



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 04:46 pm BST

PDB ID : 2V4L
Title : complex of human phosphoinositide 3-kinase catalytic subunit gamma (p110 gamma) with PIK-284
Authors : Apsel, B.; Gonzalez, B.; Blair, J.A.; Nazif, T.M.; Feldman, M.E.; Williams, R.L.; Shokat, K.M.; Knight, Z.A.
Deposited on : 2008-09-25
Resolution : 2.50 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 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

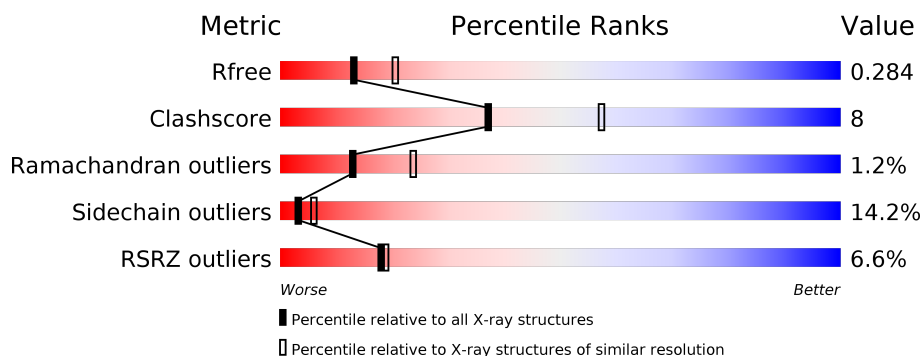
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 ≥ 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	<div> <div>6%</div> <div>63%</div> <div>19%</div> <div>5%</div> <div>13%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6920 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.

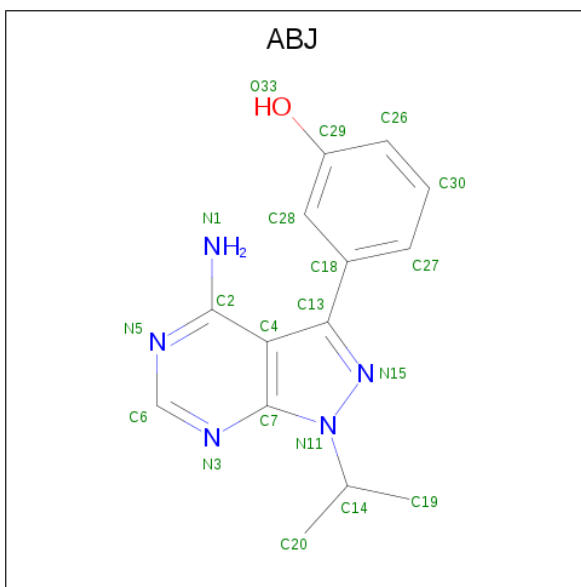
- Molecule 1 is a protein called PHOSPHATIDYLINOSITOL-4,5-BISPHOSPHATE 3-KINASE CATALYTIC SUBUNIT GAMMA ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	845	Total	C	N	O	S	0	0	1
			6850	4397	1173	1245	35			

There are 8 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
A	459	ARG	GLN	conflict	UNP P48736

- Molecule 2 is 3-[4-AMINO-1-(1-METHYLETHYL)-1H-PYRAZOLO[3,4-D]PYRIMIDIN-3-YL]PHENOL (three-letter code: ABJ) (formula: C₁₄H₁₅N₅O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			20	14	5	1		

