



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:58 PM UTC

PDB ID : 2CHZ / pdb_00002chz
Title : A pharmacological map of the PI3-K family defines a role for p110alpha in signaling: The structure of complex of phosphoinositide 3-kinase gamma with inhibitor PIK-93
Authors : Knight, Z.A.; Gonzalez, B.; Feldman, M.E.; Zunder, E.R.; Goldenberg, D.D.; Williams, O.; Loewith, R.; Stokoe, D.; Balla, A.; Toth, B.; Balla, T.; Weiss, W.A.; Williams, R.L.; Shokat, K.M.
Deposited on : 2006-03-16
Resolution : 2.60 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)

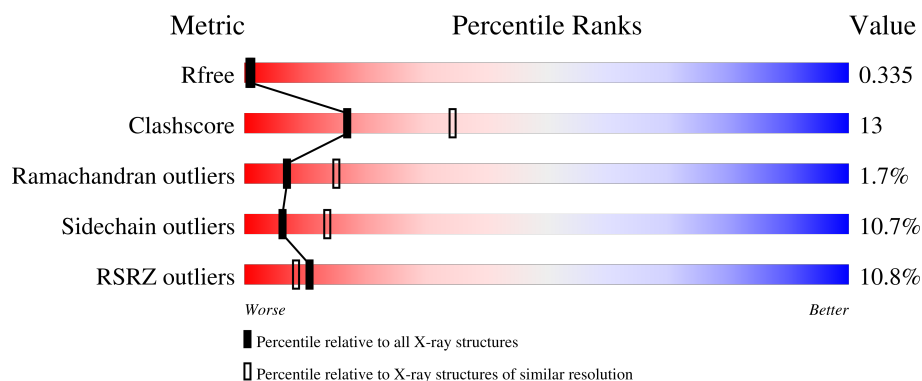
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	9% 59% 23% 5% 13%

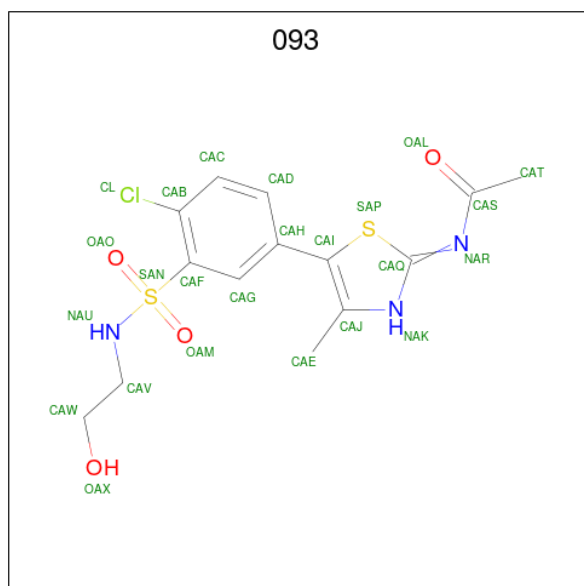
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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.

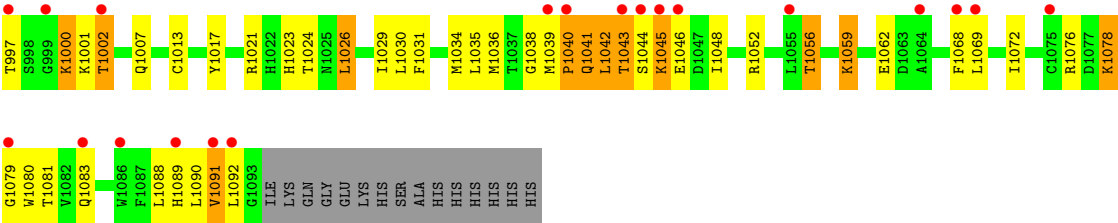
- Molecule 1 is a protein called PHOSPHATIDYLINOSITOL-4,5-BISPHOSPHATE 3-KINASE CATALYTIC SUBUNIT GAMMA ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	840	Total	C	N	O	S	0	0	1
			6802	4367	1163	1237	35			

- Molecule 2 is N-(5-(4-CHLORO-3-(2-HYDROXY-ETHYLSULFAMOYL)- PHENYLTHIA ZOLE-2-YL)-ACETAMIDE (CCD ID: 093) (formula: $C_{14}H_{16}ClN_3O_4S_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	S	0	0
			24	14	1	3	4	2		



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	144.03Å 68.11Å 106.35Å 90.00° 95.21° 90.00°	Depositor
Resolution (Å)	71.80 – 2.60 71.80 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (71.80-2.60) 99.7 (71.80-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 2.62Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.244 , 0.302 0.280 , 0.335	Depositor DCC
R_{free} test set	1306 reflections (4.10%)	wwPDB-VP
Wilson B-factor (Å ²)	60.9	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 32.7	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	0.91	EDS
Total number of atoms	6826	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.31% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 093

