



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 07:19 pm BST

PDB ID : 2CHX
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-90
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 : 2.50 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

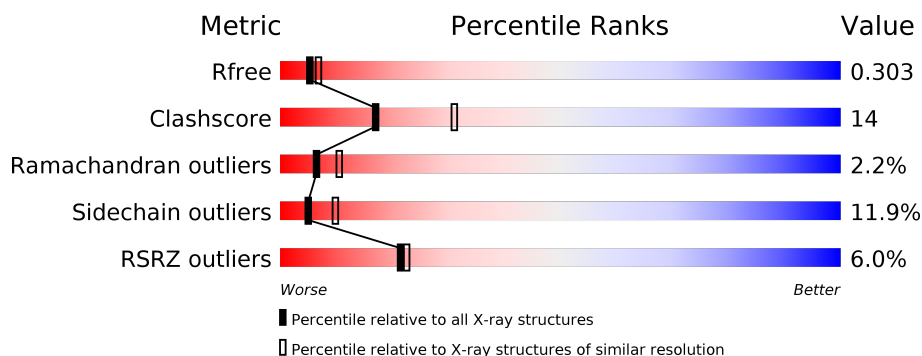
1 Overall quality at a glance

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.

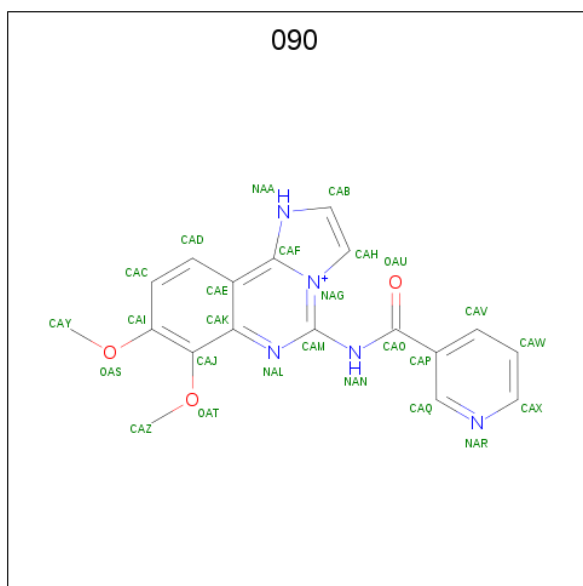
Mol	Chain	Length	Quality of chain
1	A	966	<div> <div>5%</div> <div>59%</div> <div>23%</div> <div>5%</div> <div>13%</div> </div>

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	843	Total	C	N	O	S	0	0	1
			6837	4390	1170	1242	35			

- Molecule 2 is N-(2,3-DIHYDRO-7,8-DIMETHOXYIMIDAZO[1,2-C] QUINAZOLIN-5-YL) NICOTINAMIDE (three-letter code: 090) (formula: $C_{18}H_{16}N_5O_3$).

