



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:18 PM UTC

PDB ID : 2CHW / pdb_00002chw
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 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)

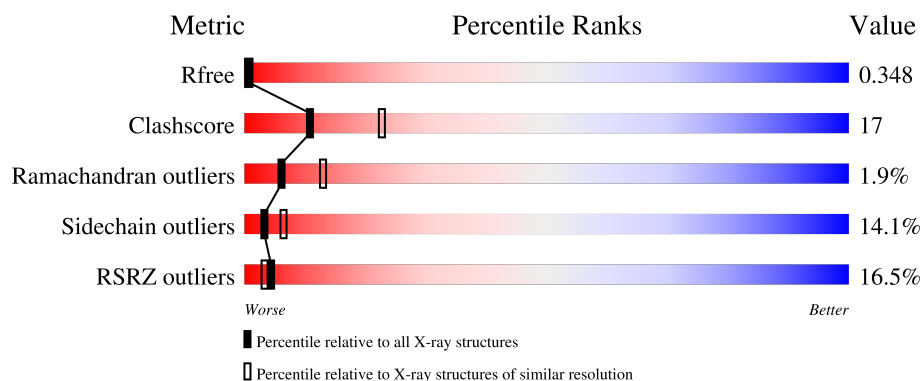
1 Overall quality at a glance

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	14% 51% 29% 6% 13%

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

2 Entry composition [i](#)

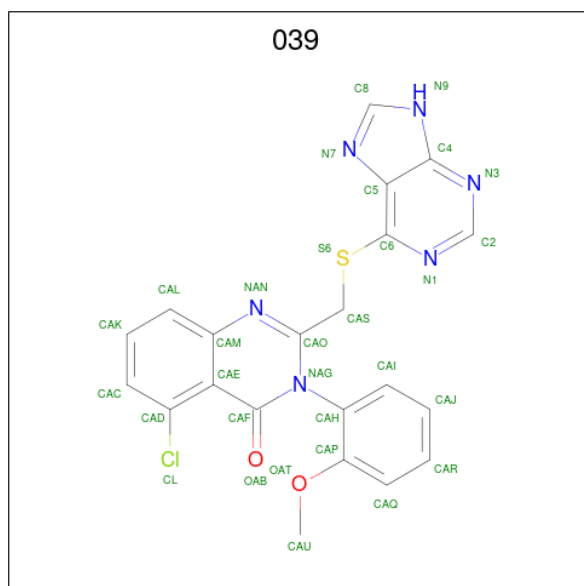
There are 3 unique types of molecules in this entry. The entry contains 6846 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: 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		