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	10/6947 (0.1%)	0.87	4/9395 (0.0%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	489	GLY	C-O	20.56	1.64	1.23
1	A	402	LYS	CG-CD	10.45	1.83	1.52
1	A	411	ASN	CG-ND2	10.16	1.54	1.33
1	A	402	LYS	CE-NZ	7.46	1.71	1.49
1	A	366	ARG	CZ-NH1	6.78	1.42	1.32
1	A	489	GLY	CA-C	6.26	1.63	1.52
1	A	1092	LEU	C-N	-6.15	1.24	1.33
1	A	410	TRP	NE1-CE2	5.89	1.44	1.37
1	A	364	LYS	CE-NZ	5.63	1.66	1.49
1	A	366	ARG	CD-NE	5.32	1.53	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	489	GLY	CA-C-O	-7.71	104.62	120.80
1	A	366	ARG	NE-CZ-NH2	7.26	125.74	119.20
1	A	527	ILE	N-CA-C	5.94	116.73	108.89
1	A	402	LYS	CB-CG-CD	-5.22	99.29	111.30

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	6802	0	6845	170	0
2	A	24	0	16	4	0
All	All	6826	0	6861	174	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 13.

All (174) 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:402:LYS:CD	1:A:402:LYS:CG	1.83	1.54
1:A:402:LYS:CE	1:A:402:LYS:NZ	1.71	1.54
1:A:489:GLY:C	1:A:489:GLY:O	1.64	1.37
2:A:2093:093:HAD	2:A:2093:093:HAE1	1.44	1.00
1:A:935:TYR:O	1:A:939:THR:HB	1.62	0.98
1:A:558:ILE:O	1:A:561:THR:HG22	1.74	0.87
1:A:410:TRP:HB3	1:A:412:VAL:HG23	1.60	0.83
1:A:804:MET:HE1	1:A:831:ILE:HG12	1.64	0.80
1:A:402:LYS:CD	1:A:402:LYS:CB	2.59	0.79
2:A:2093:093:HAD	2:A:2093:093:CAE	2.12	0.79
1:A:724:CYS:HB2	1:A:728:MET:HE3	1.65	0.78
1:A:949:ASN:H	1:A:1083:GLN:HE22	1.33	0.77
1:A:568:THR:HG22	1:A:570:GLU:H	1.51	0.76
1:A:1078:LYS:HB3	1:A:1081:THR:HB	1.69	0.74
1:A:402:LYS:CG	1:A:402:LYS:CE	2.66	0.73
1:A:629:GLN:HG2	1:A:1029:ILE:HG13	1.73	0.69
1:A:834:HIS:HB2	1:A:876:ILE:HD12	1.71	0.69
1:A:225:HIS:HE1	1:A:304:HIS:HD2	1.40	0.69
1:A:887:THR:HG22	1:A:890:LYS:H	1.57	0.69
1:A:808:LYS:HG3	1:A:833:LYS:HE2	1.74	0.69
1:A:629:GLN:CG	1:A:1029:ILE:HG13	2.25	0.66
1:A:387:ILE:HD12	1:A:418:ILE:HD13	1.79	0.65
1:A:743:GLN:NE2	1:A:876:ILE:HG23	2.12	0.64
1:A:225:HIS:CE1	1:A:304:HIS:HD2	2.15	0.64
1:A:1056:THR:O	1:A:1056:THR:HG23	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:997:THR:HG23	1:A:1001:LYS:HG3	1.80	0.63
1:A:552:ARG:HH11	1:A:552:ARG:HB2	1.63	0.63
1:A:1039:MET:HB3	1:A:1040:PRO:HD2	1.82	0.61
1:A:1001:LYS:H	1:A:1076:ARG:HH22	1.50	0.60
1:A:896:VAL:HG21	1:A:903:LYS:HB2	1.83	0.60
1:A:847:ILE:HG22	1:A:851:MET:HE2	1.85	0.59
1:A:1021:ARG:HE	1:A:1056:THR:HG22	1.66	0.59
1:A:1044:SER:O	1:A:1045:LYS:HB3	2.02	0.59
1:A:272:LEU:HB3	1:A:305:VAL:HG11	1.85	0.59
1:A:317:GLU:O	1:A:726:THR:HG23	2.03	0.58
1:A:750:LYS:HE3	1:A:834:HIS:O	2.03	0.58
1:A:548:PRO:HG2	1:A:551:LEU:HD12	1.85	0.58
1:A:1069:LEU:HD23	1:A:1072:ILE:HD12	1.86	0.57
1:A:947:ARG:NH2	1:A:963:ILE:O	2.36	0.57
1:A:416:PHE:HB3	1:A:418:ILE:HD12	1.87	0.57
1:A:464:VAL:HB	1:A:484:MET:HG2	1.87	0.56
1:A:498:ASN:OD1	1:A:498:ASN:C	2.48	0.56
1:A:844:ILE:HD13	1:A:1034:MET:SD	2.46	0.56
1:A:428:LEU:HD22	1:A:465:ASN:HB3	1.88	0.56