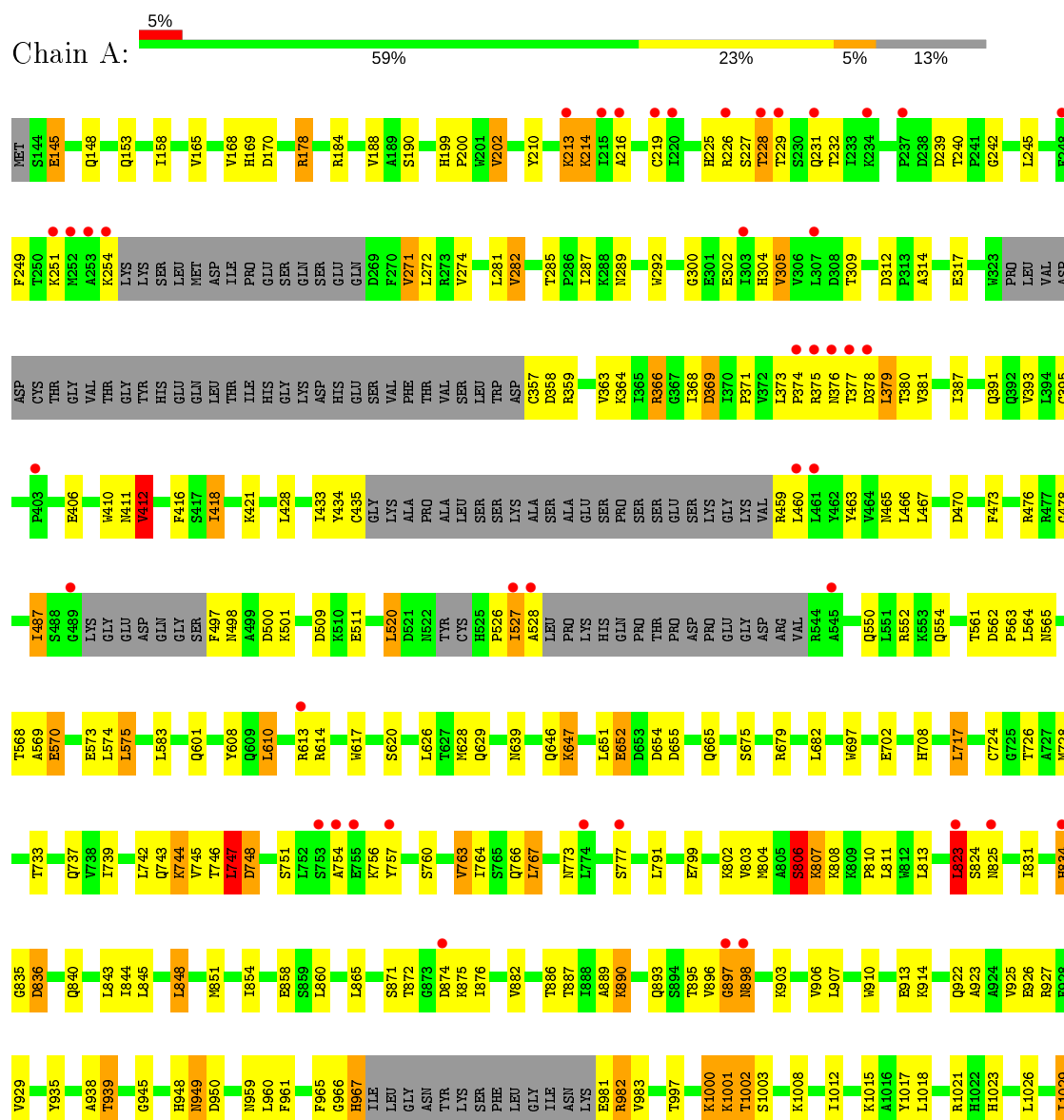


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			26	18	5	3		

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	144.49 Å 68.30 Å 106.57 Å 90.00° 95.34° 90.00°	Depositor
Resolution (Å)	57.17 – 2.50 54.29 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (57.17-2.50) 99.8 (54.29-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.51 Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.230 , 0.280 0.257 , 0.303	Depositor DCC
R_{free} test set	1483 reflections (4.12%)	wwPDB-VP
Wilson B-factor (Å ²)	51.3	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.2	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	6863	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% 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: 090

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	0.81	7/6985 (0.1%)	0.81	4/9449 (0.0%)

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 (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1000	LYS	CE-NZ	11.39	1.77	1.49
1	A	411	ASN	CG-OD1	11.36	1.49	1.24
1	A	1001	LYS	CE-NZ	9.82	1.73	1.49
1	A	411	ASN	CG-ND2	8.81	1.54	1.32
1	A	366	ARG	C-N	7.93	1.47	1.33
1	A	1000	LYS	CD-CE	5.78	1.65	1.51
1	A	364	LYS	CE-NZ	5.76	1.63	1.49

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1000	LYS	CD-CE-NZ	-7.11	95.36	111.70
1	A	823	LEU	CA-CB-CG	5.54	128.04	115.30
1	A	575	LEU	CA-CB-CG	5.40	127.73	115.30
1	A	412	VAL	CB-CA-C	-5.26	101.40	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	434	TYR	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	6837	0	6879	191	0
2	A	26	0	16	2	0
All	All	6863	0	6895	192	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 14.

