



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:29 PM UTC

PDB ID : 2WXF / pdb_00002wxf
Title : The crystal structure of the murine class IA PI 3-kinase p110delta in complex with PIK-39.
Authors : Berndt, A.; Miller, S.; Williams, O.; Lee, D.D.; Houseman, B.T.; Pacold, J.I.; Gorrec, F.; Hon, W.-C.; Liu, Y.; Rommel, C.; Gaillard, P.; Ruckle, T.; Schwarz, M.K.; Shokat, K.M.; Shaw, J.P.; Williams, R.L.
Deposited on : 2009-11-09
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

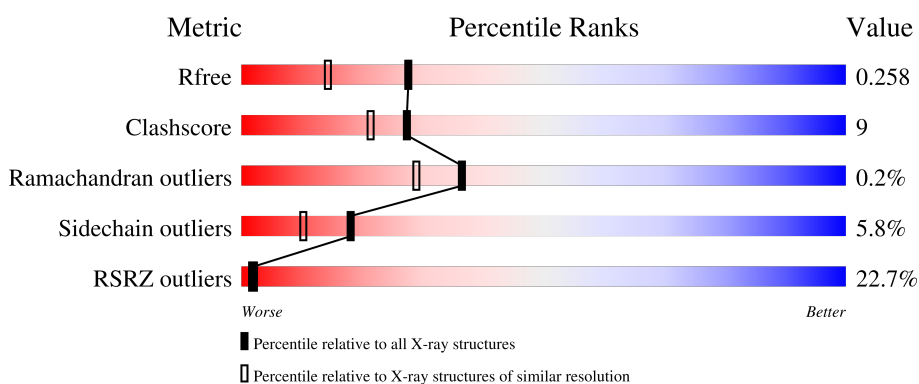
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	940	20% 72% 14% • 13%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6940 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.

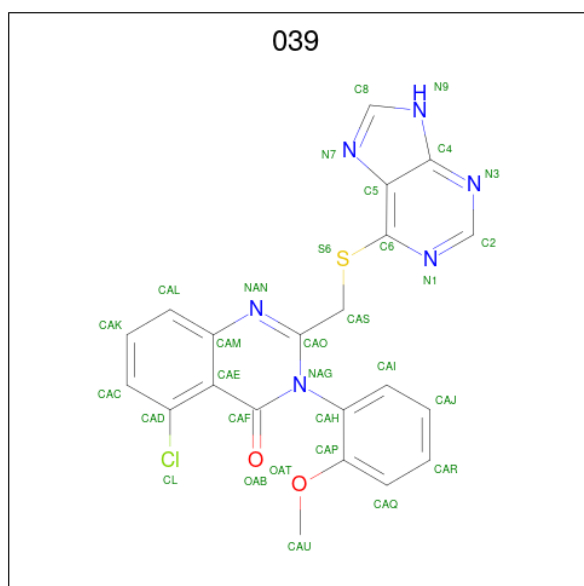
- Molecule 1 is a protein called PHOSPHATIDYLINOSITOL-4,5-BISPHOSPHATE 3-KINASE CATALYTIC SUBUNIT DELTA ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	822	Total	C	N	O	S	0	5	0
			6667	4273	1132	1206	56			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	105	GLY	-	expression tag	UNP Q3UDT3

- Molecule 2 is 2-((9H-PURIN-6-YLTHIO)METHYL)-5-CHLORO-3-(2-METHOXYPHENYL)QUINAZOLIN-4(3H)-ONE (CCD ID: 039) (formula: $C_{21}H_{15}ClN_6O_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	S	0
			31	21	1	6	2	1	0

