



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 04:00 pm BST

PDB ID : 2CHW
Title : A pharmacological map of the PI3-K family defines a role for p110 alpha in signaling: The structure of complex of phosphoinositide 3- kinase gamma with inhibitor PIK-39
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 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

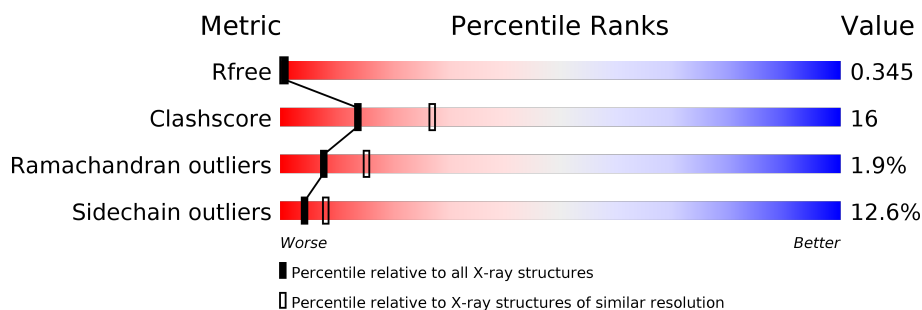
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (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 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	966	

2 Entry composition [i](#)

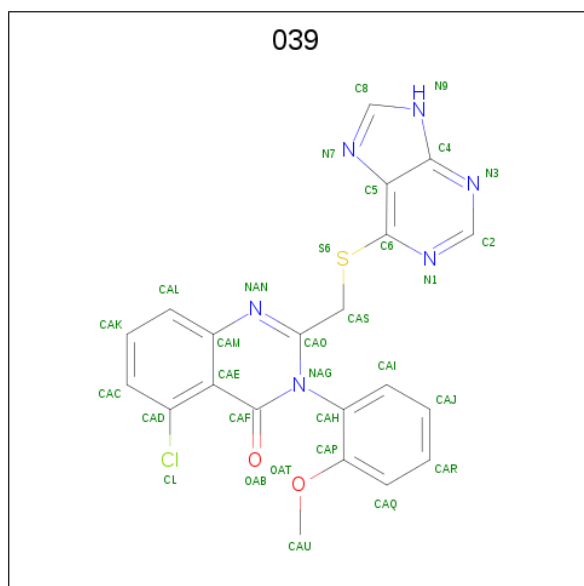
There are 3 unique types of molecules in this entry. The entry contains 6846 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	840	Total	C	N	O	S	0	0	0
			6807	4370	1163	1239	35			

- Molecule 2 is 2-((9H-PURIN-6-YLTHIO)METHYL)-5-CHLORO-3-(2-METHOXYPHENYL)QUINAZOLIN-4(3H)-ONE (three-letter code: 039) (formula: C₂₁H₁₅ClN₆O₂S).



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

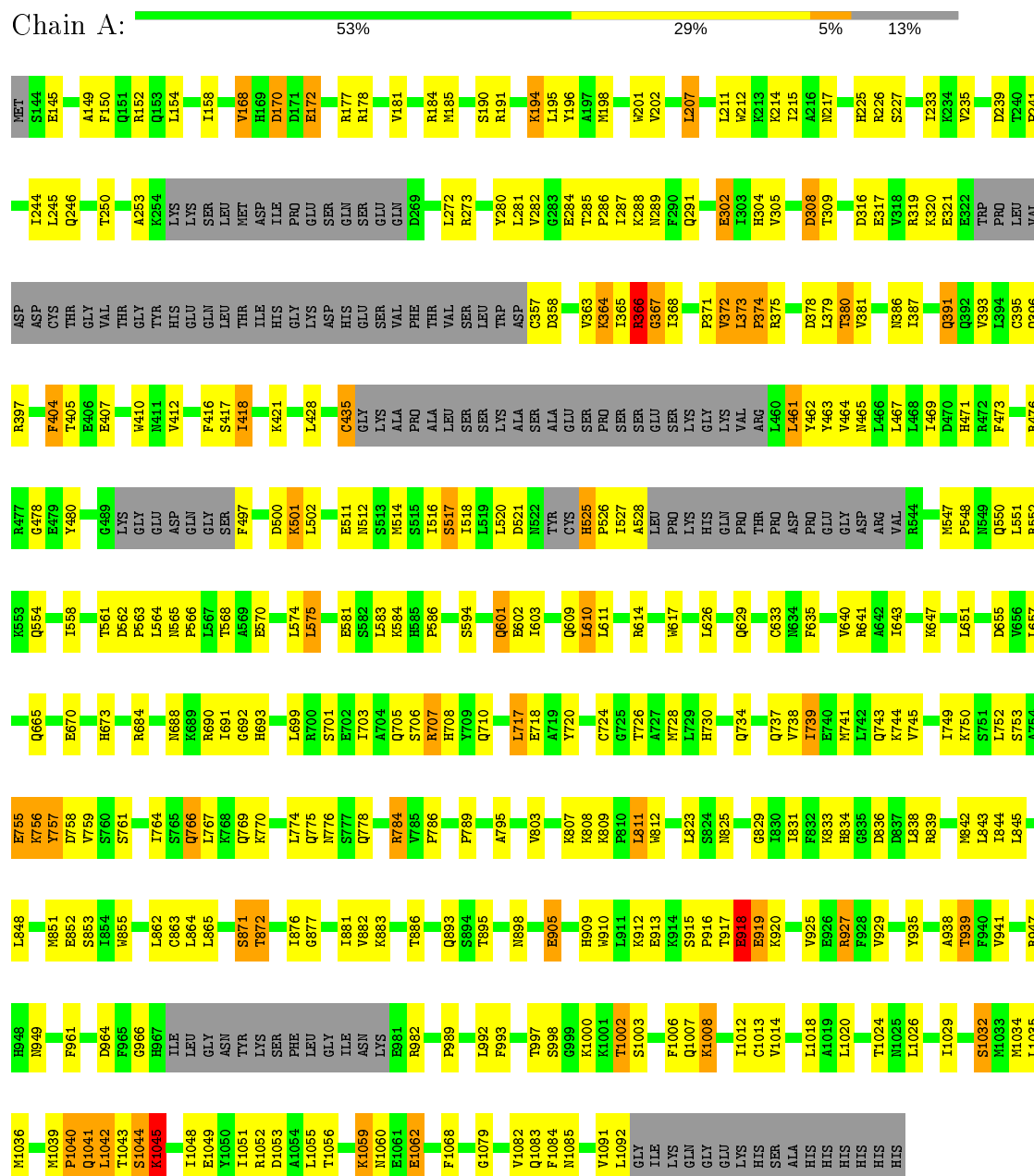
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	8	Total 8	0	0
			O 8		