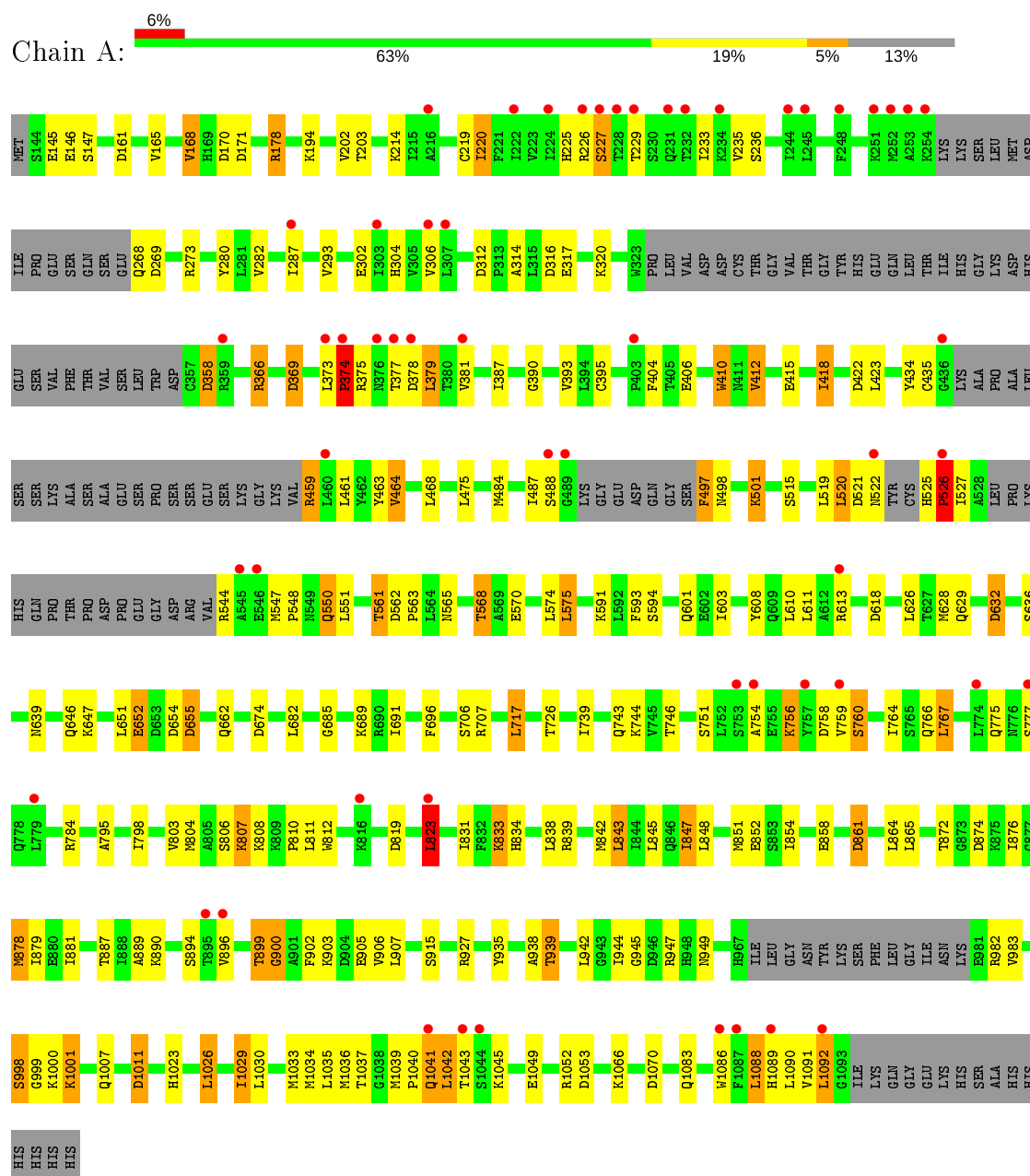
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	50	Total	O	0	0
			50	50		

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, α , β , γ	144.35Å 68.44Å 106.62Å 90.00° 95.33° 90.00°	Depositor
Resolution (Å)	54.39 – 2.50 54.36 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.2 (54.39-2.50) 97.2 (54.36-2.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.50 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.248 , 0.296 0.234 , 0.284	Depositor DCC
R_{free} test set	1440 reflections (4.10%)	wwPDB-VP
Wilson B-factor (Å ²)	50.3	Xtriage
Anisotropy	0.360	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.5	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	0.93	EDS
Total number of atoms	6920	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.68% 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: ABJ

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	0.66	3/6998 (0.0%)	0.85	21/9466 (0.2%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	900	GLY	C-O	6.99	1.34	1.23
1	A	760	SER	CB-OG	5.70	1.49	1.42
1	A	1092	LEU	C-N	-5.36	1.23	1.33

