	1040	PRO
1	A	1087	PHE
1	A	227	SER
1	A	252	MET
1	A	376	ASN
1	A	545	ALA
1	A	778	GLN
1	A	899	THR
1	A	228	THR
1	A	527	ILE
1	A	999	GLY
1	A	526	PRO
1	A	1079	GLY
1	A	374	PRO

### 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	754/858 (88%)	647 (86%)	107 (14%)	3 10

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	SER
1	A	153	GLN
1	A	168	VAL
1	A	185	MET
1	A	204	SER
1	A	207	LEU
1	A	213	LYS
1	A	215	ILE
1	A	219	CYS
1	A	226	ARG
1	A	231	GLN
1	A	247	SER
1	A	250	THR
1	A	252	MET
1	A	271	VAL
1	A	281	LEU
1	A	282	VAL
1	A	306	VAL
1	A	362	ARG
1	A	366	ARG
1	A	372	VAL
1	A	375	ARG
1	A	376	ASN
1	A	377	THR
1	A	379	LEU
1	A	380	THR
1	A	388	GLN
1	A	391	GLN
1	A	395	CYS
1	A	470	ASP
1	A	472	ARG
1	A	477	ARG
1	A	511	GLU
1	A	515	SER
1	A	520	LEU
1	A	525	HIS
1	A	527	ILE
1	A	544	ARG

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Mol	Chain	Res	Type
1	A	549	ASN
1	A	550	GLN
1	A	554	GLN
1	A	570	GLU
1	A	574	LEU
1	A	575	LEU
1	A	591	LYS
1	A	610	LEU
1	A	619	GLN
1	A	626	LEU
1	A	638	GLU
1	A	647	LYS
1	A	650	SER
1	A	662	GLN
1	A	682	LEU
1	A	701	SER
1	A	717	LEU
1	A	728	MET
1	A	731	ASP
1	A	749	ILE
1	A	756	LYS
1	A	760	SER
1	A	761	SER
1	A	764	ILE
1	A	766	GLN
1	A	767	LEU
1	A	770	LYS
1	A	778	GLN
1	A	779	LEU
1	A	782	SER
1	A	792	LYS
1	A	819	ASP
1	A	823	LEU
1	A	833	LYS
1	A	838	LEU
1	A	843	LEU
1	A	845	LEU
1	A	848	LEU
1	A	865	LEU
1	A	871	SER
1	A	875	LYS
1	A	883	LYS

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Mol	Chain	Res	Type
1	A	887	THR
1	A	888	ILE
1	A	895	THR
1	A	899	THR
1	A	907	LEU
1	A	926	GLU
1	A	939	THR
1	A	946	ASP
1	A	982	ARG
1	A	988	THR
1	A	1001	LYS
1	A	1002	THR
1	A	1008	LYS
1	A	1026	LEU
1	A	1029	ILE
1	A	1032	SER
1	A	1042	LEU
1	A	1043	THR
1	A	1044	SER
1	A	1046	GLU
1	A	1048	ILE
1	A	1049	GLU
1	A	1052	ARG
1	A	1053	ASP
1	A	1087	PHE
1	A	1088	LEU
1	A	1089	HIS

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

Mol	Chain	Res	Type
1	A	218	ASN
1	A	231	GLN
1	A	391	GLN
1	A	483	HIS
1	A	601	GLN
1	A	609	GLN
1	A	646	GLN
1	A	734	GLN
1	A	743	GLN
1	A	766	GLN
1	A	778	GLN

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Mol	Chain	Res	Type
1	A	825	ASN
1	A	908	ASN
1	A	959	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 carbohydrates 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	GD9	A	1	-	37,40,40	2.04	12 (32%)	43,59,59	2.57	15 (34%)

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	GD9	A	1	-	-	2/17/36/36	0/6/6/6