All (192) 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:1001:LYS:CE	1:A:1001:LYS:NZ	1.73	1.46
1:A:1000:LYS:NZ	1:A:1000:LYS:CE	1.77	1.43
1:A:629:GLN:HG2	1:A:1029:ILE:HG13	1.44	0.99
1:A:1039:MET:HB3	1:A:1040:PRO:HD2	1.49	0.94
1:A:949:ASN:H	1:A:1083:GLN:HE22	1.08	0.94
1:A:652:GLU:OE1	1:A:654:ASP:HB3	1.67	0.94
1:A:240:THR:HG22	1:A:242:GLY:H	1.35	0.92
1:A:724:CYS:HB2	1:A:728:MET:HE3	1.58	0.85
1:A:724:CYS:HB2	1:A:728:MET:CE	2.09	0.82
1:A:848:LEU:HD12	1:A:851:MET:HE1	1.62	0.80
1:A:380:THR:O	1:A:435:CYS:SG	2.42	0.77
1:A:874:ASP:O	1:A:875:LYS:HB2	1.83	0.76
1:A:550:GLN:O	1:A:554:GLN:HG3	1.87	0.75
1:A:561:THR:CG2	1:A:565:ASN:HB3	2.18	0.74
1:A:379:LEU:HD12	1:A:435:CYS:HB2	1.71	0.73
1:A:312:ASP:OD2	1:A:314:ALA:HB3	1.90	0.71
1:A:1000:LYS:CD	1:A:1000:LYS:NZ	2.53	0.70
1:A:949:ASN:H	1:A:1083:GLN:NE2	1.87	0.70
1:A:497:PHE:HD1	1:A:1041:GLN:HE21	1.37	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1089:HIS:O	1:A:1092:LEU:N	2.24	0.70
1:A:165:VAL:HG12	1:A:165:VAL:O	1.91	0.70
1:A:225:HIS:CE1	1:A:304:HIS:HD2	2.09	0.70
1:A:848:LEU:HD12	1:A:851:MET:CE	2.21	0.69
1:A:184:ARG:O	1:A:188:VAL:HG23	1.94	0.68
1:A:823:LEU:HD12	1:A:823:LEU:H	1.58	0.67
1:A:225:HIS:HE1	1:A:304:HIS:HD2	1.42	0.67
1:A:1021:ARG:HE	1:A:1056:THR:CG2	2.07	0.66
1:A:848:LEU:HA	1:A:851:MET:HE2	1.76	0.66
1:A:935:TYR:O	1:A:939:THR:HB	1.96	0.65
1:A:1089:HIS:C	1:A:1091:VAL:H	2.00	0.65
1:A:882:VAL:H	2:A:2093:090:HAA	1.44	0.64
1:A:652:GLU:OE1	1:A:654:ASP:CB	2.44	0.64
1:A:981:GLU:HA	1:A:982:ARG:CZ	2.28	0.64
1:A:860:LEU:HD21	1:A:1015:LYS:HE2	1.79	0.64
1:A:1089:HIS:O	1:A:1091:VAL:N	2.32	0.63
1:A:387:ILE:HG13	1:A:418:ILE:CD1	2.28	0.63
1:A:807:LYS:H	1:A:807:LYS:HE3	1.64	0.63
1:A:834:HIS:CD2	1:A:834:HIS:C	2.72	0.63
1:A:834:HIS:CD2	1:A:835:GLY:N	2.67	0.63
1:A:743:GLN:O	1:A:747:LEU:HB2	1.99	0.62
1:A:1002:THR:HG23	1:A:1003:SER:N	2.16	0.60
1:A:1039:MET:HB3	1:A:1040:PRO:CD	2.29	0.60
1:A:608:TYR:CZ	1:A:639:ASN:ND2	2.70	0.60
1:A:371:PRO:HG2	1:A:511:GLU:O	2.02	0.59
1:A:410:TRP:HB3	1:A:412:VAL:CG2	2.32	0.59
1:A:767:LEU:HD12	1:A:803:VAL:HG23	1.84	0.59
1:A:178:ARG:NH1	1:A:178:ARG:HG3	2.17	0.59
1:A:675:SER:O	1:A:679:ARG:HG3	2.03	0.59
1:A:226:ARG:HD2	1:A:229:THR:HB	1.85	0.58
1:A:202:VAL:HG22	1:A:285:THR:HG21	1.85	0.58
1:A:1089:HIS:C	1:A:1091:VAL:N	2.57	0.57
1:A:1002:THR:CG2	1:A:1003:SER:N	2.67	0.57
1:A:1021:ARG:HE	1:A:1056:THR:HG23	1.66	0.57
1:A:395:CYS:HB3	1:A:418:ILE:HD11	1.87	0.57
1:A:939:THR:HG23	1:A:945:GLY:HA2	1.87	0.56
1:A:628:MET:HB2	1:A:1029:ILE:HG21	1.88	0.56
1:A:614:ARG:HG2	1:A:617:TRP:HB3	1.87	0.56
1:A:380:THR:O	1:A:435:CYS:CB	2.54	0.56
1:A:854:ILE:HG23	1:A:1023:HIS:CD2	2.41	0.56
1:A:927:ARG:HE	1:A:959:ASN:HD22	1.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:PRO:O	1:A:527:ILE:HG13	2.05	0.56
1:A:473:PHE:O	1:A:527:ILE:HD12	2.06	0.55
1:A:478:GLY:N	1:A:520:LEU:O	2.29	0.55
1:A:893:GLN:HA	1:A:897:GLY:CA	2.37	0.55