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1092	LEU	O-C-N	-12.00	102.81	123.20
1	A	861	ASP	CB-CG-OD2	7.39	124.95	118.30
1	A	632	ASP	CB-CG-OD1	7.37	124.94	118.30
1	A	1070	ASP	CB-CG-OD2	7.27	124.84	118.30
1	A	655	ASP	CB-CG-OD2	6.88	124.49	118.30
1	A	874	ASP	CB-CG-OD2	6.22	123.90	118.30
1	A	575	LEU	CA-CB-CG	5.67	128.35	115.30
1	A	758	ASP	CB-CG-OD2	5.63	123.37	118.30
1	A	171	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	520	LEU	CA-CB-CG	5.57	128.10	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	526	PRO	N-CA-C	5.51	126.44	112.10
1	A	674	ASP	CB-CG-OD1	5.46	123.22	118.30
1	A	819	ASP	CB-CG-OD2	5.46	123.22	118.30
1	A	1092	LEU	CA-C-N	5.46	127.12	116.20
1	A	521	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	823	LEU	CA-CB-CG	5.38	127.67	115.30
1	A	358	ASP	CB-CG-OD2	5.34	123.10	118.30
1	A	1053	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	161	ASP	CB-CG-OD2	5.24	123.02	118.30
1	A	422	ASP	CB-CG-OD2	5.04	122.83	118.30
1	A	618	ASP	CB-CG-OD2	5.02	122.82	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	526	PRO	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	6850	0	6890	106	1
2	A	20	0	14	1	0
3	A	50	0	0	2	0
All	All	6920	0	6904	107	1

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 8.