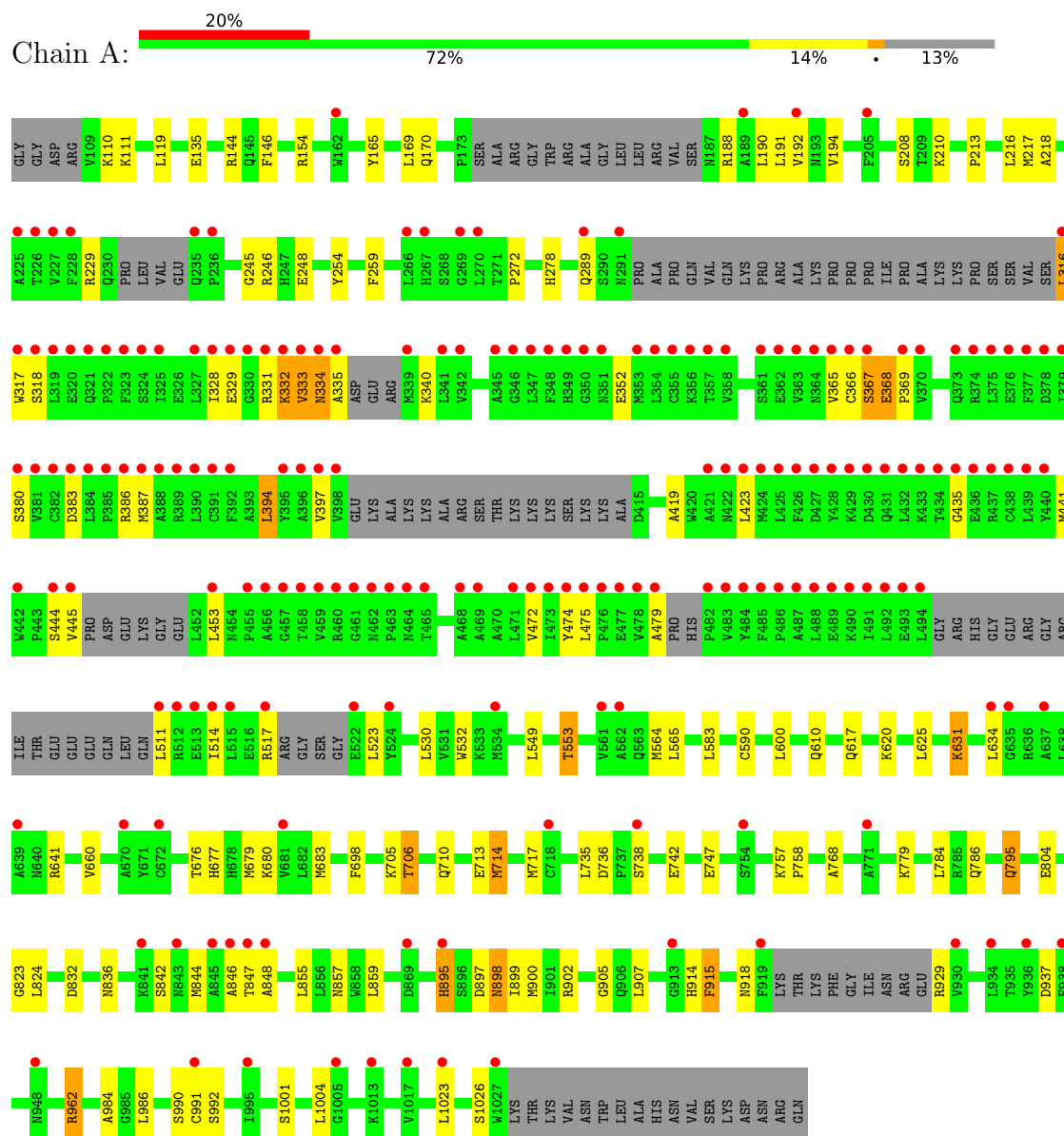
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	242	Total 242	O 242	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 DELTA ISOFORM



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	142.42Å 65.01Å 116.69Å 90.00° 103.53° 90.00°	Depositor
Resolution (Å)	38.95 – 1.90 38.95 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.4 (38.95-1.90) 98.4 (38.95-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.5.0046	Depositor
R, R_{free}	0.210 , 0.240 0.230 , 0.258	Depositor DCC
R_{free} test set	2436 reflections (2.99%)	wwPDB-VP
Wilson B-factor (Å ²)	32.4	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.3	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	6940	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% 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:
039

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	0.70	2/6810 (0.0%)	0.82	3/9188 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	479	ALA	C-O	12.63	1.48	1.23
1	A	757	LYS	C-O	-9.32	1.19	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	334	ASN	N-CA-C	7.26	118.18	108.38
1	A	444	SER	N-CA-C	5.73	118.01	108.20
1	A	848	ALA	N-CA-C	5.50	118.36	109.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	6667	0	6642	121	1
2	A	31	0	15	2	0
3	A	242	0	0	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6940	0	6657	121	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 9.