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. 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. 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	143.80Å 67.52Å 106.31Å 90.00° 95.45° 90.00°	Depositor
Resolution (Å)	62.14 – 2.60 62.09 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (62.14-2.60) 99.8 (62.09-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.237 , 0.299 0.290 , 0.345	Depositor DCC
R_{free} test set	1295 reflections (4.12%)	wwPDB-VP
Wilson B-factor (Å ²)	63.3	Xtriage
Anisotropy	0.386	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 54.1	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	0.90	EDS
Total number of atoms	6846	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.66% 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	0.76	20/6953 (0.3%)	0.72	3/9403 (0.0%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	366	ARG	CZ-NH1	17.63	1.55	1.33
1	A	364	LYS	CE-NZ	12.34	1.79	1.49
1	A	366	ARG	NE-CZ	10.85	1.47	1.33
1	A	366	ARG	CG-CD	10.24	1.77	1.51
1	A	918	GLU	CG-CD	9.46	1.66	1.51
1	A	918	GLU	CD-OE1	9.30	1.35	1.25
1	A	405	THR	CB-OG1	8.83	1.60	1.43
1	A	407	GLU	CD-OE1	7.80	1.34	1.25
1	A	364	LYS	C-N	7.27	1.50	1.34
1	A	366	ARG	C-O	7.18	1.36	1.23
1	A	410	TRP	NE1-CE2	6.91	1.46	1.37
1	A	407	GLU	CD-OE2	6.68	1.32	1.25
1	A	364	LYS	C-O	6.49	1.35	1.23
1	A	1008	LYS	CB-CG	6.47	1.70	1.52
1	A	367	GLY	C-O	6.06	1.33	1.23
1	A	410	TRP	CD2-CE3	5.61	1.48	1.40
1	A	366	ARG	C-N	5.60	1.43	1.33
1	A	410	TRP	CZ2-CH2	5.42	1.47	1.37
1	A	1008	LYS	CE-NZ	5.39	1.62	1.49
1	A	367	GLY	CA-C	5.08	1.59	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	366	ARG	NE-CZ-NH2	-15.97	112.31	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	366	ARG	NE-CZ-NH1	13.97	127.28	120.30
1	A	575	LEU	CA-CB-CG	6.46	130.16	115.30

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	6807	0	6851	216	0
2	A	31	0	15	5	0
3	A	8	0	0	3	0
All	All	6846	0	6866	217	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 16.