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	GD9	S2-N5	7.10	1.72	1.63
2	A	1	GD9	C8-C3	-3.59	1.39	1.48
2	A	1	GD9	C11-N5	-2.95	1.44	1.47
2	A	1	GD9	C5-S1	-2.92	1.68	1.74
2	A	1	GD9	C13-S2	2.91	1.82	1.75
2	A	1	GD9	C22-C21	-2.87	1.34	1.42
2	A	1	GD9	C4-N2	2.84	1.36	1.32
2	A	1	GD9	N7-N6	2.72	1.43	1.37
2	A	1	GD9	O2-S2	2.57	1.47	1.43
2	A	1	GD9	O1-S2	2.50	1.47	1.43
2	A	1	GD9	C2-N1	-2.35	1.33	1.37
2	A	1	GD9	C8-C22	-2.33	1.37	1.42

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	GD9	C11-N5-S2	-7.76	106.75	116.30
2	A	1	GD9	N1-C3-N2	-6.35	121.12	126.11
2	A	1	GD9	O1-S2-O2	-5.86	110.24	118.59
2	A	1	GD9	C12-C11-N5	-5.48	104.72	108.91
2	A	1	GD9	C11-C12-N4	-4.31	101.81	110.64
2	A	1	GD9	O1-S2-N5	3.73	110.17	107.03
2	A	1	GD9	C8-C3-N2	3.20	122.67	117.46
2	A	1	GD9	C10-N5-S2	-2.96	112.67	116.30
2	A	1	GD9	C3-N1-C2	2.75	118.37	116.50
2	A	1	GD9	C4-N2-C3	2.55	122.14	116.17
2	A	1	GD9	C1-C4-N2	-2.48	116.37	122.60
2	A	1	GD9	C16-C17-N3	-2.41	105.58	110.02
2	A	1	GD9	O2-S2-C13	2.39	111.65	108.44
2	A	1	GD9	C3-C8-C22	-2.18	120.91	123.46
2	A	1	GD9	C17-N3-C14	2.08	116.11	111.52

There are no chirality outliers.

All (2) torsion outliers are listed below:

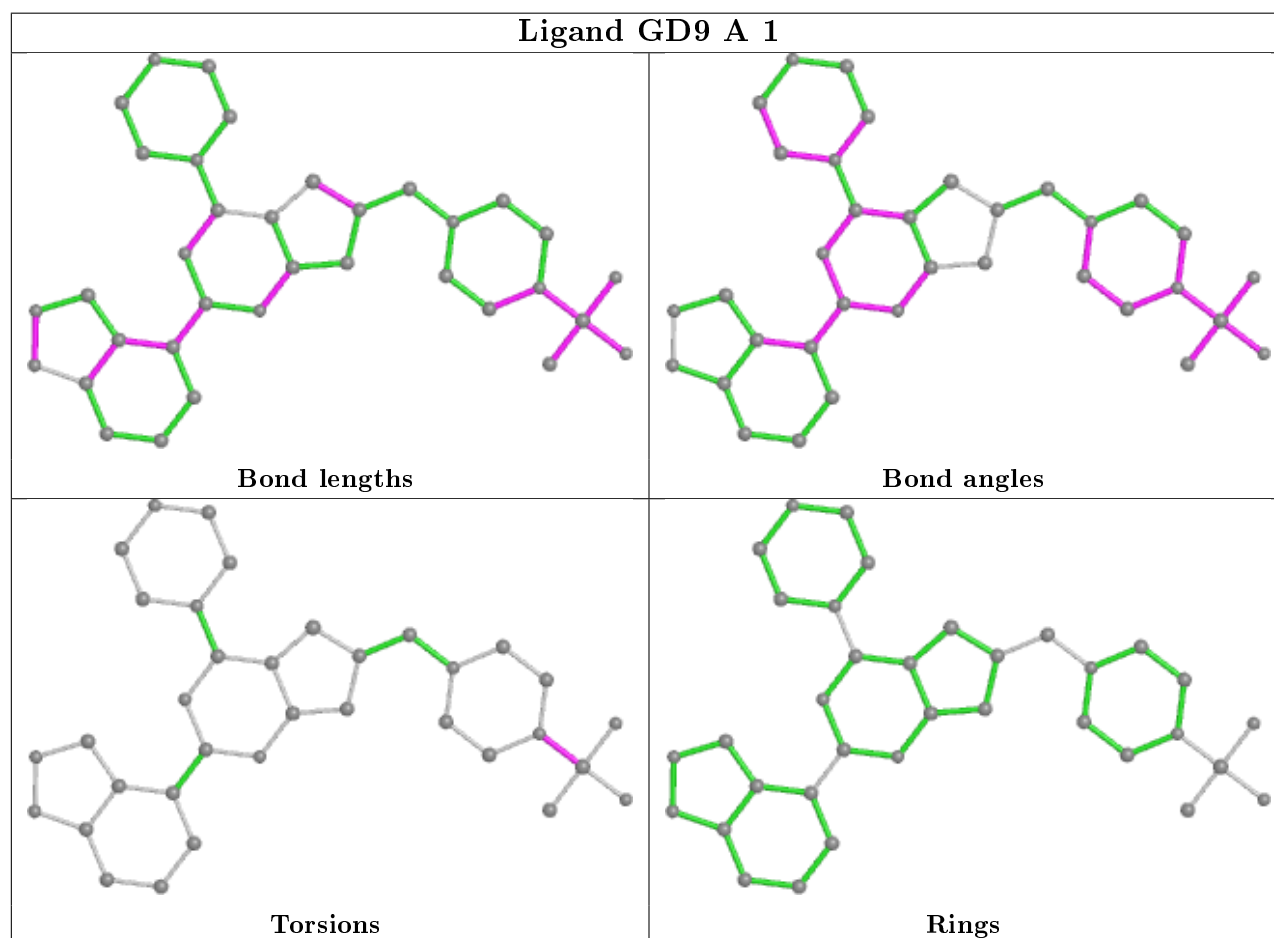
Mol	Chain	Res	Type	Atoms
2	A	1	GD9	C11-N5-S2-C13
2	A	1	GD9	C11-N5-S2-O2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	GD9	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 ⓘ