All (107) 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:525:HIS:HB3	1:A:526:PRO:HD3	1.09	1.07
1:A:525:HIS:HB3	1:A:526:PRO:CD	1.91	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:VAL:HG22	1:A:435:CYS:SG	2.06	0.95
1:A:525:HIS:CB	1:A:526:PRO:HD3	2.02	0.88
1:A:1086:TRP:CH2	1:A:1090:LEU:HD11	2.12	0.83
1:A:652:GLU:OE1	1:A:654:ASP:HB3	1.80	0.81
1:A:935:TYR:O	1:A:939:THR:HB	1.87	0.75
1:A:395:CYS:HB3	1:A:418:ILE:HD11	1.70	0.74
1:A:1089:HIS:O	1:A:1092:LEU:N	2.21	0.73
1:A:662:GLN:HG2	3:A:2049:HOH:O	1.89	0.73
1:A:775:GLN:HE22	1:A:795:ALA:HB1	1.55	0.72
1:A:949:ASN:H	1:A:1083:GLN:HE22	1.35	0.71
1:A:316:ASP:OD1	1:A:689:LYS:NZ	2.22	0.69
1:A:381:VAL:CG2	1:A:435:CYS:SG	2.80	0.68
1:A:168:VAL:HG13	1:A:170:ASP:O	1.95	0.66
1:A:899:THR:CG2	1:A:899:THR:O	2.44	0.65
1:A:410:TRP:HB3	1:A:412:VAL:HG23	1.78	0.65
1:A:743:GLN:NE2	1:A:872:THR:OG1	2.30	0.65
1:A:851:MET:HE1	1:A:938:ALA:HB1	1.79	0.64
1:A:1042:LEU:HD13	1:A:1042:LEU:H	1.62	0.64
1:A:1089:HIS:HA	1:A:1092:LEU:HB2	1.80	0.64
1:A:464:VAL:HB	1:A:484:MET:HG2	1.80	0.62
1:A:629:GLN:HG2	1:A:1029:ILE:HG13	1.83	0.60
1:A:317:GLU:O	1:A:726:THR:HG23	2.02	0.59
1:A:899:THR:HG22	1:A:899:THR:O	2.03	0.59
1:A:561:THR:HG21	1:A:565:ASN:HD22	1.69	0.58
1:A:775:GLN:NE2	1:A:795:ALA:HB1	2.18	0.58
1:A:548:PRO:CG	1:A:551:LEU:HD12	2.35	0.57
1:A:497:PHE:O	1:A:1042:LEU:HD13	2.04	0.56
1:A:165:VAL:HG12	1:A:165:VAL:O	2.05	0.56
1:A:593:PHE:CZ	1:A:611:LEU:HD21	2.40	0.56
1:A:498:ASN:C	1:A:498:ASN:OD1	2.45	0.55
1:A:1041:GLN:HA	1:A:1041:GLN:NE2	2.21	0.54
1:A:525:HIS:CB	1:A:526:PRO:CD	2.70	0.54
1:A:373:LEU:O	1:A:374:PRO:O	2.26	0.54
1:A:226:ARG:O	1:A:227:SER:C	2.46	0.54
1:A:1088:LEU:O	1:A:1091:VAL:HG22	2.08	0.53
1:A:939:THR:HG23	1:A:945:GLY:HA2	1.91	0.53
1:A:395:CYS:CB	1:A:418:ILE:HD11	2.39	0.53
1:A:939:THR:HG23	1:A:945:GLY:CA	2.39	0.53
1:A:823:LEU:H	1:A:823:LEU:HD12	1.75	0.52
1:A:854:ILE:HG23	1:A:1023:HIS:CD2	2.45	0.52
1:A:812:TRP:CE2	1:A:881:ILE:HD13	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:PHE:HB3	1:A:1041:GLN:NE2	2.25	0.50
1:A:608:TYR:CZ	1:A:639:ASN:ND2	2.77	0.50
1:A:628:MET:HB2	1:A:1029:ILE:HG21	1.93	0.50
1:A:562:ASP:HB2	1:A:563:PRO:CD	2.41	0.50
1:A:807:LYS:HZ2	1:A:807:LYS:H	1.60	0.49
1:A:848:LEU:HA	1:A:851:MET:HE2	1.94	0.49
1:A:834:HIS:HB2	1:A:876:ILE:HD12	1.93	0.49
1:A:561:THR:HG22	1:A:591:LYS:NZ	2.28	0.49
1:A:685:GLY:HA2	1:A:691:ILE:HG22	1.96	0.48
1:A:1026:LEU:O	1:A:1030:LEU:HG	2.13	0.48
1:A:393:VAL:O	1:A:393:VAL:HG23	2.12	0.48
1:A:168:VAL:CG1	1:A:170:ASP:O	2.62	0.48
1:A:852:GLU:HG3	1:A:864:LEU:HD12	1.95	0.47
1:A:759:VAL:HG12	1:A:764:ILE:HD11	1.96	0.47
1:A:369:ASP:OD1	1:A:369:ASP:N	2.47	0.47
1:A:381:VAL:HG23	1:A:404:PHE:HB2	1.97	0.47
1:A:651:LEU:HD22	1:A:655:ASP:HB3	1.98	0.46
1:A:1033:MET:O	1:A:1037:THR:HG23	2.15	0.46
1:A:312:ASP:OD2	1:A:314:ALA:HB3	2.15	0.46
1:A:810:PRO:HB3	1:A:833:LYS:HB3	1.98	0.46
1:A:1042:LEU:CD1	1:A:1042:LEU:H	2.27	0.45
1:A:1036:MET:HA	1:A:1042:LEU:HD11	1.98	0.45
1:A:390:GLY:N	1:A:636:SER:OG	2.49	0.45
1:A:804:MET:HE2	1:A:831:ILE:HG12	1.99	0.45
1:A:463:TYR:CE1	1:A:501:LYS:HA	2.51	0.45
1:A:902:PHE:N	3:A:2034:HOH:O	2.49	0.45
1:A:998:SER:O	1:A:1001:LYS:NZ	2.49	0.45
1:A:1035:LEU:HB3	1:A:1042:LEU:HG	1.97	0.45
1:A:220:ILE:N	1:A:235:VAL:O	2.48	0.44
1:A:804:MET:HE1	1:A:810:PRO:HB2	1.98	0.44
1:A:165:VAL:CG1	1:A:165:VAL:O	2.65	0.44
1:A:287:ILE:HG23	1:A:293:VAL:HG21	1.98	0.44
1:A:746:THR:HG23	1:A:811:LEU:HD13	1.99	0.44
1:A:847:ILE:HG21	1:A:942:LEU:HD21	1.99	0.44
1:A:434:TYR:HA	1:A:459:ARG:O	2.16	0.44
1:A:1011:ASP:OD1	1:A:1011:ASP:C	2.56	0.44
1:A:839:ARG:HA	1:A:842:MET:CE	2.48	0.44
1:A:568:THR:HG22	1:A:570:GLU:N	2.33	0.43
1:A:839:ARG:HA	1:A:842:MET:HE2	2.00	0.43
1:A:548:PRO:HG3	1:A:551:LEU:HD12	2.01	0.43
1:A:861:ASP:C	1:A:861:ASP:OD1	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:887:THR:HG22	1:A:889:ALA:N	2.34	0.43
1:A:273:ARG:HB2	1:A:280:TYR:CE2	2.54	0.43
1:A:225:HIS:CE1	1:A:304:HIS:HD2	2.37	0.42
1:A:423:LEU:HD22	1:A:468:LEU:CD1	2.48	0.42
1:A:811:LEU:HD12	1:A:811:LEU:N	2.34	0.42
1:A:944:ILE:O	1:A:947:ARG:HD3	2.19	0.42
1:A:1091:VAL:O	1:A:1091:VAL:HG23	2.20	0.42
1:A:366:ARG:HH12	1:A:519:LEU:HD22	1.84	0.42
2:A:2093:ABJ:H12N	2:A:2093:ABJ:C27	2.32	0.42
1:A:878:MET:C	1:A:879:ILE:HG13	2.40	0.41
1:A:804:MET:HE1	1:A:831:ILE:HG23	2.02	0.41
1:A:767:LEU:HD12	1:A:803:VAL:HG23	2.01	0.41
1:A:233:ILE:HG22	1:A:235:VAL:HG23	2.03	0.41
1:A:178:ARG:NH1	1:A:178:ARG:HG3	2.35	0.41
1:A:435:CYS:SG	1:A:461:LEU:HD12	2.61	0.41
1:A:475:LEU:HD21	1:A:522:ASN:CB	2.51	0.41
1:A:843:LEU:HG	1:A:1034:MET:HG3	2.03	0.40
1:A:381:VAL:HG21	1:A:404:PHE:CG	2.56	0.40
1:A:804:MET:CE	1:A:810:PRO:HB2	2.49	0.40
1:A:903:LYS:HD3	1:A:906:VAL:CG2	2.52	0.40
1:A:900:GLY:O	1:A:902:PHE:CD1	2.74	0.40
1:A:302:GLU:OE1	1:A:304:HIS:HE1	2.05	0.40
1:A:696:PHE:CD1	1:A:717:LEU:HD21	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:GLN:NE2	1:A:570:GLU:OE1[2_555]	2.09	0.11