1:A:271:VAL:HG21	1:A:282:VAL:HG11	1.89	0.55
1:A:271:VAL:HG22	1:A:282:VAL:CG1	2.37	0.55
1:A:922:GLN:HA	1:A:922:GLN:OE1	2.06	0.54
1:A:178:ARG:HH11	1:A:178:ARG:HG3	1.71	0.54
1:A:428:LEU:HD22	1:A:465:ASN:HB3	1.90	0.54
1:A:145:GLU:HA	1:A:148:GLN:HE21	1.72	0.54
1:A:745:VAL:C	1:A:747:LEU:N	2.61	0.53
1:A:1042:LEU:O	1:A:1042:LEU:HD22	2.08	0.53
1:A:561:THR:HG23	1:A:565:ASN:HB3	1.87	0.53
1:A:1035:LEU:HB3	1:A:1042:LEU:HG	1.89	0.53
1:A:806:SER:O	1:A:808:LYS:O	2.27	0.53
1:A:836:ASP:O	1:A:875:LYS:HA	2.08	0.53
1:A:651:LEU:HD22	1:A:655:ASP:HB3	1.91	0.53
1:A:804:MET:HE1	1:A:810:PRO:HB2	1.91	0.53
1:A:733:THR:O	1:A:737:GLN:HG3	2.08	0.52
1:A:1055:LEU:O	1:A:1056:THR:HG22	2.09	0.52
1:A:745:VAL:O	1:A:747:LEU:N	2.42	0.52
1:A:851:MET:HE1	1:A:938:ALA:HB1	1.91	0.52
1:A:887:THR:HG22	1:A:890:LYS:H	1.74	0.52
1:A:834:HIS:CG	1:A:835:GLY:N	2.77	0.51
1:A:214:LYS:NZ	1:A:300:GLY:HA2	2.25	0.51
1:A:225:HIS:HE1	1:A:304:HIS:CD2	2.24	0.51
1:A:527:ILE:HG22	1:A:528:ALA:N	2.25	0.51
1:A:368:ILE:HG21	1:A:433:ILE:HD11	1.92	0.51
1:A:357:CYS:N	1:A:421:LYS:HD3	2.26	0.51
1:A:824:SER:C	1:A:825:ASN:HD22	2.14	0.51
1:A:939:THR:HG23	1:A:945:GLY:CA	2.40	0.51
1:A:272:LEU:HD22	1:A:305:VAL:CG1	2.41	0.50
1:A:965:PHE:O	1:A:967:HIS:N	2.45	0.50
1:A:825:ASN:HD22	1:A:825:ASN:N	2.10	0.50
1:A:898:ASN:N	1:A:898:ASN:HD22	2.08	0.50
1:A:927:ARG:NE	1:A:959:ASN:HD22	2.09	0.50
1:A:387:ILE:HG13	1:A:418:ILE:HD13	1.94	0.49
1:A:747:LEU:HB3	1:A:748:ASP:OD1	2.11	0.49
1:A:165:VAL:O	1:A:165:VAL:CG1	2.58	0.49
1:A:844:ILE:HD13	1:A:1034:MET:SD	2.52	0.49
1:A:378:ASP:O	1:A:379:LEU:C	2.51	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:764:ILE:O	1:A:764:ILE:HG22	2.12	0.49
1:A:564:LEU:HD11	1:A:1048:ILE:HG22	1.95	0.49
1:A:874:ASP:O	1:A:875:LYS:CB	2.58	0.49
1:A:1008:LYS:O	1:A:1012:ILE:HG13	2.12	0.49
1:A:285:THR:HG22	1:A:289:ASN:HB2	1.95	0.49
1:A:898:ASN:N	1:A:898:ASN:ND2	2.60	0.49
1:A:903:LYS:HB2	1:A:906:VAL:HG23	1.94	0.49
1:A:948:HIS:HD2	1:A:950:ASP:HB2	1.78	0.49
1:A:302:GLU:OE1	1:A:304:HIS:HE1	1.95	0.48
1:A:210:TYR:O	1:A:213:LYS:HD2	2.13	0.48
1:A:620:SER:O	1:A:647:LYS:NZ	2.43	0.48
1:A:807:LYS:HZ2	1:A:808:LYS:H	1.61	0.48
1:A:274:VAL:HG21	1:A:292:TRP:CD1	2.48	0.48
1:A:583:LEU:HD22	1:A:610:LEU:HD22	1.95	0.48
1:A:271:VAL:CG2	1:A:282:VAL:CG1	2.91	0.48
1:A:178:ARG:HH11	1:A:178:ARG:CG	2.26	0.48
1:A:387:ILE:HG13	1:A:418:ILE:HD11	1.96	0.48
1:A:421:LYS:HA	1:A:421:LYS:HD2	1.59	0.48
1:A:925:VAL:O	1:A:929:VAL:HG23	2.14	0.48
1:A:1045:LYS:O	1:A:1046:GLU:HG3	2.14	0.48
1:A:1035:LEU:HD12	1:A:1048:ILE:HD13	1.96	0.47
1:A:840:GLN:HG2	1:A:1039:MET:HE2	1.96	0.47
1:A:823:LEU:CD1	1:A:823:LEU:H	2.26	0.47
1:A:1001:LYS:CD	1:A:1001:LYS:NZ	2.70	0.47
1:A:743:GLN:HG2	1:A:876:ILE:HD11	1.96	0.47
1:A:1043:THR:HB	1:A:1046:GLU:HB2	1.97	0.47
1:A:231:GLN:HE21	1:A:232:THR:H	1.62	0.47
1:A:804:MET:HE1	1:A:831:ILE:HG23	1.97	0.46