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	841/960 (87%)	0.27	60 (7%) 16 9	31, 48, 62, 88	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	376	ASN	11.8
1	A	528	ALA	9.8
1	A	1044	SER	9.4
1	A	377	THR	6.0
1	A	896	VAL	5.8
1	A	143	MET	5.4
1	A	374	PRO	5.0
1	A	907	LEU	4.9
1	A	221	PHE	4.6
1	A	220	ILE	4.5
1	A	212	TRP	4.4
1	A	899	THR	4.3
1	A	1088	LEU	4.0
1	A	375	ARG	4.0
1	A	527	ILE	3.8
1	A	222	ILE	3.7
1	A	998	SER	3.5
1	A	895	THR	3.5
1	A	253	ALA	3.4
1	A	544	ARG	3.4
1	A	766	GLN	3.3
1	A	1089	HIS	3.3
1	A	1091	VAL	3.3
1	A	378	ASP	3.3
1	A	234	LYS	3.2
1	A	373	LEU	3.2
1	A	320	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	987	LEU	3.1
1	A	248	PHE	3.1
1	A	900	GLY	3.0
1	A	281	LEU	3.0
1	A	988	THR	2.8
1	A	489	GLY	2.8
1	A	303	ILE	2.7
1	A	1068	PHE	2.7
1	A	948	HIS	2.7
1	A	404	PHE	2.7
1	A	232	THR	2.6
1	A	1043	THR	2.6
1	A	272	LEU	2.6
1	A	1045	LYS	2.6
1	A	995	MET	2.5
1	A	267	GLU	2.5
1	A	991	PHE	2.3
1	A	898	ASN	2.3
1	A	823	LEU	2.3
1	A	990	ASP	2.3
1	A	233	ILE	2.3
1	A	550	GLN	2.2
1	A	1041	GLN	2.2
1	A	282	VAL	2.2
1	A	251	LYS	2.2
1	A	216	ALA	2.2
1	A	215	ILE	2.1
1	A	989	PRO	2.1
1	A	994	VAL	2.1
1	A	1086	TRP	2.1
1	A	321	GLU	2.0
1	A	902	PHE	2.0
1	A	778	GLN	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