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	829/966 (86%)	770 (93%)	49 (6%)	10 (1%)	13	24

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	227	SER
1	A	374	PRO
1	A	527	ILE
1	A	999	GLY
1	A	378	ASP
1	A	379	LEU
1	A	1040	PRO
1	A	754	ALA
1	A	756	LYS
1	A	1000	LYS

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	758/864 (88%)	650 (86%)	108 (14%)	3	6

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145	GLU
1	A	146	GLU
1	A	147	SER
1	A	168	VAL
1	A	178	ARG
1	A	194	LYS
1	A	202	VAL
1	A	203	THR
1	A	214	LYS
1	A	219	CYS
1	A	220	ILE

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Mol	Chain	Res	Type
1	A	229	THR
1	A	236	SER
1	A	268	GLN
1	A	269	ASP
1	A	282	VAL
1	A	306	VAL
1	A	320	LYS
1	A	358	ASP
1	A	366	ARG
1	A	369	ASP
1	A	374	PRO
1	A	375	ARG
1	A	377	THR
1	A	379	LEU
1	A	387	ILE
1	A	406	GLU
1	A	410	TRP
1	A	412	VAL
1	A	415	GLU
1	A	418	ILE
1	A	459	ARG
1	A	464	VAL
1	A	487	ILE
1	A	488	SER
1	A	497	PHE
1	A	501	LYS
1	A	515	SER
1	A	520	LEU
1	A	544	ARG
1	A	547	MET
1	A	550	GLN
1	A	561	THR
1	A	568	THR
1	A	574	LEU
1	A	575	LEU
1	A	594	SER
1	A	601	GLN
1	A	603	ILE
1	A	610	LEU
1	A	613	ARG
1	A	626	LEU
1	A	632	ASP