1:A:1031:PHE:HE2	1:A:1048:ILE:HA	1.71	0.56
1:A:852:GLU:HG3	1:A:864:LEU:HD12	1.88	0.55
1:A:802:LYS:HG3	1:A:812:TRP:HB3	1.88	0.55
2:A:2093:093:HAE1	2:A:2093:093:CAD	2.28	0.55
1:A:552:ARG:HB2	1:A:552:ARG:NH1	2.22	0.55
1:A:652:GLU:OE1	1:A:654:ASP:HB3	2.07	0.54
1:A:1013:CYS:HB3	1:A:1068:PHE:HE2	1.71	0.54
1:A:939:THR:HG23	1:A:945:GLY:CA	2.38	0.54
1:A:1089:HIS:C	1:A:1091:VAL:H	2.16	0.54
1:A:181:VAL:O	1:A:185:MET:HG3	2.08	0.53
1:A:806:SER:O	1:A:808:LYS:O	2.26	0.53
1:A:620:SER:O	1:A:647:LYS:NZ	2.41	0.53
1:A:1013:CYS:HB3	1:A:1068:PHE:CE2	2.44	0.53
1:A:561:THR:HG23	1:A:591:LYS:NZ	2.23	0.53
1:A:357:CYS:SG	1:A:358:ASP:N	2.72	0.52
1:A:743:GLN:C	1:A:745:VAL:H	2.16	0.52
1:A:378:ASP:HB2	1:A:404:PHE:HB3	1.91	0.52
1:A:745:VAL:HG22	1:A:770:LYS:HE2	1.92	0.52
1:A:887:THR:CG2	1:A:950:ASP:HA	2.40	0.52
1:A:421:LYS:HE3	1:A:528:ALA:HB3	1.92	0.52
1:A:848:LEU:HD12	1:A:851:MET:CE	2.39	0.51
1:A:395:CYS:SG	1:A:417:SER:OG	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.92	0.51
1:A:1017:TYR:CE2	1:A:1021:ARG:HD2	2.45	0.51
1:A:1043:THR:HB	1:A:1046:GLU:HB2	1.93	0.51
1:A:466:LEU:HD11	1:A:476:ARG:HD3	1.93	0.51
2:A:2093:093:CAE	2:A:2093:093:CAD	2.88	0.51
1:A:702:GLU:OE1	1:A:839:ARG:NH1	2.45	0.50
1:A:525:HIS:CB	1:A:526:PRO:HD3	2.42	0.50
1:A:989:PRO:HA	1:A:992:LEU:HD12	1.93	0.50
1:A:1000:LYS:H	1:A:1076:ARG:NH1	2.10	0.49
1:A:373:LEU:N	1:A:374:PRO:HD2	2.26	0.49
1:A:569:ALA:O	1:A:573:GLU:HG3	2.12	0.49
1:A:561:THR:HG23	1:A:591:LYS:HZ1	1.78	0.49
1:A:220:ILE:N	1:A:235:VAL:O	2.43	0.49
1:A:402:LYS:CD	1:A:402:LYS:NZ	2.67	0.49
1:A:480:TYR:O	1:A:517:SER:HA	2.13	0.49
1:A:1078:LYS:O	1:A:1080:TRP:N	2.46	0.49
1:A:525:HIS:HB2	1:A:526:PRO:HD3	1.95	0.49
1:A:1078:LYS:HB3	1:A:1081:THR:CB	2.40	0.49
1:A:161:ASP:OD2	1:A:164:ASP:HB2	2.13	0.48
1:A:735:GLN:O	1:A:739:ILE:HG23	2.13	0.48
1:A:1041:GLN:HE21	1:A:1041:GLN:HA	1.78	0.48
1:A:158:ILE:HG12	1:A:717:LEU:HD13	1.95	0.48
1:A:145:GLU:HA	1:A:148:GLN:HE21	1.78	0.48
1:A:774:LEU:HA	1:A:778:GLN:OE1	2.13	0.48
1:A:939:THR:HG23	1:A:945:GLY:HA2	1.96	0.48
1:A:848:LEU:HD12	1:A:851:MET:HE3	1.95	0.48
1:A:375:ARG:NH1	1:A:376:ASN:HB2	2.28	0.48
1:A:845:LEU:HD23	1:A:869:CYS:HB3	1.95	0.48
1:A:641:ARG:HE	1:A:670:GLU:CD	2.22	0.47
1:A:660:LEU:O	1:A:664:VAL:HG23	2.13	0.47
1:A:568:THR:HG22	1:A:570:GLU:N	2.25	0.47
1:A:395:CYS:CB	1:A:418:ILE:HD11	2.44	0.47
1:A:922:GLN:HA	1:A:922:GLN:OE1	2.13	0.47
1:A:872:THR:OG1	1:A:877:GLY:HA2	2.13	0.47
1:A:198:MET:SD	1:A:282:VAL:HG11	2.54	0.47
1:A:653:ASP:CG	1:A:684:ARG:HH21	2.21	0.47
1:A:622:LEU:HD21	1:A:651:LEU:HG	1.97	0.47
1:A:184:ARG:HH21	1:A:321:GLU:CD	2.23	0.47
1:A:168:VAL:HG13	1:A:169:HIS:N	2.31	0.46
1:A:1059:LYS:HA	1:A:1059:LYS:HE3	1.97	0.46
1:A:629:GLN:HG2	1:A:1029:ILE:CG1	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:CYS:HG	1:A:417:SER:HG	1.42	0.46
1:A:839:ARG:HG2	1:A:842:MET:HE2	1.98	0.46
1:A:1035:LEU:HB3	1:A:1042:LEU:HG	1.98	0.46