All (121) 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:899:ILE:CG2	1:A:907[B]:LEU:HD11	1.48	1.41
1:A:367:SER:HB3	1:A:368:GLU:C	1.51	1.34
1:A:367:SER:HB3	1:A:369:PRO:N	1.52	1.24
1:A:549:LEU:HG	1:A:564:MET:HE1	1.27	1.17
1:A:386:ARG:HG3	1:A:387:MET:HE2	1.34	1.07
1:A:899:ILE:HG21	1:A:907[B]:LEU:HD11	1.36	1.07
1:A:367:SER:CB	1:A:368:GLU:C	2.30	1.04
1:A:899:ILE:HG22	1:A:907[B]:LEU:HD11	1.39	1.02
1:A:899:ILE:CG2	1:A:907[B]:LEU:CD1	2.38	1.02
1:A:795:GLN:HG2	3:A:2151:HOH:O	1.59	1.01
1:A:706:THR:OG1	1:A:710:GLN:NE2	2.06	0.89
1:A:899:ILE:HG22	1:A:907[B]:LEU:CD1	2.03	0.85
1:A:929:ARG:NH2	1:A:1001[B]:SER:OG	2.09	0.84
1:A:847:THR:HG22	3:A:2194:HOH:O	1.79	0.81
1:A:368:GLU:N	1:A:369:PRO:CD	2.46	0.78
1:A:549:LEU:CG	1:A:564:MET:HE1	2.11	0.77
1:A:962:ARG:HG2	1:A:962:ARG:HH11	1.51	0.75
1:A:367:SER:HB3	1:A:369:PRO:CA	2.16	0.75
1:A:367:SER:HA	1:A:368:GLU:CB	2.18	0.74
1:A:902:ARG:HD2	3:A:2182:HOH:O	1.88	0.74
1:A:914:HIS:HB3	1:A:918:ASN:O	1.88	0.73
1:A:367:SER:C	1:A:369:PRO:HD3	2.13	0.73
1:A:367:SER:HA	1:A:368:GLU:HB3	1.71	0.72
1:A:895:HIS:H	1:A:898:ASN:HD21	1.37	0.71
1:A:902:ARG:CD	3:A:2182:HOH:O	2.39	0.71
1:A:366:CYS:O	1:A:367:SER:CB	2.38	0.71
1:A:553:THR:CG2	1:A:564:MET:HE3	2.21	0.71
1:A:387:MET:HE3	1:A:590:CYS:HB3	1.74	0.70
1:A:246:ARG:NH1	1:A:248:GLU:OE1	2.25	0.69
1:A:387:MET:HE3	1:A:590:CYS:SG	2.33	0.69
1:A:610:GLN:OE1	1:A:795:GLN:NE2	2.26	0.68
1:A:549:LEU:HG	1:A:564:MET:CE	2.17	0.68
1:A:747:GLU:OE1	3:A:2127:HOH:O	2.12	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:899:ILE:HG23	1:A:907[B]:LEU:HD11	1.67	0.67
1:A:110:LYS:NZ	1:A:144:ARG:HH12	1.94	0.65
1:A:900:MET:O	1:A:907[B]:LEU:HD12	1.97	0.65
1:A:929:ARG:HH22	1:A:1001[A]:SER:HB3	1.62	0.65
1:A:991:CYS:HB2	3:A:2238:HOH:O	1.96	0.64
1:A:786:GLN:OE1	3:A:2145:HOH:O	2.14	0.64
1:A:328:ILE:HB	1:A:472:VAL:HG23	1.79	0.63
1:A:859:LEU:HD21	1:A:905:GLY:HA2	1.80	0.63
1:A:386:ARG:CG	1:A:387:MET:HE2	2.23	0.60
1:A:368:GLU:N	1:A:369:PRO:HD3	2.15	0.59
1:A:367:SER:HB3	1:A:369:PRO:CD	2.32	0.59
1:A:553:THR:HG21	1:A:564:MET:HE3	1.84	0.59
1:A:146:PHE:CE1	1:A:631:LYS:HD2	2.37	0.59
1:A:679:MET:O	1:A:683:MET:HG3	2.03	0.59
1:A:747:GLU:HG2	3:A:2128:HOH:O	2.01	0.59
1:A:387:MET:HE3	1:A:590:CYS:CB	2.34	0.57
1:A:366:CYS:O	1:A:367:SER:HB2	2.04	0.57
1:A:641:ARG:NH2	3:A:2082:HOH:O	2.39	0.56
1:A:367:SER:CB	1:A:368:GLU:O	2.54	0.56
1:A:583:LEU:HD11	1:A:600:LEU:HD11	1.88	0.55
1:A:895:HIS:H	1:A:898:ASN:ND2	2.03	0.55
1:A:617:GLN:HE22	1:A:620:LYS:NZ	2.05	0.55
1:A:419:ALA:HB3	1:A:441:MET:HE3	1.86	0.55
1:A:435:GLY:HA2	1:A:475:LEU:O	2.08	0.54
1:A:329:GLU:HB2	1:A:369:PRO:O	2.08	0.53
1:A:532:TRP:HZ3	1:A:564:MET:HE2	1.74	0.53
1:A:902:ARG:HD3	3:A:2182:HOH:O	2.07	0.53
1:A:119:LEU:HD23	1:A:683:MET:HE3	1.89	0.53