All (217) 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:366:ARG:CG	1:A:366:ARG:CD	1.77	1.62
1:A:364:LYS:NZ	1:A:364:LYS:CE	1.79	1.44
1:A:366:ARG:HG3	1:A:366:ARG:HH11	1.28	0.98
1:A:851:MET:HE1	1:A:938:ALA:CB	1.97	0.95
1:A:851:MET:HE1	1:A:938:ALA:HB1	1.50	0.92
1:A:1039:MET:HB2	3:A:2008:HOH:O	1.74	0.88
1:A:949:ASN:H	1:A:1083:GLN:HE22	1.23	0.86
1:A:882:VAL:H	2:A:2093:039:H9	1.21	0.85
1:A:935:TYR:O	1:A:939:THR:HB	1.79	0.82
1:A:178:ARG:HH11	1:A:178:ARG:HB2	1.45	0.80
1:A:629:GLN:HG3	1:A:1029:ILE:HG13	1.61	0.80
1:A:239:ASP:O	1:A:287:ILE:HG23	1.84	0.77
1:A:149:ALA:HA	1:A:152:ARG:HD3	1.68	0.76
1:A:366:ARG:HG3	1:A:366:ARG:NH1	1.99	0.75
1:A:395:CYS:CB	1:A:418:ILE:HD11	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:ILE:HD12	1:A:418:ILE:HD13	1.74	0.70
1:A:386:ASN:OD1	1:A:396:GLN:HG3	1.92	0.70
1:A:568:THR:HG22	1:A:570:GLU:N	2.07	0.70
1:A:629:GLN:CG	1:A:1029:ILE:HG13	2.21	0.70
1:A:366:ARG:CB	1:A:366:ARG:CD	2.69	0.69
1:A:525:HIS:N	1:A:525:HIS:HD1	1.90	0.69
1:A:558:ILE:O	1:A:561:THR:HG22	1.93	0.68
1:A:372:VAL:HG13	1:A:374:PRO:HD3	1.76	0.68
1:A:461:LEU:HD22	1:A:462:TYR:CE2	2.29	0.67
1:A:178:ARG:HB2	1:A:178:ARG:NH1	2.10	0.67
1:A:1042:LEU:HD12	3:A:2008:HOH:O	1.95	0.66
1:A:833:LYS:HE3	1:A:836:ASP:OD2	1.95	0.66
1:A:181:VAL:HG22	1:A:184:ARG:HH22	1.60	0.65
1:A:812:TRP:HB2	2:A:2093:039:CAC	2.26	0.65
1:A:1039:MET:HB3	1:A:1040:PRO:HD2	1.79	0.65
1:A:158:ILE:HG12	1:A:717:LEU:HD13	1.79	0.64
1:A:317:GLU:O	1:A:726:THR:HG23	1.97	0.64
1:A:851:MET:CE	1:A:938:ALA:CB	2.73	0.64
1:A:701:SER:OG	1:A:871:SER:HB3	1.97	0.64
1:A:1041:GLN:HE21	1:A:1042:LEU:H	1.45	0.64
1:A:357:CYS:HA	1:A:421:LYS:HB2	1.79	0.64
1:A:568:THR:HG22	1:A:570:GLU:H	1.62	0.64
1:A:1014:VAL:O	1:A:1018:LEU:HG	1.98	0.63
1:A:614:ARG:HG2	1:A:617:TRP:HB3	1.79	0.63
1:A:851:MET:HE1	1:A:938:ALA:HB2	1.79	0.63
1:A:225:HIS:CE1	1:A:304:HIS:HD2	2.16	0.63
1:A:601:GLN:HG3	1:A:602:GLU:N	2.14	0.62
1:A:364:LYS:O	1:A:518:ILE:HA	1.99	0.62
1:A:851:MET:CE	1:A:938:ALA:HB2	2.29	0.62
1:A:395:CYS:HB3	1:A:418:ILE:HD11	1.83	0.61
1:A:272:LEU:HD22	1:A:305:VAL:HG11	1.83	0.60
1:A:525:HIS:N	1:A:525:HIS:ND1	2.49	0.60
1:A:416:PHE:HB3	1:A:418:ILE:HD12	1.83	0.60
1:A:1041:GLN:HE21	1:A:1042:LEU:N	1.99	0.60
1:A:724:CYS:HB2	1:A:728:MET:HE3	1.84	0.59
1:A:872:THR:OG1	1:A:877:GLY:HA2	2.02	0.59
1:A:750:LYS:NZ	1:A:834:HIS:HD2	2.00	0.59
1:A:1042:LEU:H	1:A:1042:LEU:HD13	1.68	0.59
1:A:393:VAL:O	1:A:393:VAL:HG23	2.03	0.59
1:A:368:ILE:HB	1:A:514:MET:SD	2.43	0.59
1:A:1032:SER:HB2	1:A:1048:ILE:CG2	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1062:GLU:N	1:A:1062:GLU:CD	2.56	0.58
1:A:753:SER:HB2	1:A:809:LYS:HE3	1.86	0.58
1:A:308:ASP:N	1:A:308:ASP:OD1	2.37	0.58
1:A:882:VAL:N	2:A:2093:039:H9	1.99	0.57
1:A:395:CYS:HB2	1:A:418:ILE:HD11	1.86	0.57
1:A:463:TYR:CE1	1:A:501:LYS:HA	2.40	0.57
1:A:1056:THR:HG23	1:A:1056:THR:O	2.04	0.56
1:A:1062:GLU:H	1:A:1062:GLU:CD	2.08	0.56
1:A:839:ARG:HA	1:A:842:MET:HE2	1.86	0.56
1:A:941:VAL:HG21	1:A:1020:LEU:HD12	1.86	0.56
1:A:428:LEU:HD22	1:A:465:ASN:HB3	1.87	0.56
1:A:177:ARG:NH2	1:A:718:GLU:OE2	2.29	0.56
1:A:750:LYS:NZ	1:A:834:HIS:CD2	2.74	0.56
1:A:366:ARG:CG	1:A:366:ARG:NH1	2.67	0.56
1:A:1013:CYS:HB3	1:A:1068:PHE:CE2	2.40	0.56
1:A:467:LEU:O	1:A:476:ARG:NH1	2.39	0.56