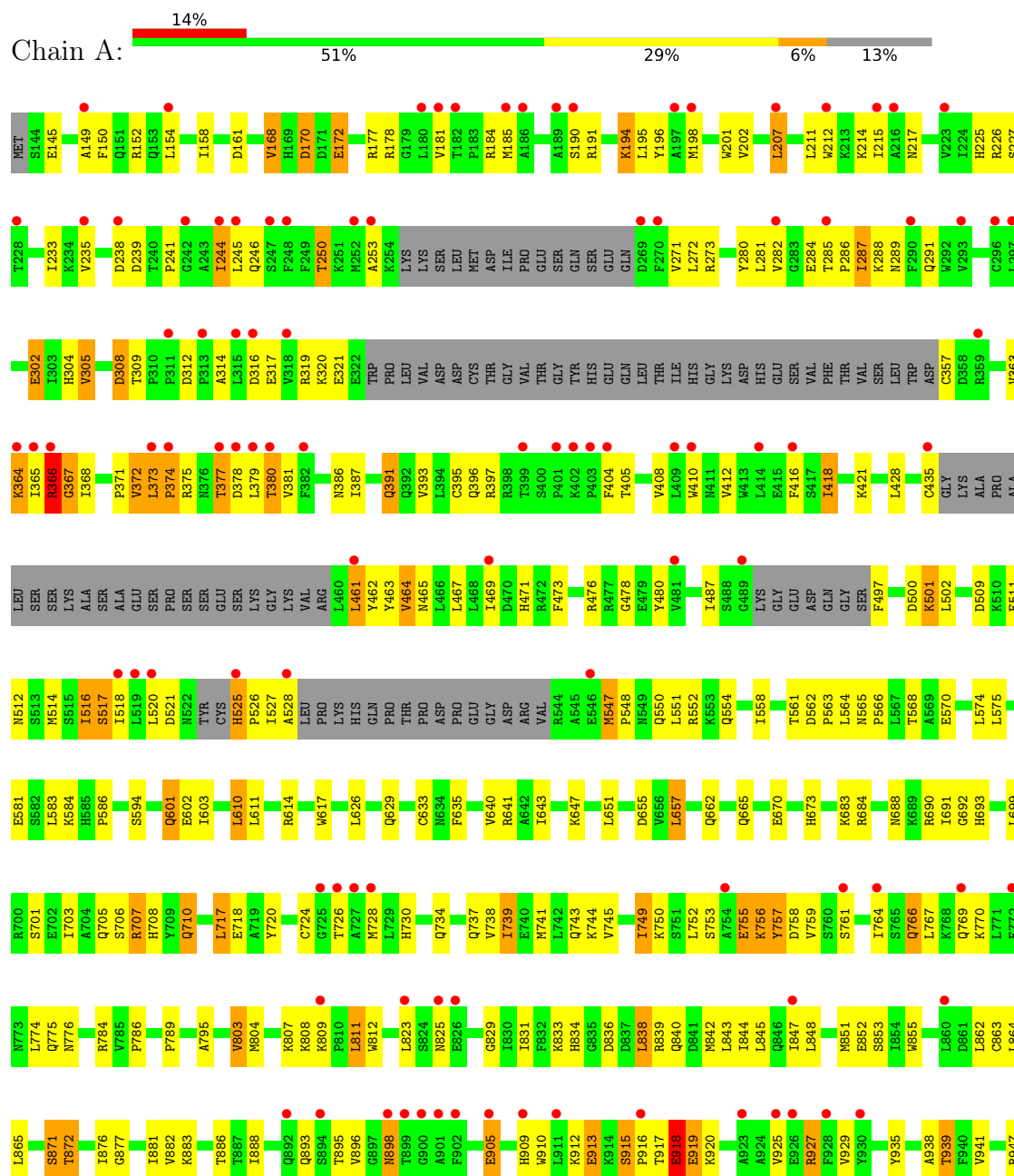
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	8	Total O 8 8	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 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 62.14 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (62.14-2.60) 99.8 (62.14-2.60)	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 0.292 , 0.348	Depositor DCC
R_{free} test set	1295 reflections (4.11%)	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)	0.34 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	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

5.1 Standard geometry

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	0.88	21/6953 (0.3%)	0.98	16/9403 (0.2%)

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	366	ARG	CZ-NH1	16.58	1.55	1.32
1	A	364	LYS	C-N	16.41	1.50	1.33
1	A	366	ARG	NE-CZ	12.82	1.47	1.33
1	A	366	ARG	C-O	11.23	1.36	1.24
1	A	405	THR	CB-OG1	10.72	1.60	1.43
1	A	364	LYS	CE-NZ	10.19	1.79	1.49
1	A	364	LYS	C-O	9.79	1.35	1.24
1	A	366	ARG	CG-CD	8.37	1.77	1.52
1	A	410	TRP	NE1-CE2	8.26	1.46	1.37
1	A	410	TRP	C-N	8.23	1.44	1.33
1	A	366	ARG	C-N	8.04	1.43	1.33
1	A	367	GLY	CA-C	7.24	1.59	1.51
1	A	367	GLY	C-O	6.83	1.33	1.23
1	A	408	VAL	CA-CB	6.40	1.62	1.54
1	A	464	VAL	CA-CB	5.91	1.61	1.55
1	A	1008	LYS	CB-CG	5.86	1.70	1.52
1	A	918	GLU	CG-CD	5.63	1.66	1.52
1	A	918	GLU	CD-OE1	5.54	1.35	1.25
1	A	410	TRP	CZ2-CH2	5.47	1.47	1.37
1	A	410	TRP	CD2-CE3	5.32	1.48	1.40
1	A	1029	ILE	CA-CB	-5.05	1.48	1.54