1:A:617:GLN:HE21	1:A:984:ALA:HA	1.74	0.52
1:A:915:PHE:CD2	1:A:915:PHE:C	2.88	0.52
1:A:146:PHE:CZ	1:A:631:LYS:HD2	2.45	0.52
1:A:110:LYS:HZ1	1:A:144:ARG:HH12	1.58	0.51
1:A:329:GLU:HG2	1:A:472:VAL:CG2	2.41	0.51
1:A:154:ARG:HD2	1:A:165:TYR:CZ	2.46	0.51
1:A:367:SER:CA	1:A:368:GLU:CB	2.87	0.51
1:A:192:VAL:HG13	1:A:272:PRO:HB2	1.94	0.50
1:A:380:SER:HB3	1:A:383:ASP:OD1	2.11	0.50
1:A:553:THR:HG22	1:A:564:MET:HE3	1.92	0.50
1:A:154:ARG:HD2	1:A:165:TYR:CE2	2.47	0.50
1:A:170:GLN:HG2	3:A:2019:HOH:O	2.11	0.50
1:A:836[A]:ASN:HD22	2:A:1500:039:HAR	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:736:ASP:CG	1:A:738:SER:HG	2.22	0.48
1:A:366:CYS:O	1:A:367:SER:OG	2.30	0.48
1:A:929:ARG:HH22	1:A:1001[B]:SER:HG	1.54	0.48
1:A:367:SER:OG	1:A:368:GLU:O	2.30	0.48
1:A:194:VAL:HG21	1:A:216:LEU:HD21	1.95	0.48
1:A:617:GLN:NE2	1:A:984:ALA:HA	2.29	0.48
1:A:895:HIS:ND1	1:A:897:ASP:OD1	2.47	0.47
1:A:962:ARG:HG2	1:A:962:ARG:NH1	2.26	0.47
1:A:676:THR:HG22	1:A:680:LYS:HE2	1.96	0.47
1:A:836[A]:ASN:ND2	2:A:1500:039:HAR	2.30	0.47
1:A:698:PHE:HZ	1:A:714:MET:HG2	1.80	0.47
1:A:842:SER:O	1:A:844:MET:HG2	2.16	0.45
1:A:620:LYS:HE2	1:A:660:VAL:HG11	1.99	0.45
1:A:553:THR:CG2	1:A:564:MET:CE	2.93	0.45
1:A:278:HIS:HE1	3:A:2022:HOH:O	2.00	0.45
1:A:334:ASN:CG	1:A:335:ALA:H	2.24	0.45
1:A:713:GLU:O	1:A:717:MET:HG3	2.16	0.44
1:A:698:PHE:HZ	1:A:714:MET:CG	2.29	0.44
1:A:832:ASP:OD2	1:A:836[B]:ASN:ND2	2.48	0.44
1:A:334:ASN:ND2	1:A:335:ALA:H	2.16	0.44
1:A:218:ALA:HB3	3:A:2021:HOH:O	2.17	0.43
1:A:367:SER:CB	1:A:369:PRO:CA	2.91	0.43
1:A:169:LEU:HD22	1:A:259:PHE:HE1	1.84	0.43
1:A:289:GLN:HG2	1:A:677:HIS:CD2	2.53	0.43
1:A:191:LEU:O	1:A:272:PRO:HD2	2.18	0.43
1:A:367:SER:CA	1:A:368:GLU:C	2.91	0.43
1:A:895:HIS:CE1	1:A:898:ASN:OD1	2.72	0.43
1:A:735:LEU:HD11	1:A:824:LEU:HB3	2.00	0.42
1:A:328:ILE:HD11	1:A:474:TYR:HB2	2.01	0.42
1:A:245:GLY:HA3	1:A:768:ALA:HB2	2.02	0.42
1:A:368:GLU:N	1:A:369:PRO:HD2	2.28	0.42
1:A:316:LEU:C	1:A:318:SER:H	2.28	0.42
1:A:1023:LEU:O	1:A:1026:SER:HB3	2.20	0.42
1:A:213:PRO:HD3	1:A:254:TYR:O	2.20	0.42
1:A:898:ASN:HD22	1:A:898:ASN:C	2.27	0.42
1:A:110:LYS:HZ3	1:A:144:ARG:HH12	1.63	0.41
1:A:394:LEU:HD22	1:A:441:MET:HE1	2.02	0.41
1:A:135:GLU:HG2	1:A:625:LEU:HD12	2.02	0.41
1:A:915:PHE:C	1:A:915:PHE:HD2	2.27	0.41
1:A:929:ARG:HH22	1:A:1001[A]:SER:CB	2.25	0.41
1:A:213:PRO:O	1:A:217:MET:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:784:LEU:HD12	1:A:823:GLY:HA3	2.02	0.41
1:A:846:ALA:HA	1:A:857:ASN:HB3	2.03	0.40
1:A:332:LYS:HE3	1:A:333:VAL:N	2.36	0.40
1:A:758:PRO:HB3	1:A:779:LYS:HG2	2.03	0.40
1:A:208:SER:OG	1:A:210:LYS:HG2	2.21	0.40
1:A:367:SER:CB	1:A:369:PRO:HA	2.51	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:714:MET:CE	1:A:714:MET:CE[2_555]	1.79	0.41