1:A:760:SER:O	1:A:763:VAL:HG12	2.14	0.46
1:A:359:ARG:HG2	1:A:359:ARG:HH11	1.81	0.46
1:A:239:ASP:O	1:A:287:ILE:HG13	2.16	0.45
1:A:271:VAL:CG2	1:A:282:VAL:HG11	2.46	0.45
1:A:896:VAL:HG23	1:A:897:GLY:H	1.81	0.45
1:A:228:THR:CG2	1:A:228:THR:O	2.64	0.45
1:A:742:LEU:HD22	1:A:813:LEU:HD11	1.98	0.45
1:A:896:VAL:CG2	1:A:903:LYS:HD2	2.46	0.45
1:A:498:ASN:C	1:A:498:ASN:OD1	2.55	0.45
1:A:939:THR:CG2	1:A:945:GLY:HA2	2.46	0.45
1:A:1088:LEU:O	1:A:1091:VAL:HG22	2.16	0.45
1:A:665:GLN:NE2	1:A:702:GLU:OE2	2.36	0.45
1:A:743:GLN:C	1:A:745:VAL:H	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:887:THR:HG22	1:A:889:ALA:N	2.33	0.44
1:A:910:TRP:O	1:A:914:LYS:HG2	2.18	0.44
1:A:1040:PRO:HB2	1:A:1041:GLN:H	1.65	0.43
1:A:369:ASP:OD1	1:A:369:ASP:N	2.51	0.43
1:A:923:ALA:O	1:A:926:GLU:HB3	2.17	0.43
1:A:317:GLU:O	1:A:726:THR:HG23	2.18	0.43
1:A:466:LEU:HD11	1:A:476:ARG:HD3	2.00	0.43
1:A:745:VAL:C	1:A:747:LEU:H	2.21	0.43
1:A:1017:TYR:OH	1:A:1056:THR:HG22	2.19	0.43
1:A:287:ILE:HG13	1:A:287:ILE:H	1.68	0.43
1:A:697:TRP:CZ3	1:A:872:THR:HG22	2.54	0.43
1:A:168:VAL:HG13	1:A:170:ASP:O	2.18	0.43
1:A:378:ASP:O	1:A:379:LEU:O	2.36	0.43
1:A:552:ARG:HB2	1:A:552:ARG:CZ	2.49	0.43
1:A:743:GLN:C	1:A:745:VAL:N	2.72	0.43
1:A:363:VAL:HG23	1:A:520:LEU:HD13	2.00	0.42
1:A:804:MET:HB2	1:A:810:PRO:HG2	2.01	0.42
1:A:834:HIS:CD2	1:A:835:GLY:CA	3.02	0.42
1:A:497:PHE:HD1	1:A:1041:GLN:NE2	2.10	0.42
1:A:910:TRP:HA	1:A:913:GLU:HG2	2.01	0.42
1:A:562:ASP:HB2	1:A:563:PRO:CD	2.50	0.42
1:A:470:ASP:HB3	1:A:476:ARG:NH2	2.34	0.41
1:A:1055:LEU:C	1:A:1056:THR:HG22	2.41	0.41
1:A:199:HIS:O	1:A:200:PRO:C	2.59	0.41
1:A:410:TRP:HB3	1:A:412:VAL:HG22	2.00	0.41
1:A:467:LEU:HB2	1:A:476:ARG:HH12	1.85	0.41
1:A:561:THR:HG23	1:A:565:ASN:CB	2.50	0.41
1:A:460:LEU:HG	1:A:487:ILE:HD13	2.03	0.41
1:A:500:ASP:HB3	1:A:708:HIS:CD2	2.55	0.41
1:A:724:CYS:HB2	1:A:728:MET:HE2	1.99	0.41
1:A:960:LEU:HD23	1:A:961:PHE:N	2.36	0.41
1:A:497:PHE:HB3	1:A:1041:GLN:HE22	1.84	0.41
1:A:463:TYR:CE1	1:A:501:LYS:HA	2.55	0.41
1:A:158:ILE:HG12	1:A:717:LEU:HD13	2.02	0.41
1:A:1045:LYS:O	1:A:1046:GLU:CG	2.69	0.41
1:A:245:LEU:O	1:A:249:PHE:HD1	2.03	0.41
1:A:416:PHE:HB3	1:A:418:ILE:HD12	2.02	0.41
1:A:1091:VAL:O	1:A:1091:VAL:HG23	2.21	0.41
2:A:2093:090:NAL	2:A:2093:090:OAU	2.51	0.41
1:A:168:VAL:HG13	1:A:169:HIS:N	2.35	0.41
1:A:178:ARG:NH1	1:A:178:ARG:CG	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:569:ALA:O	1:A:573:GLU:HG3	2.20	0.41
1:A:1092:LEU:HD23	1:A:1093:GLY:N	2.36	0.41
1:A:851:MET:HB2	1:A:851:MET:HE2	1.94	0.40
1:A:724:CYS:O	1:A:728:MET:HE2	2.21	0.40
1:A:743:GLN:O	1:A:745:VAL:N	2.54	0.40
1:A:1002:THR:HG23	1:A:1003:SER:H	1.85	0.40
1:A:1041:GLN:HA	1:A:1041:GLN:OE1	2.21	0.40
1:A:568:THR:HG22	1:A:570:GLU:H	1.85	0.40
1:A:1018:LEU:HD13	1:A:1061:GLU:OE1	2.21	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	827/966 (86%)	760 (92%)	49 (6%)	18 (2%)	6 10