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	366	ARG	NE-CZ-NH2	-7.65	112.31	119.20
1	A	994	VAL	N-CA-C	-7.34	105.61	112.96
1	A	364	LYS	CA-C-N	-6.29	114.62	122.48
1	A	364	LYS	C-N-CA	-6.29	114.62	122.48
1	A	364	LYS	O-C-N	5.93	130.27	123.27
1	A	366	ARG	NE-CZ-NH1	5.78	127.28	121.50
1	A	915	SER	CA-C-N	5.73	125.41	119.05
1	A	915	SER	C-N-CA	5.73	125.41	119.05
1	A	898	ASN	N-CA-C	5.25	117.20	107.60
1	A	377	THR	N-CA-C	-5.20	102.35	110.10
1	A	847	ILE	N-CA-C	-5.17	105.50	110.72
1	A	250	THR	N-CA-C	-5.16	106.67	113.17
1	A	1008	LYS	CB-CG-CD	-5.06	99.67	111.30
1	A	547	MET	CA-C-N	5.01	124.94	119.78
1	A	547	MET	C-N-CA	5.01	124.94	119.78
1	A	662	GLN	CA-CB-CG	-5.00	104.09	114.10

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	226	0
2	A	31	0	15	6	0
3	A	8	0	0	3	0
All	All	6846	0	6866	227	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 17.

All (227) 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:CD	1:A:366:ARG:CG	1.77	1.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:LYS:CE	1:A:364:LYS:NZ	1.79	1.44
1:A:851:MET:HE1	1:A:938:ALA:CB	1.77	1.15
1:A:366:ARG:HG3	1:A:366:ARG:HH11	1.28	0.98
1:A:851:MET:HE1	1:A:938:ALA:HB2	1.46	0.96
1:A:851:MET:HE1	1:A:938:ALA:HB1	1.54	0.88
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:724:CYS:HB2	1:A:728:MET:HE3	1.59	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
1:A:368:ILE:HD13	1:A:514:MET:HE1	1.72	0.71
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:CD	1:A:366:ARG:CB	2.69	0.69
1:A:525:HIS:HD1	1:A:525:HIS:N	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:833:LYS:HE3	1:A:836:ASP:OD2	1.95	0.66
1:A:1042:LEU:HD12	3:A:2008:HOH:O	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: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:614:ARG:HG2	1:A:617:TRP:HB3	1.79	0.63
1:A:1014:VAL:O	1:A:1018:LEU:HG	1.98	0.63
1:A:225:HIS:CE1	1:A:304:HIS:HD2	2.16	0.63