1:A:1038:GLY:C	1:A:1039:MET:HE2	2.40	0.46
1:A:363:VAL:HG12	1:A:416:PHE:HE1	1.81	0.45
1:A:219:CYS:HA	1:A:235:VAL:O	2.17	0.45
1:A:1002:THR:HG22	1:A:1007:GLN:HG3	1.98	0.45
1:A:382:PHE:HE2	1:A:398:ARG:HH11	1.62	0.45
1:A:274:VAL:HG21	1:A:292:TRP:CD1	2.52	0.45
1:A:371:PRO:HG2	1:A:511:GLU:O	2.15	0.45
1:A:434:TYR:CE1	1:A:460:LEU:HB2	2.51	0.45
1:A:480:TYR:HB2	1:A:518:ILE:CG1	2.46	0.45
1:A:839:ARG:HA	1:A:842:MET:HE2	1.98	0.45
1:A:641:ARG:NE	1:A:670:GLU:OE1	2.40	0.45
1:A:737:GLN:O	1:A:741:MET:HG3	2.17	0.45
1:A:848:LEU:HA	1:A:851:MET:HE3	1.98	0.45
1:A:489:GLY:O	1:A:489:GLY:CA	2.59	0.44
1:A:241:PRO:HD2	1:A:285:THR:O	2.17	0.44
1:A:548:PRO:CG	1:A:551:LEU:HD12	2.46	0.44
1:A:601:GLN:HG3	1:A:602:GLU:N	2.31	0.44
1:A:887:THR:HG21	1:A:950:ASP:HA	2.00	0.44
1:A:764:ILE:H	1:A:764:ILE:HG13	1.59	0.44
1:A:1089:HIS:C	1:A:1091:VAL:N	2.75	0.44
1:A:364:LYS:O	1:A:518:ILE:HA	2.17	0.44
1:A:369:ASP:N	1:A:369:ASP:OD1	2.50	0.44
1:A:812:TRP:C	1:A:812:TRP:CD1	2.96	0.44
1:A:1056:THR:O	1:A:1056:THR:CG2	2.64	0.44
1:A:147:SER:HA	1:A:319:ARG:HH12	1.83	0.43
1:A:903:LYS:HG2	1:A:905:GLU:OE2	2.18	0.43
1:A:997:THR:HG23	1:A:1001:LYS:CG	2.48	0.43
1:A:945:GLY:HA3	1:A:984:PRO:O	2.19	0.43
1:A:960:LEU:HD11	1:A:991:PHE:CE2	2.54	0.43
1:A:561:THR:HG21	1:A:565:ASN:HD22	1.84	0.43
1:A:433:ILE:HB	1:A:462:TYR:HB2	2.00	0.43
1:A:887:THR:HG23	1:A:950:ASP:HA	2.01	0.42
1:A:960:LEU:HD11	1:A:991:PHE:HE2	1.85	0.42
1:A:629:GLN:HG3	1:A:1029:ILE:HG13	1.97	0.42
1:A:798:ILE:HD12	1:A:798:ILE:H	1.84	0.42
1:A:246:GLN:C	1:A:248:PHE:H	2.27	0.42
1:A:834:HIS:HB2	1:A:876:ILE:CD1	2.45	0.42
1:A:497:PHE:HB3	1:A:1041:GLN:NE2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:892:GLN:NE2	1:A:903:LYS:O	2.53	0.42
1:A:205:LYS:O	1:A:206:PRO:O	2.38	0.42
1:A:915:SER:HA	1:A:916:PRO:HD3	1.77	0.42
1:A:1026:LEU:O	1:A:1030:LEU:HG	2.19	0.42
1:A:253:ALA:O	1:A:254:LYS:HB2	2.20	0.42
1:A:589:TYR:CD2	1:A:593:PHE:HE1	2.38	0.42
1:A:840:GLN:O	1:A:844:ILE:HG12	2.20	0.42
1:A:165:VAL:HG12	1:A:165:VAL:O	2.20	0.41
1:A:378:ASP:CB	1:A:404:PHE:HB3	2.49	0.41
1:A:389:HIS:O	1:A:392:GLN:HB3	2.20	0.41
1:A:939:THR:CG2	1:A:945:GLY:HA2	2.50	0.41
1:A:807:LYS:HE3	1:A:808:LYS:HG2	2.03	0.41
1:A:854:ILE:HG23	1:A:1023:HIS:CD2	2.55	0.41
1:A:274:VAL:HG11	1:A:292:TRP:CE2	2.56	0.41
1:A:387:ILE:HD12	1:A:418:ILE:CD1	2.49	0.41
1:A:1021:ARG:NE	1:A:1056:THR:HG22	2.34	0.41
1:A:475:LEU:HD21	1:A:522:ASN:HB2	2.02	0.41
1:A:233:ILE:HG22	1:A:235:VAL:HG23	2.02	0.41
1:A:651:LEU:HD22	1:A:655:ASP:HB3	2.01	0.41
1:A:804:MET:HE2	1:A:812:TRP:HB2	2.02	0.41
1:A:271:VAL:CG2	1:A:282:VAL:HG12	2.51	0.41
1:A:583:LEU:HD22	1:A:610:LEU:HD22	2.02	0.41
1:A:774:LEU:HD22	1:A:779:LEU:HD13	2.01	0.40
1:A:580:TYR:HE2	1:A:613:ARG:HD3	1.86	0.40
1:A:1036:MET:HA	1:A:1042:LEU:HD11	2.03	0.40
1:A:904:ASP:OD2	1:A:904:ASP:N	2.55	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	822/966 (85%)	745 (91%)	63 (8%)	14 (2%)	7	15