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Mol	Chain	Res	Type
1	A	646	GLN
1	A	647	LYS
1	A	652	GLU
1	A	682	LEU
1	A	706	SER
1	A	707	ARG
1	A	717	LEU
1	A	739	ILE
1	A	744	LYS
1	A	751	SER
1	A	756	LYS
1	A	760	SER
1	A	766	GLN
1	A	767	LEU
1	A	777	SER
1	A	784	ARG
1	A	798	ILE
1	A	806	SER
1	A	807	LYS
1	A	808	LYS
1	A	823	LEU
1	A	833	LYS
1	A	838	LEU
1	A	843	LEU
1	A	845	LEU
1	A	847	ILE
1	A	858	GLU
1	A	865	LEU
1	A	878	MET
1	A	890	LYS
1	A	894	SER
1	A	896	VAL
1	A	899	THR
1	A	905	GLU
1	A	907	LEU
1	A	915	SER
1	A	927	ARG
1	A	939	THR
1	A	982	ARG
1	A	983	VAL
1	A	998	SER
1	A	1001	LYS

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Mol	Chain	Res	Type
1	A	1007	GLN
1	A	1011	ASP
1	A	1026	LEU
1	A	1029	ILE
1	A	1039	MET
1	A	1041	GLN
1	A	1042	LEU
1	A	1043	THR
1	A	1045	LYS
1	A	1049	GLU
1	A	1052	ARG
1	A	1066	LYS
1	A	1088	LEU

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

Mol	Chain	Res	Type
1	A	231	GLN
1	A	268	GLN
1	A	304	HIS
1	A	389	HIS
1	A	486	GLN
1	A	554	GLN
1	A	565	ASN
1	A	705	GLN
1	A	743	GLN
1	A	766	GLN
1	A	778	GLN
1	A	834	HIS
1	A	898	ASN
1	A	959	ASN
1	A	1023	HIS
1	A	1041	GLN
1	A	1083	GLN

5.3.3 RNA ⓘ

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	ABJ	A	2093	-	20,22,22	2.96	2 (10%)	20,32,32	2.29	3 (15%)

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	ABJ	A	2093	-	-	2/8/8/8	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2093	ABJ	N15-N11	-11.17	1.23	1.37
2	A	2093	ABJ	C18-C13	-6.53	1.40	1.49

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2093	ABJ	C13-N15-N11	7.78	111.38	105.17
2	A	2093	ABJ	N3-C6-N5	-4.91	121.01	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2093	ABJ	C18-C13-N15	2.67	125.35	120.78

There are no chirality outliers.

All (2) torsion outliers are listed below:

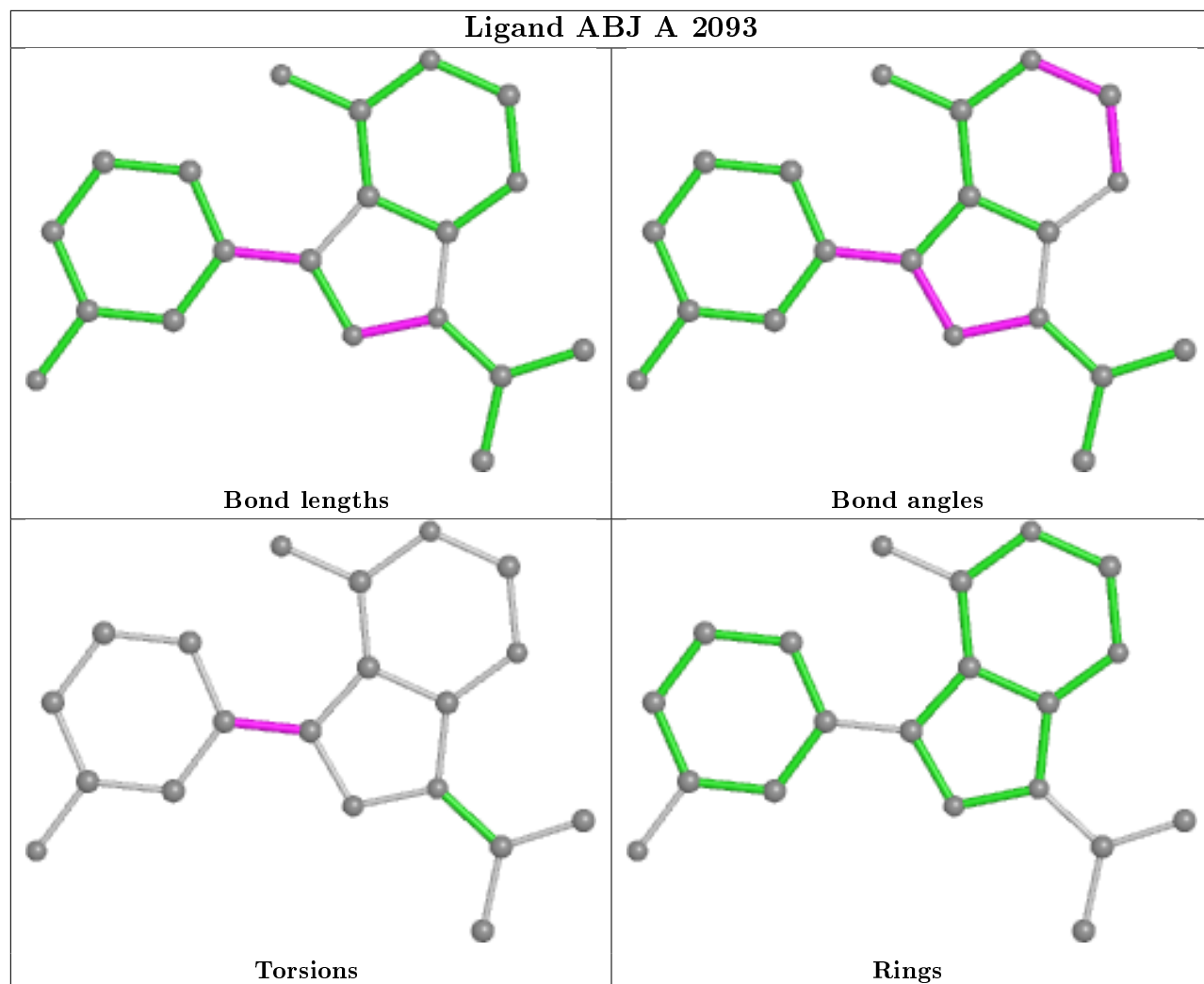
Mol	Chain	Res	Type	Atoms
2	A	2093	ABJ	N15-C13-C18-C27
2	A	2093	ABJ	N15-C13-C18-C28

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2093	ABJ	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 [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	845/966 (87%)	0.34	56 (6%) 18 19	12, 21, 28, 55	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1044	SER	8.7
1	A	1092	LEU	6.0
1	A	254	LYS	5.9
1	A	376	ASN	5.3
1	A	526	PRO	5.1
1	A	248	PHE	4.7
1	A	216	ALA	4.3
1	A	1043	THR	4.1
1	A	779	LEU	4.0
1	A	436	GLY	4.0
1	A	374	PRO	3.8
1	A	307	LEU	3.8
1	A	252	MET	3.7
1	A	754	ALA	3.6
1	A	895	THR	3.5
1	A	373	LEU	3.4
1	A	378	ASP	3.3
1	A	757	TYR	3.2
1	A	522	ASN	3.2
1	A	234	LYS	3.2
1	A	777	SER	3.0
1	A	545	ALA	2.9
1	A	613	ARG	2.9
1	A	306	VAL	2.9
1	A	228	THR	2.8
1	A	1089	HIS	2.8
1	A	253	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	381	VAL	2.8
1	A	227	SER	2.8
1	A	823	LEU	2.6
1	A	231	GLN	2.6
1	A	774	LEU	2.6
1	A	1041	GLN	2.6
1	A	251	LYS	2.6
1	A	1086	TRP	2.6
1	A	489	GLY	2.5
1	A	303	ILE	2.5
1	A	377	THR	2.5
1	A	753	SER	2.4
1	A	546	GLU	2.3
1	A	229	THR	2.3
1	A	403	PRO	2.3
1	A	245	LEU	2.3
1	A	287	ILE	2.3
1	A	226	ARG	2.3
1	A	359	ARG	2.3
1	A	222	ILE	2.3
1	A	1087	PHE	2.2
1	A	244	ILE	2.1
1	A	816	LYS	2.1
1	A	759	VAL	2.1
1	A	488	SER	2.1
1	A	232	THR	2.0
1	A	896	VAL	2.0
1	A	224	ILE	2.0
1	A	460	LEU	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 ⓘ