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	376	ASN
1	A	754	ALA
1	A	966	GLY
1	A	1040	PRO
1	A	1090	LEU
1	A	527	ILE
1	A	744	LYS
1	A	746	THR
1	A	806	SER
1	A	949	ASN
1	A	1046	GLU
1	A	374	PRO

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Mol	Chain	Res	Type
1	A	747	LEU
1	A	1092	LEU
1	A	216	ALA
1	A	251	LYS
1	A	509	ASP
1	A	897	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	757/864 (88%)	667 (88%)	90 (12%)	5 10

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145	GLU
1	A	153	GLN
1	A	178	ARG
1	A	190	SER
1	A	202	VAL
1	A	213	LYS
1	A	214	LYS
1	A	219	CYS
1	A	227	SER
1	A	228	THR
1	A	254	LYS
1	A	271	VAL
1	A	281	LEU
1	A	282	VAL
1	A	305	VAL
1	A	309	THR
1	A	358	ASP
1	A	366	ARG
1	A	369	ASP
1	A	373	LEU

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Mol	Chain	Res	Type
1	A	375	ARG
1	A	377	THR
1	A	379	LEU
1	A	381	VAL
1	A	391	GLN
1	A	393	VAL
1	A	406	GLU
1	A	412	VAL
1	A	418	ILE
1	A	459	ARG
1	A	487	ILE
1	A	520	LEU
1	A	570	GLU
1	A	574	LEU
1	A	575	LEU
1	A	601	GLN
1	A	610	LEU
1	A	613	ARG
1	A	626	LEU
1	A	646	GLN
1	A	647	LYS
1	A	652	GLU
1	A	682	LEU
1	A	717	LEU
1	A	739	ILE
1	A	744	LYS
1	A	747	LEU
1	A	748	ASP
1	A	751	SER
1	A	756	LYS
1	A	757	TYR
1	A	763	VAL
1	A	766	GLN
1	A	767	LEU
1	A	773	ASN
1	A	777	SER
1	A	791	LEU
1	A	799	GLU
1	A	802	LYS
1	A	806	SER
1	A	807	LYS
1	A	811	LEU

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Mol	Chain	Res	Type
1	A	823	LEU
1	A	834	HIS
1	A	836	ASP
1	A	843	LEU
1	A	845	LEU
1	A	848	LEU
1	A	858	GLU
1	A	865	LEU
1	A	871	SER
1	A	886	THR
1	A	890	LYS
1	A	895	THR
1	A	898	ASN
1	A	907	LEU
1	A	939	THR
1	A	967	HIS
1	A	982	ARG
1	A	983	VAL
1	A	997	THR
1	A	1002	THR
1	A	1026	LEU
1	A	1029	ILE
1	A	1041	GLN
1	A	1042	LEU
1	A	1043	THR
1	A	1045	LYS
1	A	1052	ARG
1	A	1078	LYS

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	148	GLN
1	A	225	HIS
1	A	231	GLN
1	A	304	HIS
1	A	639	ASN
1	A	766	GLN
1	A	773	ASN
1	A	775	GLN
1	A	825	ASN
1	A	834	HIS

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Mol	Chain	Res	Type
1	A	898	ASN
1	A	948	HIS
1	A	959	ASN
1	A	1007	GLN
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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates 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	090	A	2093	-	25,29,29	1.24	2 (8%)	31,41,41	1.98	7 (22%)