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	374	PRO
1	A	379	LEU
1	A	897	GLY
1	A	1040	PRO
1	A	1045	LYS
1	A	1079	GLY
1	A	206	PRO
1	A	758	ASP
1	A	319	ARG
1	A	949	ASN
1	A	1000	LYS
1	A	1090	LEU
1	A	227	SER
1	A	526	PRO

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%)	673 (89%)	81 (11%)	6	14

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145	GLU
1	A	163	THR
1	A	168	VAL
1	A	214	LYS
1	A	215	ILE
1	A	220	ILE
1	A	226	ARG

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Mol	Chain	Res	Type
1	A	250	THR
1	A	251	LYS
1	A	281	LEU
1	A	287	ILE
1	A	358	ASP
1	A	359	ARG
1	A	373	LEU
1	A	375	ARG
1	A	378	ASP
1	A	381	VAL
1	A	387	ILE
1	A	406	GLU
1	A	418	ILE
1	A	464	VAL
1	A	487	ILE
1	A	574	LEU
1	A	575	LEU
1	A	601	GLN
1	A	610	LEU
1	A	613	ARG
1	A	647	LYS
1	A	652	GLU
1	A	682	LEU
1	A	705	GLN
1	A	717	LEU
1	A	739	ILE
1	A	748	ASP
1	A	755	GLU
1	A	756	LYS
1	A	764	ILE
1	A	766	GLN
1	A	767	LEU
1	A	769	GLN
1	A	770	LYS
1	A	774	LEU
1	A	792	LYS
1	A	799	GLU
1	A	804	MET
1	A	807	LYS
1	A	811	LEU
1	A	814	GLU
1	A	823	LEU