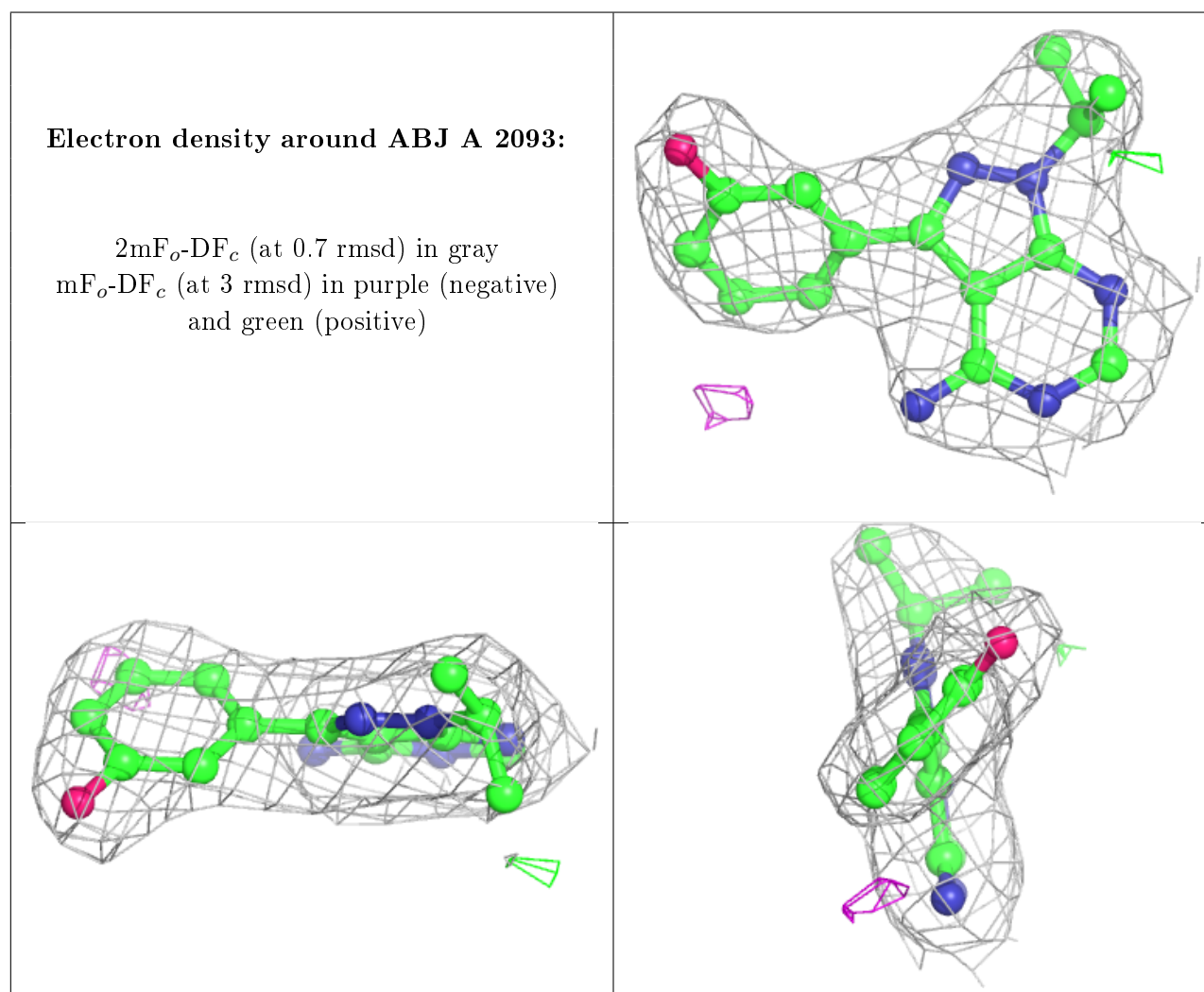
There are no carbohydrates in this entry.

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, 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(\AA^2)	Q<0.9
2	ABJ	A	2093	20/20	0.96	0.12	44,46,47,48	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.