1:A:752:LEU:HD13	1:A:766:GLN:HG2	1.88	0.56
1:A:497:PHE:HB3	1:A:1041:GLN:HE22	1.72	0.55
1:A:767:LEU:CD1	1:A:803:VAL:HG23	2.36	0.55
1:A:775:GLN:HE22	1:A:795:ALA:HB1	1.72	0.55
1:A:640:VAL:O	1:A:643:ILE:HG12	2.07	0.54
1:A:665:GLN:NE2	3:A:2004:HOH:O	2.39	0.54
1:A:246:GLN:O	1:A:250:THR:OG1	2.23	0.54
1:A:480:TYR:O	1:A:517:SER:HA	2.08	0.54
1:A:692:GLY:HA3	1:A:720:TYR:OH	2.08	0.54
1:A:500:ASP:HB3	1:A:708:HIS:CD2	2.42	0.54
1:A:564:LEU:HD11	1:A:1048:ILE:HG22	1.90	0.54
1:A:1082:VAL:HA	1:A:1085:ASN:HD22	1.73	0.54
1:A:583:LEU:HD22	1:A:610:LEU:HD22	1.90	0.53
1:A:1008:LYS:HG2	1:A:1012:ILE:HD11	1.90	0.53
1:A:364:LYS:NZ	1:A:364:LYS:CD	2.70	0.53
1:A:741:MET:O	1:A:744:LYS:HB2	2.09	0.53
1:A:757:TYR:CE2	1:A:807:LYS:HG3	2.44	0.53
1:A:844:ILE:HD13	1:A:1034:MET:SD	2.49	0.53
1:A:396:GLN:O	1:A:397:ARG:NH1	2.42	0.52
1:A:657:LEU:HG	1:A:691:ILE:HG12	1.90	0.52
1:A:225:HIS:CE1	1:A:304:HIS:CD2	2.98	0.52
1:A:833:LYS:CE	1:A:836:ASP:OD2	2.58	0.52
1:A:500:ASP:O	1:A:502:LEU:N	2.43	0.52
1:A:473:PHE:HD2	1:A:527:ILE:HD12	1.73	0.52
1:A:378:ASP:OD2	1:A:404:PHE:O	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:916:PRO:HD2	1:A:920:LYS:HD2	1.92	0.51
1:A:947:ARG:NH2	1:A:964:ASP:O	2.43	0.51
1:A:1035:LEU:HD12	1:A:1048:ILE:HD13	1.91	0.51
1:A:750:LYS:HZ3	1:A:834:HIS:CD2	2.29	0.51
1:A:302:GLU:HB2	1:A:304:HIS:CE1	2.45	0.51
1:A:500:ASP:C	1:A:502:LEU:H	2.13	0.51
1:A:225:HIS:HE1	1:A:304:HIS:CD2	2.28	0.51
1:A:421:LYS:HE3	1:A:528:ALA:HB3	1.92	0.51
1:A:917:THR:C	1:A:919:GLU:H	2.15	0.50
1:A:905:GLU:HA	1:A:993:PHE:CD2	2.46	0.50
1:A:949:ASN:N	1:A:1083:GLN:HE22	2.03	0.50
1:A:562:ASP:HB2	1:A:563:PRO:CD	2.42	0.50
1:A:581:GLU:OE2	1:A:584:LYS:HD2	2.12	0.49
1:A:286:PRO:O	1:A:289:ASN:N	2.44	0.49
1:A:1056:THR:OG1	1:A:1059:LYS:HG3	2.12	0.49
1:A:172:GLU:HG3	1:A:471:HIS:ND1	2.28	0.49
1:A:373:LEU:O	1:A:373:LEU:HG	2.12	0.49
1:A:1002:THR:HG23	1:A:1006:PHE:HD2	1.77	0.48
1:A:550:GLN:HE21	1:A:554:GLN:HG3	1.77	0.48
1:A:172:GLU:HB3	1:A:673:HIS:HD2	1.77	0.48
1:A:964:ASP:C	1:A:966:GLY:H	2.17	0.48
1:A:380:THR:O	1:A:435:CYS:HB2	2.14	0.48
1:A:391:GLN:OE1	1:A:633:CYS:HB2	2.13	0.48
1:A:688:ASN:OD1	1:A:690:ARG:N	2.45	0.48
1:A:737:GLN:O	1:A:741:MET:HG3	2.14	0.48
1:A:168:VAL:HG13	1:A:170:ASP:O	2.13	0.47
1:A:395:CYS:HG	1:A:417:SER:HG	1.60	0.47
1:A:635:PHE:O	1:A:641:ARG:HD2	2.14	0.47
1:A:745:VAL:HG13	1:A:770:LYS:HD2	1.96	0.47
1:A:829:GLY:HA3	1:A:881:ILE:HB	1.97	0.46
1:A:739:ILE:O	1:A:743:GLN:HG3	2.14	0.46
1:A:838:LEU:CD2	1:A:877:GLY:HA3	2.45	0.46
1:A:910:TRP:HA	1:A:913:GLU:HG2	1.98	0.46
1:A:706:SER:O	1:A:710:GLN:HB3	2.15	0.46
1:A:212:TRP:C	1:A:214:LYS:H	2.18	0.46
1:A:749:ILE:HG21	1:A:803:VAL:HG21	1.98	0.46
1:A:755:GLU:OE1	1:A:755:GLU:HA	2.16	0.46
1:A:831:ILE:HD13	2:A:2093:039:HAL	1.98	0.46
1:A:478:GLY:N	1:A:520:LEU:O	2.45	0.46
1:A:893:GLN:HE21	1:A:898:ASN:HD22	1.64	0.46
1:A:1042:LEU:CD1	1:A:1042:LEU:N	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:ARG:HH11	1:A:178:ARG:CB	2.21	0.46
1:A:750:LYS:HE3	1:A:808:LYS:HA	1.97	0.45
1:A:925:VAL:O	1:A:929:VAL:HG23	2.16	0.45
1:A:357:CYS:HA	1:A:421:LYS:CB	2.47	0.45
1:A:1035:LEU:HD22	1:A:1039:MET:HG3	1.98	0.45
1:A:233:ILE:HG22	1:A:235:VAL:HG23	1.98	0.45
1:A:364:LYS:HA	1:A:412:VAL:O	2.17	0.45