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Mol	Chain	Res	Type
1	A	832	PHE
1	A	838	LEU
1	A	843	LEU
1	A	845	LEU
1	A	848	LEU
1	A	863	CYS
1	A	865	LEU
1	A	887	THR
1	A	888	ILE
1	A	896	VAL
1	A	899	THR
1	A	904	ASP
1	A	905	GLU
1	A	913	GLU
1	A	919	GLU
1	A	927	ARG
1	A	939	THR
1	A	957	THR
1	A	967	HIS
1	A	1002	THR
1	A	1024	THR
1	A	1026	LEU
1	A	1041	GLN
1	A	1042	LEU
1	A	1043	THR
1	A	1052	ARG
1	A	1056	THR
1	A	1059	LYS
1	A	1062	GLU
1	A	1078	LYS
1	A	1088	LEU
1	A	1091	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	GLN
1	A	151	GLN
1	A	225	HIS
1	A	291	GLN
1	A	304	HIS
1	A	376	ASN

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Mol	Chain	Res	Type
1	A	391	GLN
1	A	392	GLN
1	A	411	ASN
1	A	522	ASN
1	A	550	GLN
1	A	565	ASN
1	A	601	GLN
1	A	705	GLN
1	A	734	GLN
1	A	743	GLN
1	A	766	GLN
1	A	769	GLN
1	A	846	GLN
1	A	892	GLN
1	A	898	ASN
1	A	951	ASN
1	A	959	ASN
1	A	1023	HIS
1	A	1041	GLN
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	093	A	2093	-	25,25,25	2.24	5 (20%)	33,36,36	2.36	8 (24%)

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	093	A	2093	-	-	10/19/19/19	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2093	093	SAN-NAU	-5.91	1.52	1.61
2	A	2093	093	OAM-SAN	5.46	1.49	1.43
2	A	2093	093	OAO-SAN	5.43	1.49	1.43
2	A	2093	093	CAH-CAI	-3.73	1.40	1.48
2	A	2093	093	CAE-CAJ	2.09	1.53	1.49

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2093	093	OAO-SAN-OAM	-9.57	107.89	119.52
2	A	2093	093	CAI-CAJ-NAK	4.66	112.75	105.70
2	A	2093	093	CAS-NAR-CAQ	4.10	126.76	117.26
2	A	2093	093	CAF-SAN-NAU	3.55	112.68	107.86
2	A	2093	093	CAE-CAJ-CAI	-3.44	126.94	130.98
2	A	2093	093	CAB-CAF-SAN	-2.23	121.66	123.19
2	A	2093	093	CAW-CAV-NAU	-2.22	106.05	110.90
2	A	2093	093	OAM-SAN-NAU	2.03	110.19	107.03

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2093	093	NAU-CAV-CAW-OAX
2	A	2093	093	NAK-CAQ-NAR-CAS