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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	0.63
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:1062:GLU:CD	1:A:1062:GLU:H	2.08	0.61
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: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:393:VAL:HG23	1:A:393:VAL:O	2.03	0.59
1:A:1042:LEU:H	1:A:1042:LEU:HD13	1.68	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
1:A:753:SER:HB2	1:A:809:LYS:HE3	1.86	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:196:TYR:OH	1:A:728:MET:HE2	2.05	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:500:ASP:C	1:A:502:LEU:H	2.13	0.56
1:A:308:ASP:N	1:A:308:ASP:OD1	2.37	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: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:1013:CYS:HB3	1:A:1068:PHE:CE2	2.40	0.56
1:A:851:MET:CE	1:A:938:ALA:HB2	2.29	0.55
1:A:1034:MET:HG2	1:A:1039:MET:HE3	1.87	0.55
1:A:497:PHE:HB3	1:A:1041:GLN:HE22	1.72	0.55
1:A:917:THR:C	1:A:919:GLU:H	2.15	0.55
1:A:750:LYS:HZ2	1:A:834:HIS:CD2	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:TYR:O	1:A:517:SER:HA	2.08	0.54
1:A:500:ASP:HB3	1:A:708:HIS:CD2	2.42	0.54
1:A:692:GLY:HA3	1:A:720:TYR:OH	2.08	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:964:ASP:C	1:A:966:GLY:H	2.17	0.53
1:A:757:TYR:CE2	1:A:807:LYS:HG3	2.44	0.53
1:A:839:ARG:HA	1:A:842:MET:HE2	1.91	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:194:LYS:O	1:A:198:MET:HE3	2.09	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
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:212:TRP:C	1:A:214:LYS:H	2.18	0.51
1:A:302:GLU:HB2	1:A:304:HIS:CE1	2.45	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: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:1043:THR:C	1:A:1045:LYS:H	2.19	0.49
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: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:1056:THR:OG1	1:A:1059:LYS:HG3	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:380:THR:O	1:A:435:CYS:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:500:ASP:C	1:A:502:LEU:N	2.72	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:750:LYS:HZ2	1:A:834:HIS:HD2	1.60	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:749:ILE:HG21	1:A:803:VAL:HG21	1.98	0.46
1:A:478:GLY:N	1:A:520:LEU:O	2.45	0.46
1:A:831:ILE:HD13	2:A:2093:039:HAL	1.98	0.46
1:A:893:GLN:HE21	1:A:898:ASN:HD22	1.64	0.46
1:A:917:THR:C	1:A:919:GLU:N	2.73	0.46
1:A:178:ARG:HH11	1:A:178:ARG:CB	2.21	0.46
1:A:1042:LEU:N	1:A:1042:LEU:CD1	2.79	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:755:GLU:OE1	1:A:755:GLU:HA	2.16	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:1035:LEU:HD22	1:A:1039:MET:HG3	1.98	0.45
1:A:184:ARG:HH21	1:A:321:GLU:CD	2.24	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:987:LEU:HD11	1:A:995:MET:HE3	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:LEU:HD22	1:A:462:TYR:CZ	2.53	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: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:1060:ASN:CG	1:A:1062:GLU:HG2	2.44	0.43
1:A:312:ASP:C	1:A:314:ALA:H	2.27	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
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
1:A:915:SER:HA	1:A:916:PRO:HD3	1.90	0.42
2:A:2093:039:OAB	2:A:2093:039:CL	2.75	0.42
1:A:212:TRP:C	1:A:214:LYS:N	2.77	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:509:ASP:OD1	1:A:509:ASP:C	2.63	0.41
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:287:ILE:C	1:A:289:ASN:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:918:GLU:O	1:A:918:GLU:OE1	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:HD2	1:A:684:ARG:HA	1.86	0.41
1:A:161:ASP:OD2	1:A:161:ASP:C	2.64	0.40
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:804:MET:HE3	2:A:2093:039:HAI	2.02	0.40
1:A:1051:ILE:HG12	1:A:1055:LEU:HD12	2.02	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: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: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
1:A:1036:MET:HA	1:A:1042:LEU:HD11	2.02	0.40
1:A:1054:ALA:C	1:A:1056:THR:H	2.29	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%)	6	13

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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	754/864 (87%)	648 (86%)	106 (14%)	3 6

All (106) 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	238	ASP

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Mol	Chain	Res	Type
1	A	244	ILE
1	A	271	VAL
1	A	273	ARG
1	A	281	LEU
1	A	282	VAL
1	A	284	GLU
1	A	285	THR
1	A	287	ILE
1	A	302	GLU
1	A	305	VAL
1	A	308	ASP
1	A	309	THR
1	A	316	ASP
1	A	320	LYS
1	A	365	ILE
1	A	366	ARG
1	A	372	VAL
1	A	373	LEU
1	A	375	ARG
1	A	377	THR
1	A	380	THR
1	A	391	GLN
1	A	418	ILE
1	A	461	LEU
1	A	464	VAL
1	A	487	ILE
1	A	512	ASN
1	A	516	ILE
1	A	517	SER
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	610	LEU
1	A	626	LEU
1	A	647	LYS
1	A	657	LEU
1	A	683	LYS