1:A:834:HIS:HB2	1:A:876:ILE:HD12	1.98	0.45
1:A:1043:THR:C	1:A:1045:LYS:H	2.19	0.45
1:A:194:LYS:HD3	1:A:195:LEU:HG	1.97	0.45
1:A:207:LEU:CD2	1:A:211:LEU:HB2	2.47	0.45
1:A:838:LEU:HD23	1:A:877:GLY:HA3	1.99	0.45
1:A:707:ARG:HA	1:A:710:GLN:OE1	2.17	0.45
1:A:207:LEU:HD21	1:A:211:LEU:HB2	1.99	0.44
1:A:367:GLY:O	1:A:516:ILE:HA	2.17	0.44
1:A:371:PRO:HG2	1:A:511:GLU:O	2.16	0.44
1:A:855:TRP:CE3	1:A:862:LEU:HD23	2.52	0.44
1:A:302:GLU:HB2	1:A:304:HIS:HE1	1.82	0.44
1:A:1042:LEU:N	1:A:1042:LEU:HD13	2.31	0.44
1:A:1060:ASN:HB2	1:A:1062:GLU:OE1	2.17	0.44
1:A:366:ARG:CG	1:A:366:ARG:CZ	2.95	0.44
1:A:380:THR:O	1:A:435:CYS:HA	2.18	0.44
1:A:461:LEU:HD22	1:A:462:TYR:CZ	2.53	0.44
1:A:373:LEU:O	1:A:373:LEU:CG	2.66	0.44
1:A:641:ARG:NH1	1:A:670:GLU:OE1	2.50	0.44
1:A:366:ARG:HB2	1:A:517:SER:HB2	1.99	0.44
1:A:480:TYR:HB2	1:A:518:ILE:HG12	2.00	0.44
1:A:191:ARG:HD2	1:A:196:TYR:CD1	2.53	0.43
1:A:784:ARG:NH1	1:A:789:PRO:O	2.51	0.43
1:A:997:THR:HG22	1:A:998:SER:N	2.33	0.43
1:A:1003:SER:O	1:A:1007:GLN:HG3	2.19	0.43
1:A:500:ASP:C	1:A:502:LEU:N	2.72	0.43
1:A:154:LEU:O	1:A:158:ILE:HG13	2.18	0.43
1:A:852:GLU:HG3	1:A:864:LEU:HD12	2.01	0.43
1:A:755:GLU:OE1	1:A:807:LYS:HG2	2.18	0.42
1:A:181:VAL:O	1:A:185:MET:HG3	2.19	0.42
1:A:547:MET:HA	1:A:548:PRO:HD2	1.85	0.42
1:A:381:VAL:HG21	1:A:404:PHE:CG	2.54	0.42
1:A:201:TRP:CD1	1:A:291:GLN:HG3	2.54	0.42
1:A:379:LEU:HB3	1:A:380:THR:H	1.48	0.42
1:A:548:PRO:HG2	1:A:551:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558:ILE:HG21	1:A:575:LEU:HD21	2.00	0.42
1:A:286:PRO:O	1:A:288:LYS:N	2.52	0.42
1:A:1032:SER:HB2	1:A:1048:ILE:HG23	2.00	0.42
1:A:1042:LEU:HD22	1:A:1042:LEU:O	2.20	0.42
2:A:2093:039:OAB	2:A:2093:039:CL	2.75	0.42
1:A:915:SER:HA	1:A:916:PRO:HD3	1.90	0.42
1:A:693:HIS:NE2	1:A:786:PRO:O	2.30	0.42
1:A:941:VAL:HG21	1:A:1020:LEU:CD1	2.49	0.42
1:A:1042:LEU:HD23	1:A:1048:ILE:HD11	2.02	0.42
1:A:198:MET:HG2	1:A:280:TYR:CG	2.55	0.41
1:A:699:LEU:O	1:A:703:ILE:HG13	2.20	0.41
1:A:734:GLN:O	1:A:738:VAL:HG23	2.20	0.41
1:A:935:TYR:CE1	1:A:961:PHE:HA	2.55	0.41
1:A:989:PRO:HA	1:A:992:LEU:HD12	2.02	0.41
1:A:641:ARG:NE	1:A:670:GLU:OE1	2.50	0.41
1:A:761:SER:HA	1:A:764:ILE:HD12	2.01	0.41
1:A:851:MET:HE2	1:A:851:MET:HB2	1.89	0.41
1:A:917:THR:C	1:A:919:GLU:N	2.73	0.41
1:A:918:GLU:OE1	1:A:918:GLU:O	2.39	0.41
1:A:241:PRO:O	1:A:245:LEU:HG	2.19	0.41
1:A:150:PHE:HB2	1:A:319:ARG:NH1	2.36	0.41
1:A:469:ILE:HG21	1:A:527:ILE:HD11	2.01	0.41
1:A:172:GLU:HB3	1:A:673:HIS:CD2	2.55	0.41
1:A:651:LEU:HD22	1:A:655:ASP:HB3	2.03	0.41
1:A:684:ARG:HA	1:A:684:ARG:HD2	1.86	0.41
1:A:363:VAL:HG12	1:A:416:PHE:HE1	1.86	0.40
1:A:812:TRP:CE2	1:A:881:ILE:HD13	2.56	0.40
1:A:1051:ILE:HG12	1:A:1055:LEU:HD12	2.02	0.40
1:A:184:ARG:HH21	1:A:321:GLU:CD	2.24	0.40
1:A:705:GLN:HG2	1:A:839:ARG:CZ	2.51	0.40
1:A:758:ASP:OD1	1:A:759:VAL:N	2.54	0.40
1:A:851:MET:HE3	1:A:938:ALA:HB2	2.01	0.40
1:A:149:ALA:O	1:A:152:ARG:HB2	2.21	0.40
1:A:565:ASN:HA	1:A:566:PRO:HD3	1.86	0.40
1:A:743:GLN:NE2	1:A:872:THR:OG1	2.54	0.40
1:A:1036:MET:HA	1:A:1042:LEU:HD11	2.02	0.40
1:A:803:VAL:CG2	1:A:811:LEU:HD12	2.52	0.40
1:A:863:CYS:SG	1:A:927:ARG:NH1	2.95	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	824/966 (85%)	728 (88%)	80 (10%)	16 (2%)	8 15