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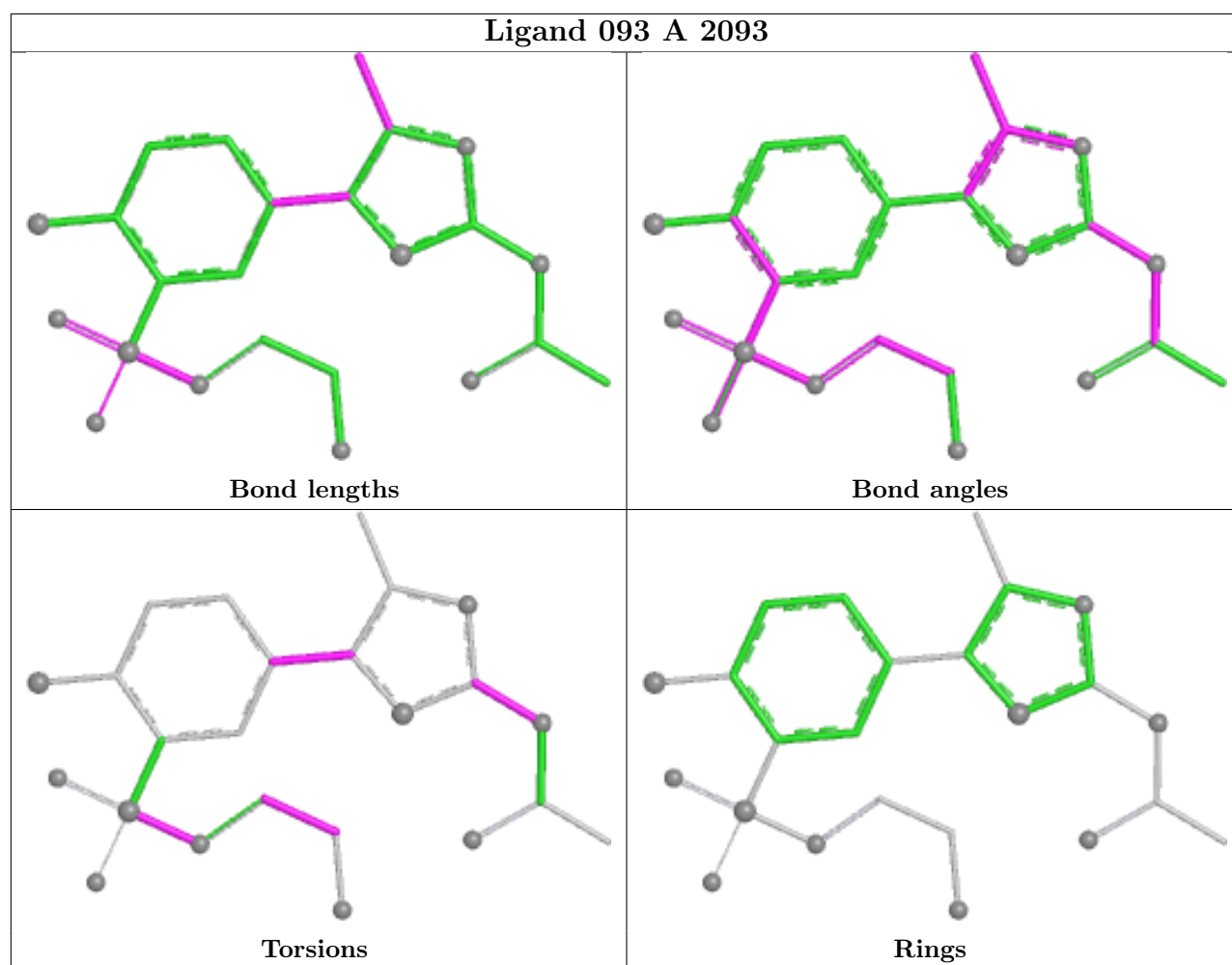
Mol	Chain	Res	Type	Atoms
2	A	2093	093	SAP-CAQ-NAR-CAS
2	A	2093	093	CAV-NAU-SAN-OAO
2	A	2093	093	CAD-CAH-CAI-CAJ
2	A	2093	093	CAG-CAH-CAI-CAJ
2	A	2093	093	CAV-NAU-SAN-CAF
2	A	2093	093	CAD-CAH-CAI-SAP
2	A	2093	093	CAG-CAH-CAI-SAP
2	A	2093	093	CAV-NAU-SAN-OAM

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2093	093	4	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	840/966 (86%)	0.92	91 (10%) 11 8	31, 61, 84, 104	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	528	ALA	4.6
1	A	900	GLY	4.0
1	A	253	ALA	4.0
1	A	379	LEU	3.9
1	A	1092	LEU	3.7
1	A	216	ALA	3.7
1	A	1086	TRP	3.7
1	A	1044	SER	3.6
1	A	403	PRO	3.3
1	A	212	TRP	3.3
1	A	210	TYR	3.2
1	A	987	LEU	3.2
1	A	1040	PRO	3.2
1	A	380	THR	3.2
1	A	215	ILE	3.1
1	A	518	ILE	3.1
1	A	811	LEU	3.0
1	A	898	ASN	3.0
1	A	381	VAL	3.0
1	A	527	ILE	3.0
1	A	909	HIS	2.9
1	A	1069	LEU	2.9
1	A	896	VAL	2.9
1	A	1002	THR	2.8
1	A	316	ASP	2.8
1	A	404	PHE	2.8
1	A	545	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	525	HIS	2.7
1	A	322	GLU	2.7
1	A	1089	HIS	2.7
1	A	805	ALA	2.7
1	A	967	HIS	2.6
1	A	285	THR	2.6
1	A	997	THR	2.6
1	A	245	LEU	2.6
1	A	517	SER	2.6
1	A	1091	VAL	2.6
1	A	760	SER	2.5
1	A	754	ALA	2.5
1	A	435	CYS	2.5
1	A	233	ILE	2.5
1	A	747	LEU	2.5
1	A	752	LEU	2.4
1	A	897	GLY	2.4
1	A	832	PHE	2.4
1	A	1064	ALA	2.4
1	A	1043	THR	2.4
1	A	304	HIS	2.4
1	A	1083	GLN	2.4
1	A	985	PHE	2.4
1	A	357	CYS	2.4
1	A	254	LYS	2.3
1	A	1045	LYS	2.3
1	A	367	GLY	2.3
1	A	290	PHE	2.3
1	A	519	LEU	2.3
1	A	409	LEU	2.3
1	A	248	PHE	2.3
1	A	1075	CYS	2.2
1	A	234	LYS	2.2
1	A	229	THR	2.2
1	A	283	GLY	2.2
1	A	767	LEU	2.2
1	A	306	VAL	2.2
1	A	149	ALA	2.2
1	A	461	LEU	2.2
1	A	223	VAL	2.2
1	A	1039	MET	2.2
1	A	926	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	242	GLY	2.2
1	A	823	LEU	2.2
1	A	230	SER	2.2
1	A	989	PRO	2.1
1	A	1079	GLY	2.1
1	A	305	VAL	2.1
1	A	1068	PHE	2.1
1	A	189	ALA	2.1
1	A	893	GLN	2.1
1	A	949	ASN	2.1
1	A	1046	GLU	2.1
1	A	315	LEU	2.1
1	A	1055	LEU	2.1
1	A	368	ILE	2.1
1	A	837	ASP	2.1
1	A	414	LEU	2.0
1	A	599	GLY	2.0
1	A	999	GLY	2.0
1	A	282	VAL	2.0
1	A	393	VAL	2.0
1	A	761	SER	2.0
1	A	228	THR	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](#)