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	805/940 (86%)	788 (98%)	15 (2%)	2 (0%)	43 36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	367	SER
1	A	742	GLU

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	733/827 (89%)	691 (94%)	42 (6%)	18	11

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	LYS
1	A	188	ARG
1	A	190	LEU
1	A	229	ARG
1	A	316	LEU
1	A	317	TRP
1	A	331	ARG
1	A	332	LYS
1	A	333	VAL
1	A	340	LYS
1	A	352	GLU
1	A	365	VAL
1	A	368	GLU
1	A	394	LEU
1	A	397	VAL
1	A	423	LEU
1	A	445	VAL
1	A	453	LEU
1	A	511	LEU
1	A	514	ILE
1	A	517	ARG
1	A	523	LEU
1	A	530	LEU
1	A	553	THR
1	A	565	LEU
1	A	631	LYS
1	A	634	LEU
1	A	705	LYS
1	A	706	THR
1	A	714	MET
1	A	795	GLN
1	A	804	GLU
1	A	855	LEU
1	A	895	HIS
1	A	898	ASN
1	A	915	PHE

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Mol	Chain	Res	Type
1	A	937	ASP
1	A	962	ARG
1	A	986	LEU
1	A	990	SER
1	A	992	SER
1	A	1004	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	GLN
1	A	170	GLN
1	A	193	ASN
1	A	206	GLN
1	A	247	HIS
1	A	273	HIS
1	A	278	HIS
1	A	291	ASN
1	A	334	ASN
1	A	344	GLN
1	A	351	ASN
1	A	536	HIS
1	A	539	GLN
1	A	617	GLN
1	A	704	GLN
1	A	710	GLN
1	A	721	GLN
1	A	792	GLN
1	A	795	GLN
1	A	851	ASN
1	A	898	ASN
1	A	943	GLN
1	A	948	ASN

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 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	039	A	1500	-	35,35,35	1.48	6 (17%)	42,50,50	2.67	17 (40%)

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	039	A	1500	-	-	0/9/11/11	0/5/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1500	039	CAO-NAN	3.04	1.34	1.29
2	A	1500	039	C5-N7	-3.00	1.33	1.39
2	A	1500	039	CAE-CAF	-2.92	1.41	1.47
2	A	1500	039	CAH-CAP	-2.70	1.36	1.40
2	A	1500	039	CAM-NAN	-2.36	1.35	1.39
2	A	1500	039	CAS-CAO	2.16	1.53	1.50

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1500	039	CAU-OAT-CAP	-9.35	103.80	117.51
2	A	1500	039	N1-C2-N3	-5.14	120.81	128.58
2	A	1500	039	CAE-CAF-NAG	4.35	119.98	115.14
2	A	1500	039	N9-C4-N3	4.21	133.52	126.69
2	A	1500	039	CAP-CAH-NAG	4.13	123.24	119.02
2	A	1500	039	S6-C6-N1	3.95	126.69	117.83
2	A	1500	039	C5-C4-N3	-3.66	120.07	126.75
2	A	1500	039	CAE-CAD-CL	3.54	124.18	119.62
2	A	1500	039	OAB-CAF-NAG	-3.49	115.73	120.38
2	A	1500	039	C4-C5-C6	3.32	119.50	116.21
2	A	1500	039	N9-C8-N7	-2.70	109.77	113.87
2	A	1500	039	C4-N9-C8	2.40	108.67	106.43
2	A	1500	039	C5-N7-C8	2.39	106.17	103.48
2	A	1500	039	CAH-NAG-CAF	2.35	119.57	117.21
2	A	1500	039	C2-N1-C6	2.30	121.41	116.23
2	A	1500	039	C5-C6-S6	-2.16	114.86	120.53
2	A	1500	039	CAI-CAH-CAP	2.03	121.63	118.62

There are no chirality outliers.