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	526	PRO
1	A	217	ASN
1	A	501	LYS
1	A	1040	PRO
1	A	1044	SER
1	A	1045	LYS
1	A	1079	GLY
1	A	253	ALA
1	A	756	LYS
1	A	776	ASN
1	A	918	GLU
1	A	227	SER
1	A	244	ILE
1	A	1049	GLU
1	A	611	LEU
1	A	374	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	754/864 (87%)	659 (87%)	95 (13%)	4 8

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145	GLU
1	A	168	VAL
1	A	170	ASP
1	A	172	GLU
1	A	190	SER
1	A	194	LYS
1	A	202	VAL
1	A	207	LEU
1	A	215	ILE
1	A	226	ARG
1	A	273	ARG
1	A	281	LEU
1	A	282	VAL
1	A	284	GLU
1	A	285	THR
1	A	302	GLU
1	A	308	ASP
1	A	309	THR
1	A	316	ASP
1	A	320	LYS
1	A	358	ASP
1	A	365	ILE
1	A	366	ARG
1	A	372	VAL
1	A	373	LEU
1	A	375	ARG
1	A	380	THR
1	A	391	GLN
1	A	404	PHE
1	A	418	ILE
1	A	435	CYS
1	A	461	LEU
1	A	464	VAL
1	A	512	ASN
1	A	517	SER