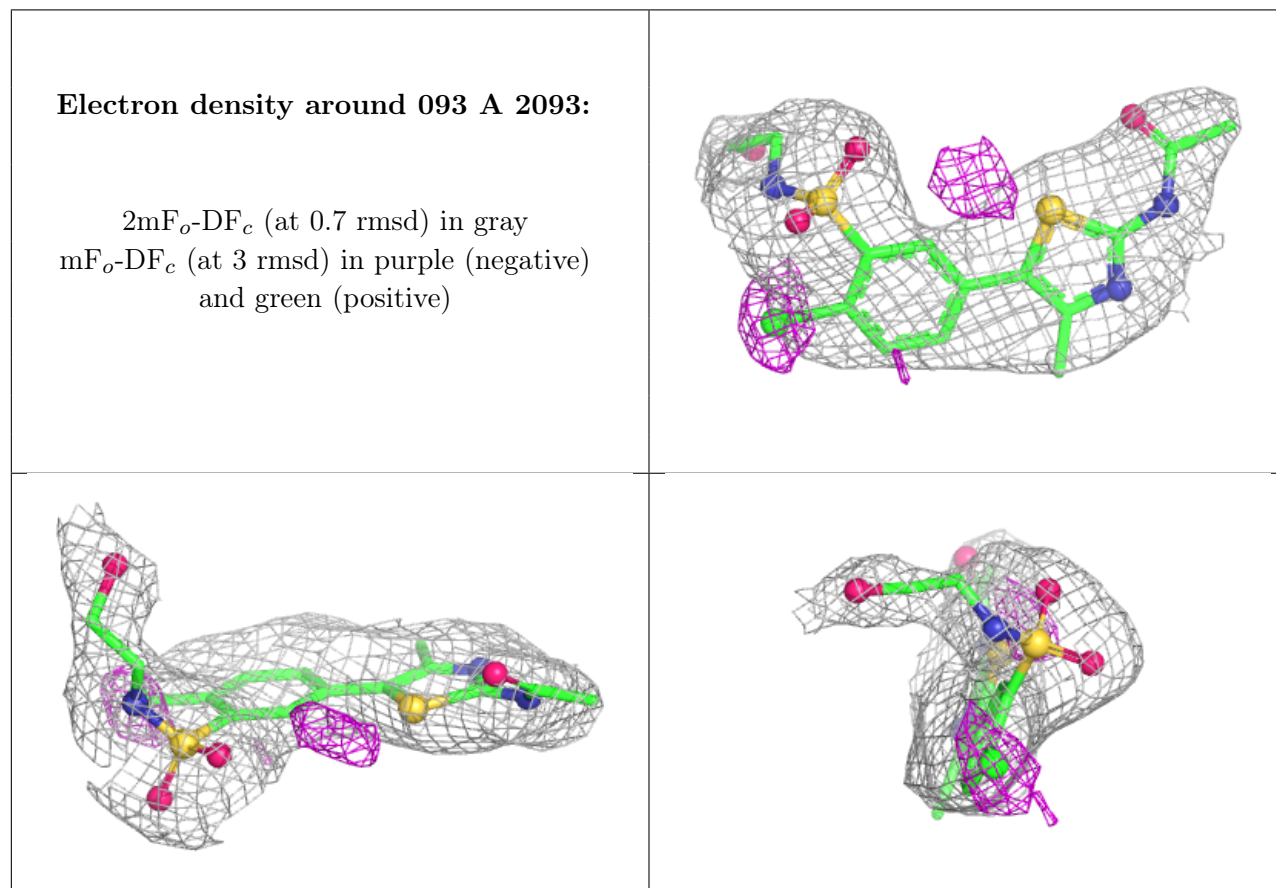
There are no oligosaccharides in this entry.

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	093	A	2093	24/24	0.80	0.19	77,79,79,80	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.