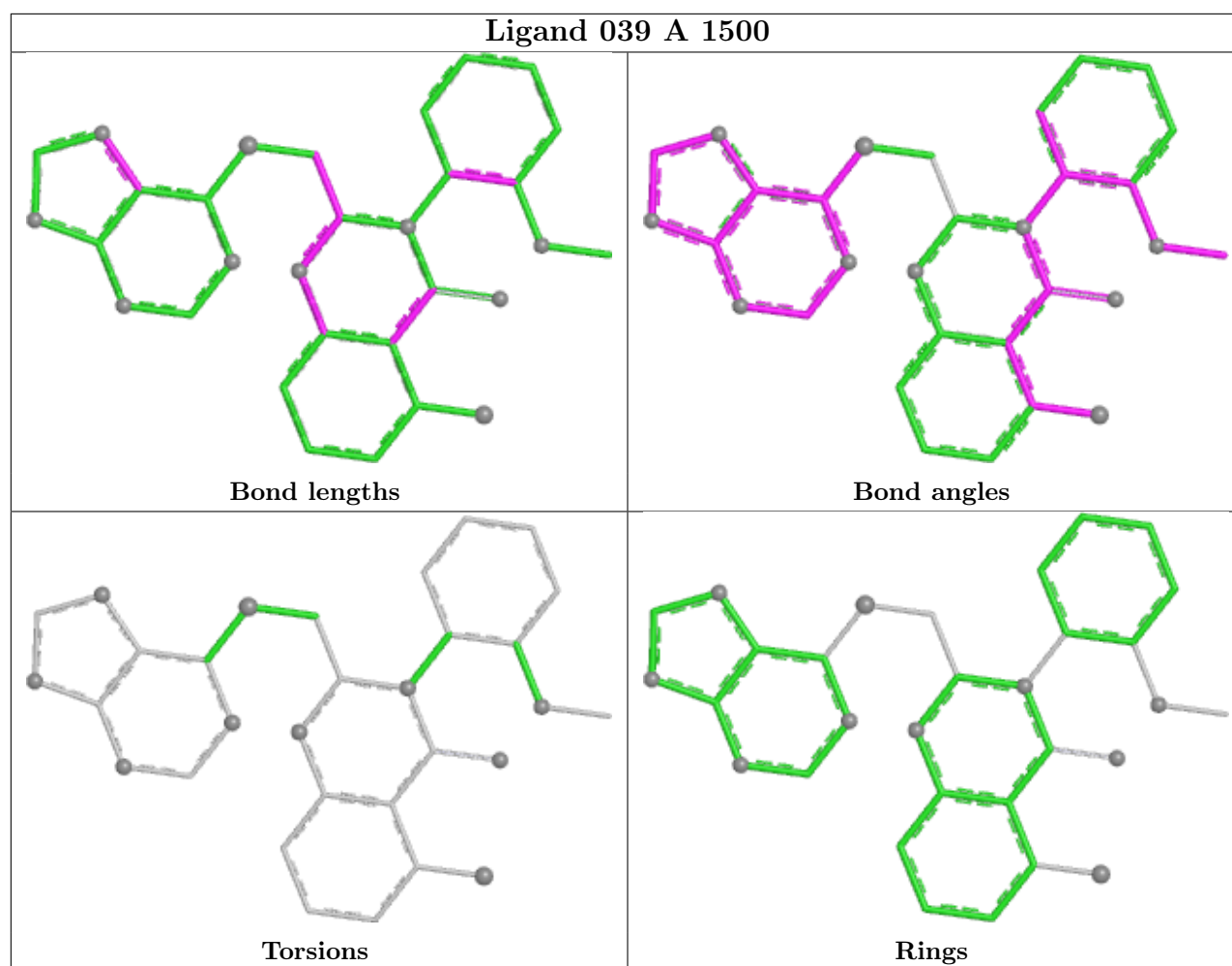
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1500	039	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	822/940 (87%)	1.43	187 (22%) 2 2	5, 17, 32, 49	5 (0%)