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Mol	Chain	Res	Type
1	A	707	ARG
1	A	710	GLN
1	A	717	LEU
1	A	730	HIS
1	A	739	ILE
1	A	749	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	803	VAL
1	A	811	LEU
1	A	823	LEU
1	A	825	ASN
1	A	838	LEU
1	A	840	GLN
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	888	ILE
1	A	895	THR
1	A	896	VAL
1	A	905	GLU
1	A	909	HIS
1	A	912	LYS
1	A	913	GLU
1	A	919	GLU
1	A	927	ARG
1	A	939	THR
1	A	982	ARG
1	A	1000	LYS
1	A	1002	THR
1	A	1024	THR
1	A	1026	LEU

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Mol	Chain	Res	Type
1	A	1032	SER
1	A	1042	LEU
1	A	1044	SER
1	A	1045	LYS
1	A	1048	ILE
1	A	1052	ARG
1	A	1057	VAL
1	A	1059	LYS
1	A	1062	GLU
1	A	1091	VAL
1	A	1092	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	GLN
1	A	169	HIS
1	A	225	HIS
1	A	231	GLN
1	A	304	HIS
1	A	376	ASN
1	A	389	HIS
1	A	411	ASN
1	A	522	ASN
1	A	550	GLN
1	A	565	ASN
1	A	600	GLN
1	A	601	GLN
1	A	705	GLN
1	A	711	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	893	GLN
1	A	898	ASN
1	A	948	HIS
1	A	1005	HIS

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Mol	Chain	Res	Type
1	A	1007	GLN
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	039	A	2093	-	35,35,35	1.69	7 (20%)	42,50,50	2.82	12 (28%)

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	-	-	2/9/11/11	0/5/5/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2093	039	C5-N7	-3.97	1.31	1.39
2	A	2093	039	CAH-NAG	-3.68	1.39	1.44
2	A	2093	039	CAE-CAF	-3.64	1.39	1.47
2	A	2093	039	CAS-CAO	3.40	1.55	1.50
2	A	2093	039	C6-S6	2.70	1.80	1.76
2	A	2093	039	CAO-NAN	2.65	1.34	1.29
2	A	2093	039	C4-N9	-2.32	1.33	1.36

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2093	039	CAS-S6-C6	13.27	116.43	100.81
2	A	2093	039	N1-C2-N3	-5.20	120.72	128.58
2	A	2093	039	CAE-CAF-NAG	4.48	120.13	115.14
2	A	2093	039	C2-N1-C6	3.32	123.70	116.23
2	A	2093	039	CAE-CAD-CL	3.27	123.83	119.62
2	A	2093	039	C5-C4-N3	-3.13	121.05	126.75
2	A	2093	039	N9-C4-N3	3.05	131.63	126.69
2	A	2093	039	C5-N7-C8	2.78	106.62	103.48
2	A	2093	039	C4-C5-C6	2.42	118.61	116.21
2	A	2093	039	NAG-CAO-NAN	-2.23	117.81	124.36
2	A	2093	039	C5-C6-N1	-2.07	116.54	119.45
2	A	2093	039	CAM-NAN-CAO	2.07	122.29	117.26

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2093	039	C5-C6-S6-CAS
2	A	2093	039	N1-C6-S6-CAS