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	090	A	2093	-	-	0/12/12/12	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2093	090	CAH-CAB	4.41	1.53	1.36
2	A	2093	090	CAJ-CAK	-2.10	1.39	1.42

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2093	090	CAB-CAH-NAG	-8.26	100.04	106.83
2	A	2093	090	CAK-CAE-CAF	-2.83	117.85	119.98
2	A	2093	090	CAX-NAR-CAQ	2.74	121.58	116.85
2	A	2093	090	CAP-CAQ-NAR	-2.70	119.50	123.49
2	A	2093	090	OAS-CAI-CAJ	2.51	120.00	116.49
2	A	2093	090	CAE-CAK-NAL	-2.26	120.21	123.33
2	A	2093	090	OAS-CAI-CAC	-2.16	120.67	124.37

There are no chirality outliers.

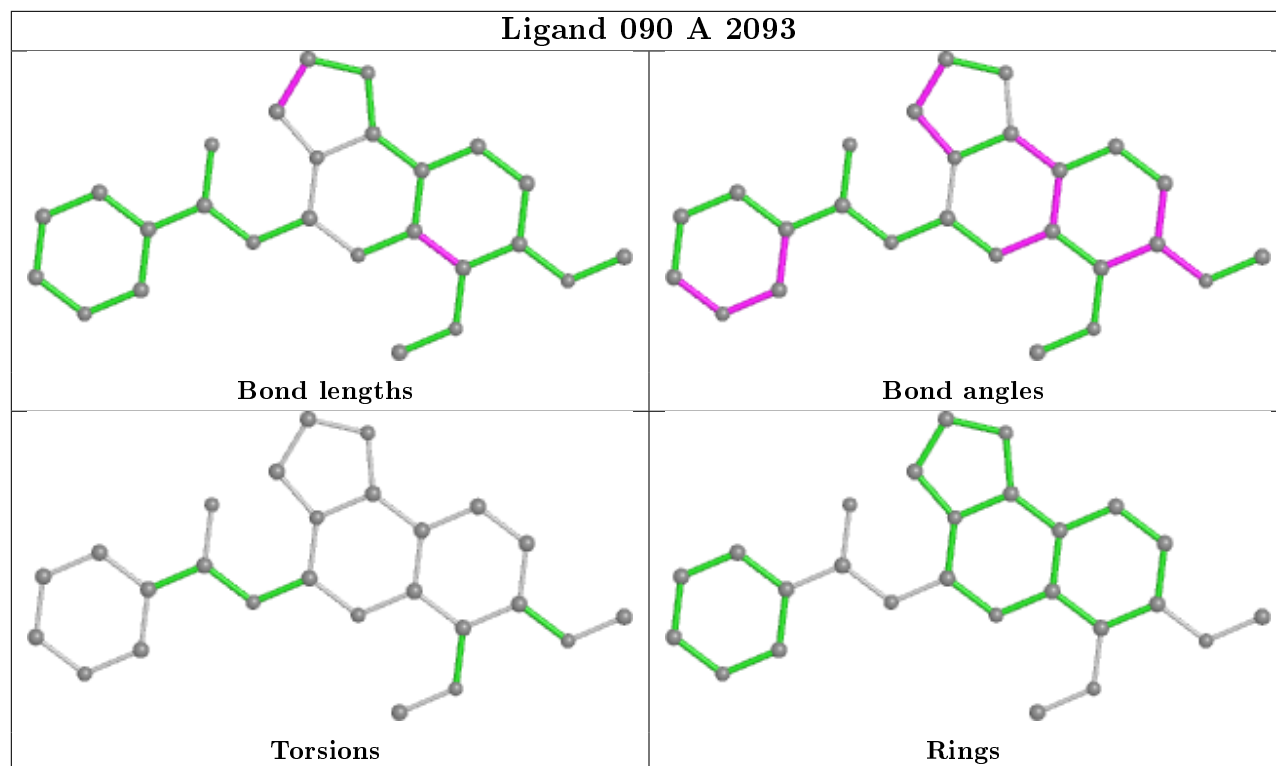
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2093	090	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	843/966 (87%)	0.54	51 (6%) 21 22	20, 46, 74, 108	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1044	SER	7.1
1	A	376	ASN	5.7
1	A	1045	LYS	5.7
1	A	374	PRO	5.6
1	A	226	ARG	5.5
1	A	757	TYR	5.2
1	A	307	LEU	4.7
1	A	216	ALA	4.5
1	A	377	THR	4.4
1	A	375	ARG	4.0
1	A	1092	LEU	3.9
1	A	254	LYS	3.8
1	A	897	GLY	3.8
1	A	825	ASN	3.7
1	A	228	THR	3.6
1	A	1086	TRP	3.6
1	A	378	ASP	3.6
1	A	777	SER	3.5
1	A	229	THR	3.3
1	A	874	ASP	3.2
1	A	234	LYS	3.1
1	A	528	ALA	3.1
1	A	489	GLY	3.0
1	A	1066	LYS	3.0
1	A	754	ALA	3.0
1	A	403	PRO	3.0
1	A	253	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	215	ILE	2.8
1	A	1043	THR	2.8
1	A	545	ALA	2.8
1	A	461	LEU	2.6
1	A	823	LEU	2.6
1	A	213	LYS	2.6
1	A	251	LYS	2.6
1	A	774	LEU	2.5
1	A	219	CYS	2.5
1	A	231	GLN	2.5
1	A	527	ILE	2.4
1	A	252	MET	2.4
1	A	220	ILE	2.3
1	A	613	ARG	2.2
1	A	303	ILE	2.2
1	A	1041	GLN	2.2
1	A	755	GLU	2.2
1	A	1046	GLU	2.2
1	A	248	PHE	2.1
1	A	753	SER	2.1
1	A	237	PRO	2.1
1	A	898	ASN	2.1
1	A	834	HIS	2.1
1	A	460	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](#)