All (187) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	479	ALA	18.5
1	A	494	LEU	14.2
1	A	428	TYR	12.6
1	A	482	PRO	11.8
1	A	318	SER	10.9
1	A	487	ALA	9.6
1	A	317	TRP	8.9
1	A	478	VAL	8.6
1	A	426	PHE	8.2
1	A	485	PHE	8.1
1	A	489	GLU	7.6
1	A	484	TYR	7.5
1	A	430	ASP	7.4
1	A	319	LEU	7.3
1	A	388	ALA	7.3
1	A	486	PRO	7.3
1	A	429	LYS	7.3
1	A	445	VAL	7.3
1	A	384	LEU	7.3
1	A	458	THR	6.9
1	A	381	VAL	6.9
1	A	477	GLU	6.8
1	A	387	MET	6.7
1	A	386	ARG	6.7
1	A	461	GLY	6.5
1	A	490	LYS	6.5
1	A	491	ILE	6.4

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Mol	Chain	Res	Type	RSRZ
1	A	385	PRO	6.3
1	A	463	PRO	6.3
1	A	459	VAL	6.3
1	A	440	TYR	6.2
1	A	382	CYS	5.9
1	A	488	LEU	5.9
1	A	422	ASN	5.9
1	A	460	ARG	5.9
1	A	379	ILE	5.7
1	A	374	ARG	5.7
1	A	437	ARG	5.7
1	A	919	PHE	5.7
1	A	1027	TRP	5.7
1	A	432	LEU	5.6
1	A	483	VAL	5.6
1	A	431	GLN	5.6
1	A	349	HIS	5.5
1	A	390	LEU	5.4
1	A	492	LEU	5.4
1	A	391	CYS	5.3
1	A	424	MET	5.2
1	A	457	GLY	5.1
1	A	380	SER	5.1
1	A	348	PHE	5.0
1	A	322	PRO	5.0
1	A	323	PHE	5.0
1	A	320	GLU	5.0
1	A	435	GLY	5.0
1	A	456	ALA	4.9
1	A	367	SER	4.8
1	A	334	ASN	4.8
1	A	189	ALA	4.8
1	A	434	THR	4.8
1	A	512	ARG	4.7
1	A	350	GLY	4.7
1	A	425	LEU	4.7
1	A	363	VAL	4.6
1	A	377	PHE	4.6
1	A	473	ILE	4.5
1	A	472	VAL	4.5
1	A	493	GLU	4.4
1	A	427	ASP	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	423	LEU	4.3
1	A	373	GLN	4.3
1	A	383	ASP	4.2
1	A	439	LEU	4.2
1	A	395	TYR	4.2
1	A	357	THR	4.2
1	A	228	PHE	4.2
1	A	846	ALA	4.2
1	A	324	SER	4.1
1	A	511	LEU	4.0
1	A	936	TYR	4.0
1	A	335	ALA	4.0
1	A	514	ILE	4.0
1	A	347	LEU	3.9
1	A	438	CYS	3.9
1	A	397	VAL	3.9
1	A	476	PRO	3.9
1	A	389	ARG	3.8
1	A	421	ALA	3.8
1	A	358	VAL	3.8
1	A	328	ILE	3.7
1	A	321	GLN	3.6
1	A	436	GLU	3.6
1	A	562	ALA	3.6
1	A	718[A]	CYS	3.6
1	A	738	SER	3.5
1	A	895	HIS	3.5
1	A	316	LEU	3.5
1	A	433	LYS	3.5
1	A	355	CYS	3.4
1	A	370	VAL	3.4
1	A	354	LEU	3.4
1	A	366	CYS	3.4
1	A	342	VAL	3.4
1	A	991	CYS	3.3
1	A	475	LEU	3.3
1	A	843	ASN	3.3
1	A	325	ILE	3.2
1	A	474	TYR	3.2
1	A	1017	VAL	3.2
1	A	270	LEU	3.2
1	A	471	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	465	THR	3.1
1	A	522	GLU	3.1
1	A	353	MET	3.1
1	A	369	PRO	3.1
1	A	327	LEU	3.0
1	A	375	LEU	3.0
1	A	1023	LEU	3.0
1	A	225	ALA	3.0
1	A	361	SER	3.0
1	A	455	PRO	2.9
1	A	442	TRP	2.9
1	A	345	ALA	2.9
1	A	332	LYS	2.9
1	A	339	MET	2.9
1	A	330	GLY	2.9
1	A	534	MET	2.9
1	A	462	ASN	2.8
1	A	468	ALA	2.8
1	A	637	ALA	2.8
1	A	1005	GLY	2.8
1	A	227	VAL	2.8
1	A	346	GLY	2.8
1	A	378	ASP	2.8
1	A	205	PHE	2.7
1	A	392	PHE	2.7
1	A	269	GLY	2.6
1	A	561	VAL	2.6
1	A	771	ALA	2.6
1	A	453	LEU	2.6
1	A	333	VAL	2.6
1	A	226	THR	2.6
1	A	331	ARG	2.5
1	A	847	THR	2.5
1	A	524	TYR	2.5
1	A	356	LYS	2.5
1	A	291	ASN	2.5
1	A	464	ASN	2.5
1	A	396	ALA	2.4
1	A	162	TRP	2.4
1	A	365	VAL	2.4
1	A	398	VAL	2.4
1	A	341	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	938	PHE	2.4
1	A	364	ASN	2.4
1	A	1013	LYS	2.4
1	A	754	SER	2.3
1	A	515	LEU	2.3
1	A	634	LEU	2.3
1	A	934	LEU	2.3
1	A	517	ARG	2.3
1	A	376	GLU	2.3
1	A	235	GLN	2.3
1	A	639	ALA	2.2
1	A	845	ALA	2.2
1	A	848	ALA	2.2
1	A	513	GLU	2.2
1	A	267	HIS	2.2
1	A	948	ASN	2.2
1	A	351	ASN	2.1
1	A	869	ASP	2.1
1	A	681	VAL	2.1
1	A	672	CYS	2.1
1	A	841	LYS	2.1
1	A	469	ALA	2.1
1	A	995	ILE	2.1
1	A	192	VAL	2.1
1	A	266	LEU	2.1
1	A	444	SER	2.1
1	A	670	ALA	2.1
1	A	329	GLU	2.0
1	A	362	GLU	2.0
1	A	289	GLN	2.0
1	A	930	VAL	2.0
1	A	635	GLY	2.0
1	A	913	GLY	2.0
1	A	236	PRO	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