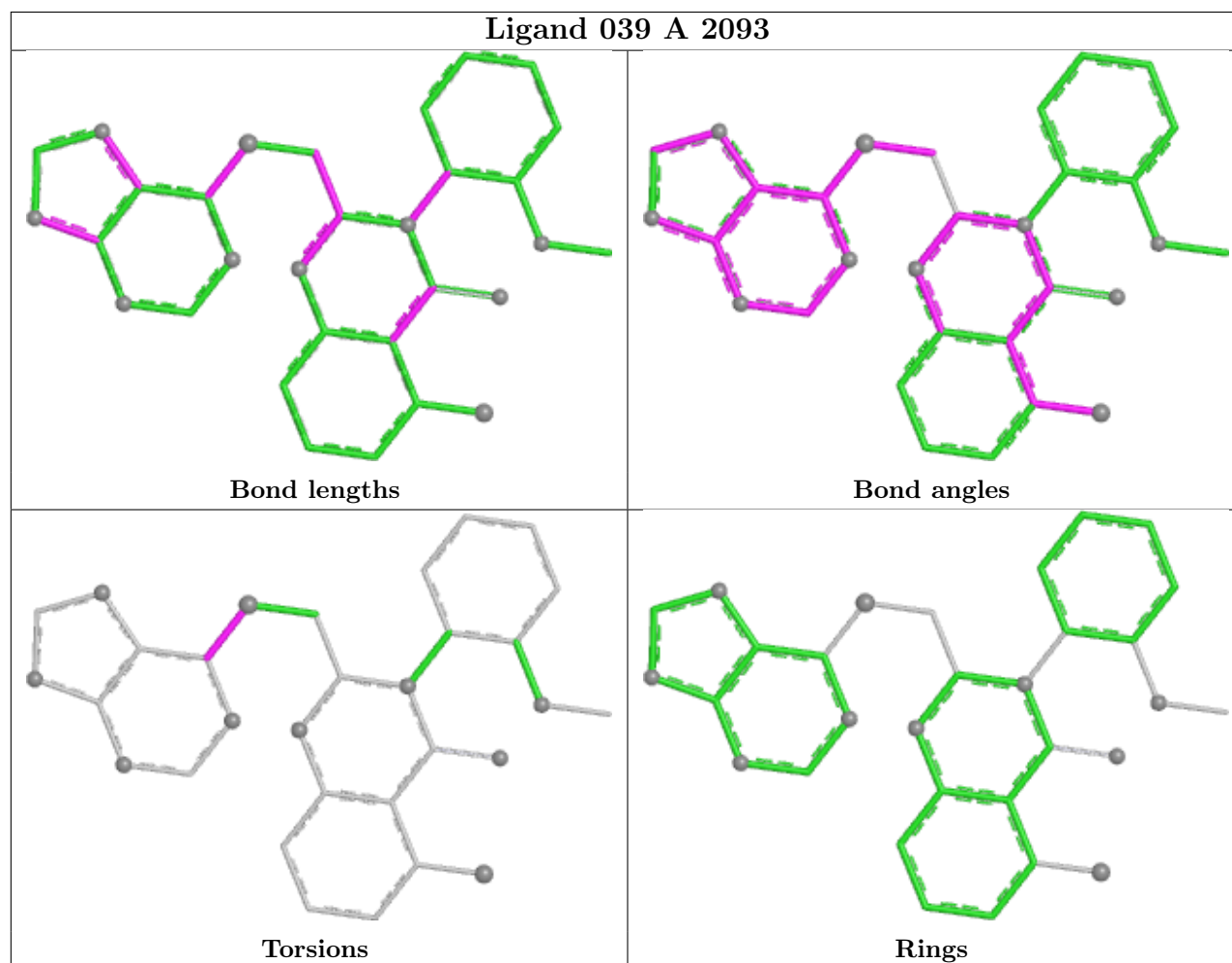
There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2093	039	6	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%)	1.19	139 (16%) 4 3	29, 62, 83, 108	0