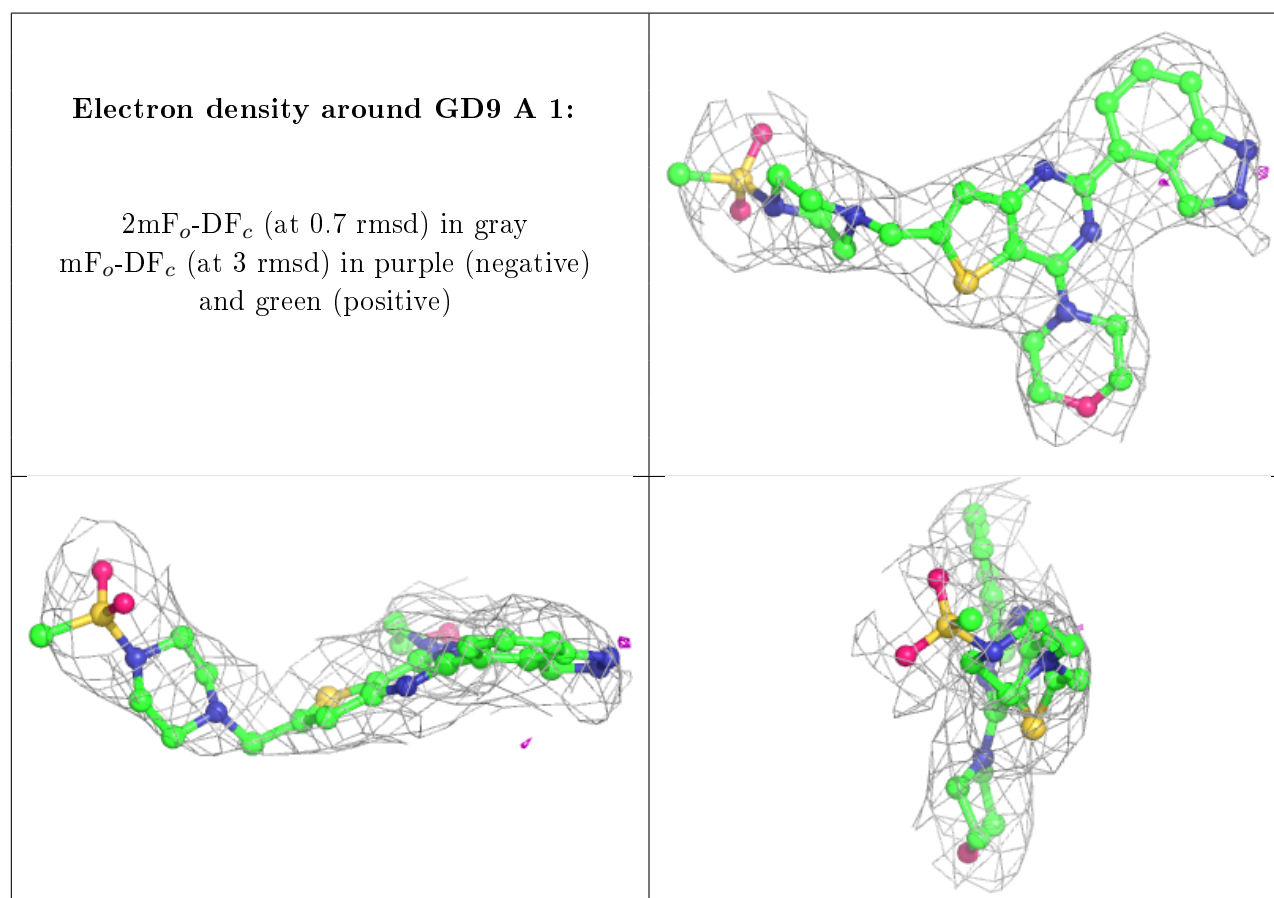
There are no carbohydrates in this entry.

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	GD9	A	1	35/35	0.95	0.15	86,91,95,97	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.