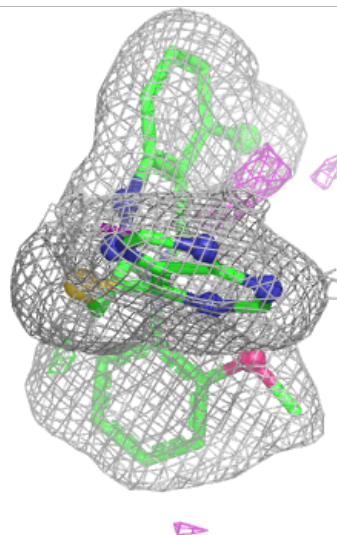
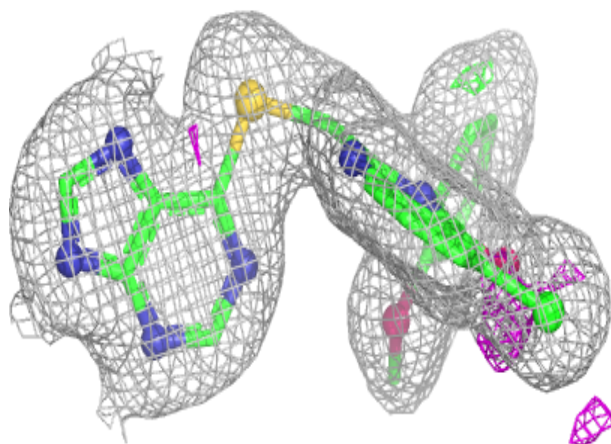
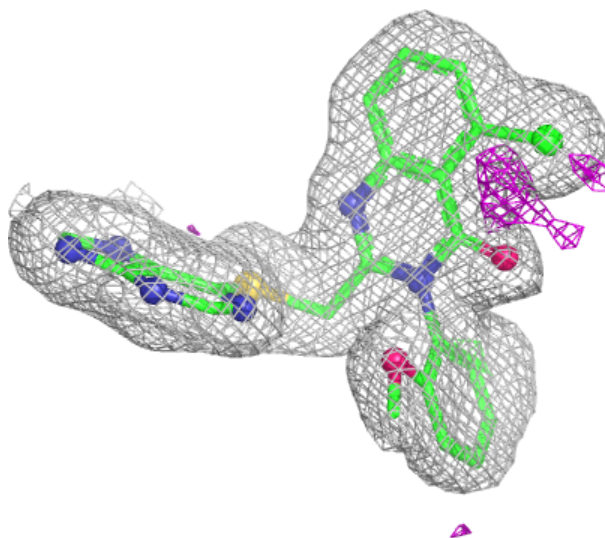
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	039	A	1500	31/31	0.95	0.08	20,25,35,38	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.

Electron density around 039 A 1500:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.