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Mol	Chain	Res	Type
1	A	521	ASP
1	A	525	HIS
1	A	552	ARG
1	A	574	LEU
1	A	586	PRO
1	A	594	SER
1	A	601	GLN
1	A	603	ILE
1	A	609	GLN
1	A	610	LEU
1	A	626	LEU
1	A	647	LYS
1	A	707	ARG
1	A	717	LEU
1	A	730	HIS
1	A	739	ILE
1	A	755	GLU
1	A	756	LYS
1	A	757	TYR
1	A	766	GLN
1	A	769	GLN
1	A	774	LEU
1	A	778	GLN
1	A	784	ARG
1	A	811	LEU
1	A	823	LEU
1	A	825	ASN
1	A	843	LEU
1	A	845	LEU
1	A	848	LEU
1	A	853	SER
1	A	865	LEU
1	A	871	SER
1	A	872	THR
1	A	883	LYS
1	A	886	THR
1	A	895	THR
1	A	905	GLU
1	A	909	HIS
1	A	912	LYS
1	A	919	GLU
1	A	927	ARG

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Mol	Chain	Res	Type
1	A	939	THR
1	A	982	ARG
1	A	1000	LYS
1	A	1002	THR
1	A	1024	THR
1	A	1026	LEU
1	A	1032	SER
1	A	1041	GLN
1	A	1042	LEU
1	A	1044	SER
1	A	1045	LYS
1	A	1052	ARG
1	A	1053	ASP
1	A	1059	LYS
1	A	1062	GLU
1	A	1084	PHE
1	A	1091	VAL
1	A	1092	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	225	HIS
1	A	231	GLN
1	A	304	HIS
1	A	389	HIS
1	A	512	ASN
1	A	522	ASN
1	A	550	GLN
1	A	565	ASN
1	A	646	GLN
1	A	705	GLN
1	A	730	HIS
1	A	734	GLN
1	A	743	GLN
1	A	766	GLN
1	A	773	ASN
1	A	775	GLN
1	A	834	HIS
1	A	840	GLN
1	A	898	ASN
1	A	948	HIS

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Mol	Chain	Res	Type
1	A	1007	GLN
1	A	1041	GLN
1	A	1083	GLN
1	A	1085	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	039	A	2093	-	32,35,35	1.85	8 (25%)	30,50,50	2.79	9 (30%)

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	2093	-	-	1/9/11/11	0/5/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2093	039	CAH-NAG	-5.26	1.39	1.45
2	A	2093	039	CAS-CAO	4.57	1.55	1.50
2	A	2093	039	C6-C5	-3.66	1.37	1.43
2	A	2093	039	C6-S6	3.17	1.80	1.76
2	A	2093	039	C6-N1	2.62	1.36	1.33
2	A	2093	039	C5-N7	-2.18	1.31	1.39
2	A	2093	039	C4-N3	-2.14	1.34	1.37
2	A	2093	039	CAO-NAG	2.08	1.41	1.36

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2093	039	CAS-S6-C6	10.97	116.43	101.52
2	A	2093	039	N3-C2-N1	-5.09	120.72	128.68
2	A	2093	039	CAO-CAS-S6	4.77	118.98	109.54
2	A	2093	039	C2-N1-C6	3.32	123.70	116.36
2	A	2093	039	C5-C6-S6	3.29	124.90	119.36
2	A	2093	039	C5-C6-N1	-3.02	116.54	122.07
2	A	2093	039	C2-N3-C4	2.53	119.37	113.45
2	A	2093	039	CAF-CAE-CAD	-2.21	123.14	126.64
2	A	2093	039	CAC-CAD-CAE	-2.16	119.19	122.58