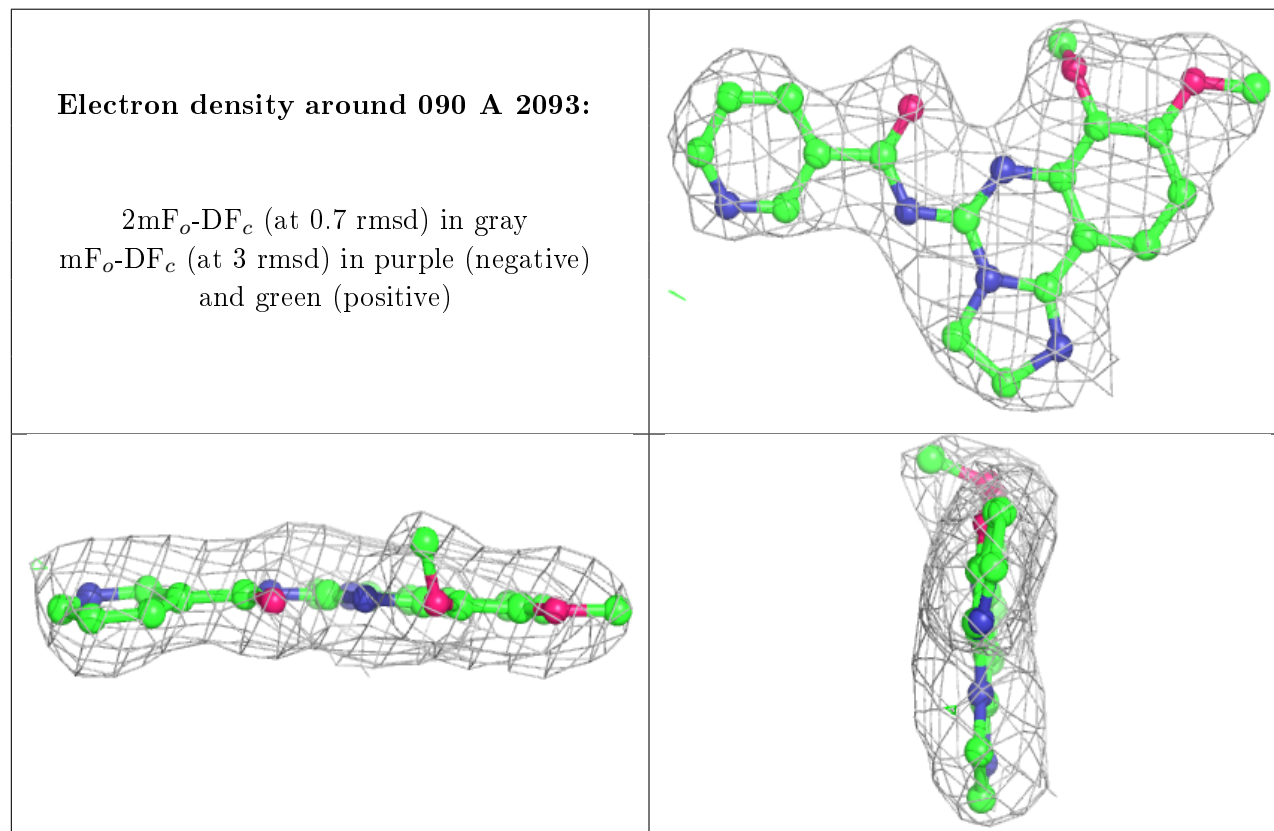
There are no carbohydrates in this entry.

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	090	A	2093	26/26	0.94	0.17	44,47,48,50	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.