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1044	SER	5.9
1	A	1091	VAL	5.2
1	A	1069	LEU	4.9
1	A	403	PRO	4.7
1	A	212	TRP	4.6
1	A	989	PRO	4.5
1	A	1079	GLY	4.3
1	A	379	LEU	4.2
1	A	528	ALA	4.2
1	A	726	THR	4.2
1	A	1084	PHE	4.1
1	A	285	THR	3.9
1	A	899	THR	3.9
1	A	900	GLY	3.9
1	A	825	ASN	3.7
1	A	215	ILE	3.7
1	A	994	VAL	3.6
1	A	1092	LEU	3.6
1	A	995	MET	3.5
1	A	987	LEU	3.5
1	A	996	GLY	3.5
1	A	1090	LEU	3.5
1	A	898	ASN	3.4
1	A	769	GLN	3.4
1	A	414	LEU	3.3
1	A	727	ALA	3.2
1	A	961	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	985	PHE	3.2
1	A	926	GLU	3.2
1	A	380	THR	3.1
1	A	1083	GLN	3.0
1	A	1064	ALA	3.0
1	A	359	ARG	3.0
1	A	1068	PHE	3.0
1	A	435	CYS	2.9
1	A	373	LEU	2.9
1	A	1070	ASP	2.9
1	A	905	GLU	2.8
1	A	1086	TRP	2.8
1	A	764	ILE	2.8
1	A	366	ARG	2.8
1	A	248	PHE	2.8
1	A	290	PHE	2.8
1	A	909	HIS	2.8
1	A	1082	VAL	2.8
1	A	1088	LEU	2.7
1	A	242	GLY	2.7
1	A	1075	CYS	2.7
1	A	894	SER	2.7
1	A	923	ALA	2.7
1	A	316	ASP	2.7
1	A	518	ILE	2.7
1	A	282	VAL	2.7
1	A	253	ALA	2.6
1	A	901	ALA	2.6
1	A	315	LEU	2.6
1	A	754	ALA	2.6
1	A	252	MET	2.6
1	A	297	LEU	2.6
1	A	525	HIS	2.6
1	A	1089	HIS	2.6
1	A	293	VAL	2.6
1	A	404	PHE	2.6
1	A	928	PHE	2.6
1	A	949	ASN	2.6
1	A	245	LEU	2.5
1	A	911	LEU	2.5
1	A	216	ALA	2.5
1	A	247	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	318	VAL	2.5
1	A	1087	PHE	2.5
1	A	198	MET	2.5
1	A	847	ILE	2.5
1	A	313	PRO	2.5
1	A	189	ALA	2.5
1	A	402	LYS	2.5
1	A	365	ILE	2.5
1	A	409	LEU	2.5
1	A	377	THR	2.4
1	A	728	MET	2.4
1	A	1007	GLN	2.4
1	A	149	ALA	2.4
1	A	416	PHE	2.4
1	A	997	THR	2.4
1	A	207	LEU	2.4
1	A	826	GLU	2.4
1	A	925	VAL	2.4
1	A	1010	GLN	2.4
1	A	1006	PHE	2.4
1	A	520	LEU	2.4
1	A	546	GLU	2.4
1	A	190	SER	2.4
1	A	269	ASP	2.4
1	A	235	VAL	2.4
1	A	860	LEU	2.3
1	A	988	THR	2.3
1	A	374	PRO	2.3
1	A	186	ALA	2.3
1	A	761	SER	2.3
1	A	519	LEU	2.3
1	A	197	ALA	2.2
1	A	296	CYS	2.2
1	A	930	TYR	2.2
1	A	990	ASP	2.2
1	A	809	LYS	2.2
1	A	993	PHE	2.2
1	A	725	GLY	2.2
1	A	399	THR	2.2
1	A	311	PRO	2.2
1	A	154	LEU	2.2
1	A	461	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	270	PHE	2.2
1	A	902	PHE	2.2
1	A	228	THR	2.2
1	A	489	GLY	2.2
1	A	378	ASP	2.2
1	A	481	VAL	2.2
1	A	180	LEU	2.1
1	A	238	ASP	2.1
1	A	244	ILE	2.1
1	A	1003	SER	2.1
1	A	772	GLU	2.1
1	A	364	LYS	2.1
1	A	181	VAL	2.1
1	A	469	ILE	2.1
1	A	948	HIS	2.1
1	A	916	PRO	2.1
1	A	892	GLN	2.1
1	A	823	LEU	2.1
1	A	991	PHE	2.1
1	A	410	TRP	2.1
1	A	182	THR	2.0
1	A	1004	PRO	2.0
1	A	382	PHE	2.0
1	A	185	MET	2.0
1	A	401	PRO	2.0
1	A	1029	ILE	2.0
1	A	1085	ASN	2.0
1	A	223	VAL	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.