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2093	039	N1-C6-S6-CAS

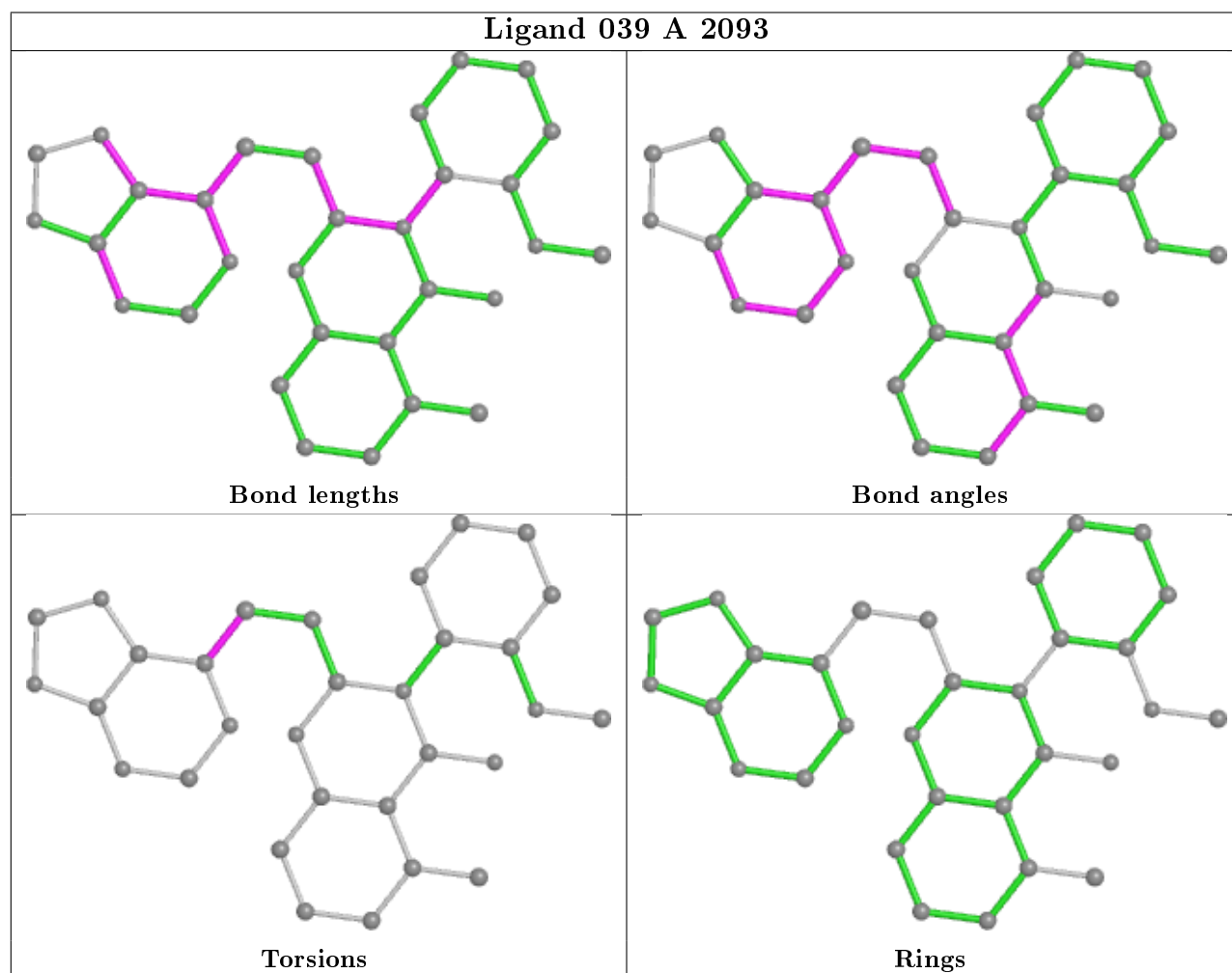
There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2093	039	5	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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

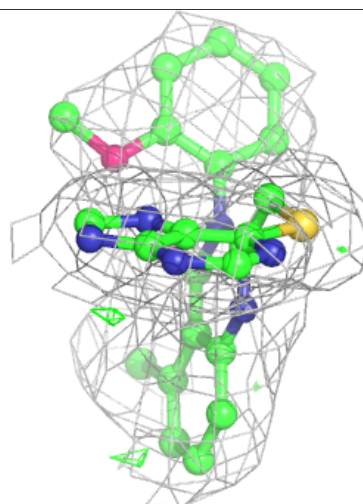
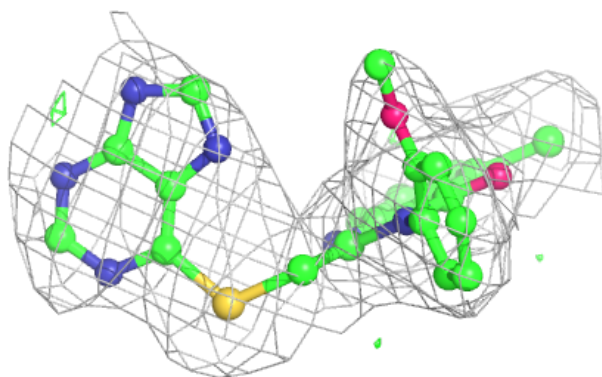
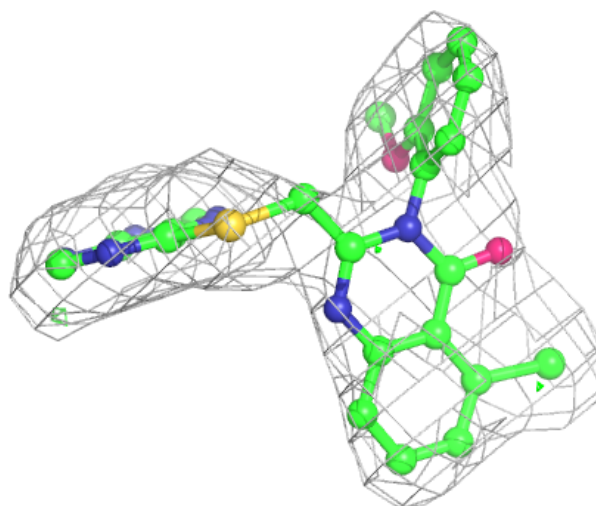
6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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 2093:

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



6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.