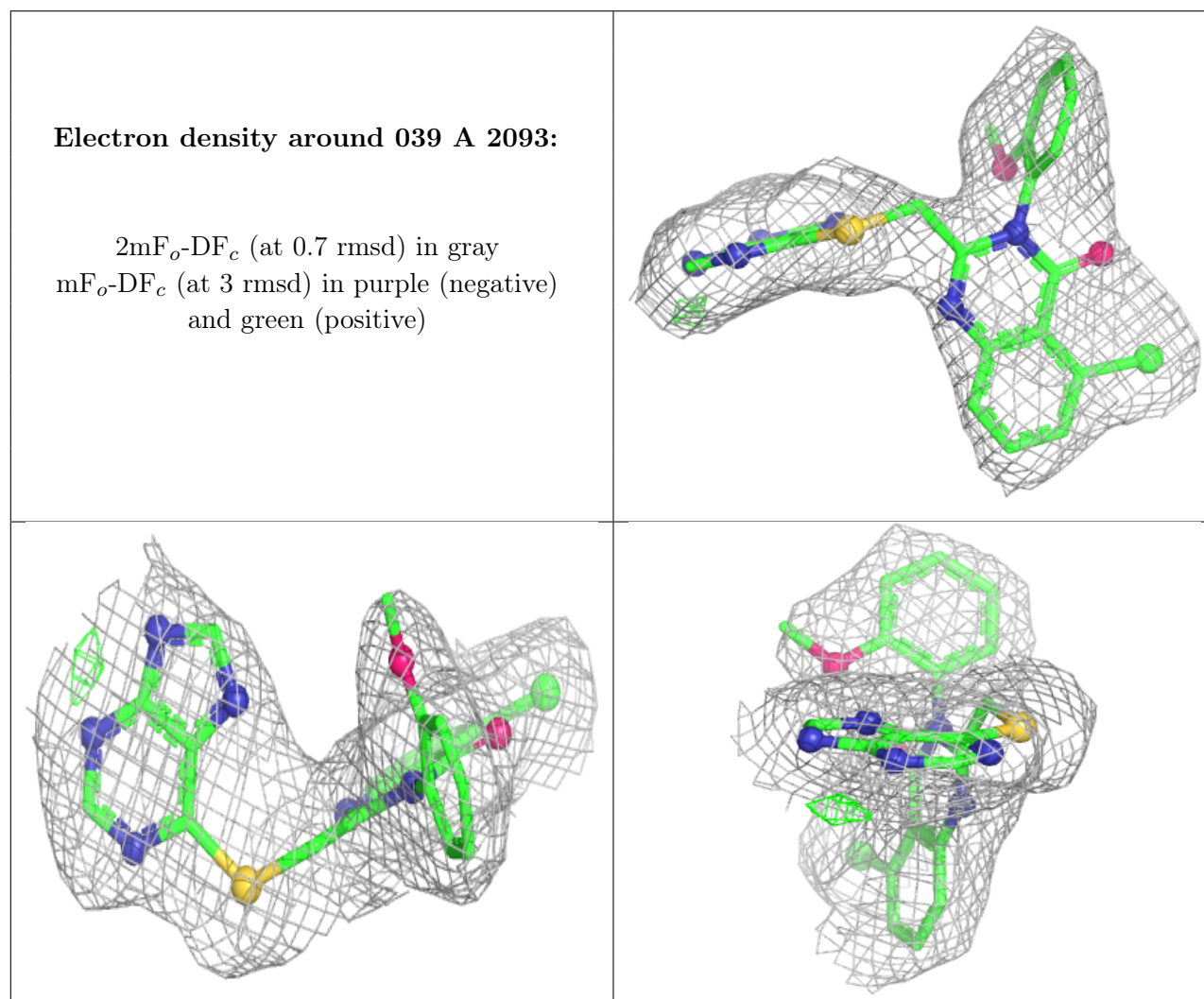
6.4 Ligands [i](#)

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(Å ²)	Q<0.9
2	039	A	2093	31/31	0.90	0.12	50,61,63,63	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.